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PRZM-3, A Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 3.12.2

by

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DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Contract No. 68-C6-0020 to HydroGeoLogic, Inc. It has been subjected to the Agency's peer and administrative review, and has been approved for publication as an EPA document. Additional peer and administration review and testing is ongoing, but not yet completed. Mention of trade names of commercial products does not constitute endorsement or recommendation for use by the U.S. Environmental Protection Agency.

FOREWORD

As environmental protection measure become more costly to implement, and the penalties of judgment errors become more severe, environmental quality management requires more efficient assessment tools based on greater knowledge of the environmental phenomena to be managed. As part of this Division's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, this Division develops management and engineering tools to help pollution control officials reach decisions on the registration and restriction of pesticides used for agricultural purposes.

The pesticide and nutrient regulatory process requires that the potential risk to human health resulting from the introduction or continued use of these chemicals be evaluated. Recently, much of this attention has been focused on human and ecosystem exposure through the leaching of pesticides and nitrogen to groundwater and the subsequent ingestion of the contaminated ground water. To provide a tool for evaluating pesticide exposure, the PRZM-2 model was developed; subsequent enhancements: expanded capabilities to include nitrogen simulation. PRZM-3 simulates the fate and transport of field-applied pesticides in the crop root zone down throughout the vadose zone, taking into account the effects of agricultural management practices. The model provides estimates of probable exposure concentrations by taking into account the variability in the natural system and the uncertainties in system properties and processes. To enable evaluation of nitrogen (particularly nitrate) exposure via groundwater, PRZM-3 includes a septic system module and capabilities for modeling soil nitrogen fate and transport.

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ABSTRACT

This publication contains documentation for the PRZM-3 model. PRZM-3 is the most recent version of a modeling system that links two subordinate models – PRZM and VADOFT – in order to predict pesticide transport and transformation down through the crop root and unsaturated soil zones. Enhancements to Release 3.0 reported herein include algorithms that also enable modeling of the nitrogen cycle soil kinetic processes, with the ability to track nitrogen discharges from a septic tank into the soil environment and its subsequent movement to groundwater. Additional included enhancements enable better simulation of physicochemical processes, increased flexibility in representing agronomic practices, and improved post-processing and data interpretation aids.

PRZM is a one-dimensional, finite-difference model that accounts for pesticide and nitrogen fate in the crop root zone. PRZM-3 includes modeling capabilities for such phenomena as soil temperature simulation, volatilization and vapor phase transport in soils, irrigation simulation, microbial transformation, and a method of characteristics (MOC) algorithm to eliminate numerical dispersion. PRZM is capable of simulating the transport and the transformation of a given parent compound, and at most as two daughter species. VADOFT is a one-dimensional, finite-element code that solves the Richard's equation for flow in the unsaturated zone. The user can use constitutive relationships between pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT can simulate the fate of two parent compounds, each with two daughter products. The PRZM and VADOFT codes are linked together with the aid of a flexible execution supervisor that allows the user to build loading models tailored to the user's site-specific situations. In order to perform probability-based exposure assessments, the code is also equipped with a Monte Carlo pre- and post-processor.

ACKNOWLEDGMENTS

The manual for PRZM-3 β was written by R.F. Carousel (USEPA), J.C. Imhoff, P.R. Hummel (AQUA TERRA Consultants), and J.M. Cheplick (Waterborne Environmental), and A.S. Donigian, Jr.(AQUA TERRA Consultants). This edition represents a major rewrite.

PRZM-3 is the result of fifteen years of focused model development effort. The original PRZM model was released in 1984, with the accompanying user's manual written by R.F. Carousel (EPA), C.N. Smith (EPA), L.A. Mulkey (EPA), J.D. Dean (Anderson Nichols) and P. Jowise (Anderson Nichols).

Release 2.0 (PRZM-2) became the official version of PRZM in the early 1990's. Several components of PRZM-2 were excerpted from the RUSTIC model. The following contributors to the RUSTIC model are acknowledged: Mr. K.A. Voos of Woodward-Clyde Consultants (WCC) programmed the execution supervisor and linked the models. The linkage was conceived by Mr. J.D. Dean and Dr. Atul Salhotra of WCC and Dr. P.S. Huyakorn of HydroGeoLogic. Dr. Huyakorn and his staff wrote the time/space bridging subroutines for the linkage. Mr. R.W. Schanz (WCC) and Y.J. Meeks (WCC) wrote the irrigation and MOC algorithms. The volatilization routines were written by Dr. J. Lin and Mr. S. Raju of AQUA TERRA Consultants. Mr. Dean wrote the daughter products algorithms that were implemented by Dr. Lin. Mr. J.L. Kittle implemented modifications to allow multiple segment (zone) simulation capability.

The original VADOFT code was written and documented by Dr. Huyakorn, Mr. H. White, Mr. J. Buckley, and Mr. T. Wadsworth of HydroGeoLogic. The Monte Carlo pre- and post-processors were written by Dr. Salhotra, Mr. P. Mineart, and Mr. Schanz of WCC.

Final assembly of the PRZM-2 model code, documentation and model testing were performed by AScI Corporation. The authors of the PRZM-2 user's manual (1993) were J.A. Mullins (AScI), R.F. Carousel (EPA), J.E. Scarbrough (AScI) and A.M. Ivery (AScI).

Prior to the release of PRZM-3, the model underwent a series of enhancements that resulted in intermediate releases. Changes were related to linking PRZM-2 with the HSPF, WASP and PATRIOT modeling systems, and the linking of PRZM-2 with the WDM database structure. Modifications to the soil moisture depth for runoff and surface pesticide 'mixing zone' calculations were documented in an addendum to the PRZM-2 user's manual written by A.S. Donigian, Jr. (AQUA TERRA), R.F. Carousel (EPA), J.C. Imhoff (AQUA TERRA) and P.R. Hummel (AQUA TERRA). Changes related to a non-uniform extraction algorithm for estimating pesticide runoff, the bi-phase transformation of a parent compound and its metabolites, the ability to transform parent compounds ins an adsorbed phase to metabolites, the metabolite loading transfer into EXAMS-2.98, the enhanced flexibility in chemical applications, and the improved output functions were implemented by Waterborne Environmental, Inc. and documented by R.F. Carousel (EPA), J.M. Cheplick (Waterborne) and W.M. Williams (Waterborne).

PRZM-2 evolved into PRZM-3 in 1995 when a septic system loading module On-site Wastewater Disposal System (OSWDS) and algorithms for modeling soil nitrogen fate and transport were added to the PRZM modeling system to provide a tool for defining wellhead protection strategies relative to nitrate contamination. This latter work was performed and documented by J.C. Imhoff, P.R. Hummel, A.S. Donigian and B.R. Bicknell, all of AQUA TERRA Consultants.

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SECTION 1
Introduction

This publication contains documentation for a soil column to groundwater loading model, PRZM-3, for the simulation of chemical contaminant transport down through the crop root and vadose zones. PRZM-3 enables modeling of organic chemicals, such as pesticides, as well as organic and inorganic nitrogen species. This release of PRZM-3 incorporates several new features in addition to those presented in the previous release of the model (PRZM-2.2): a nonuniform extraction algorithm for estimating pesticide runoff; bi-phase transformation of parent compound and metabolites; the ability to transform a parent compound in a sorbed phase to metabolites; metabolite loading transfer into EXAMS v. 2.98; enhanced flexibility in chemical applications; improved output features; and inclusion of nitrogen routines for assessing septic tank waste effluent.

A brief section on the background and objectives for the PRZM-3 model development effort follows in this introduction (Section 1.1). Section 1.2 gives a synopsis of risk and exposure assessment concepts. The reader who has sufficient background in these concepts may prefer to proceed to Section 1.3, that provides an overview of the PRZM-3 modeling system, including its major features and limitations.

1.1 Background and Objectives

The U.S. Environmental Protection Agency is continually faced with issues concerning the registration and restriction of pesticides used for agricultural purposes. Each of these regulatory processes requires that the potential risk to human health resulting from the introduction or continued use of such chemicals be evaluated. Recently, much of this attention has been focused on exposure through leaching of pesticides and nitrates to groundwater and subsequent ingestion of contaminated water.

The capability to simulate the potential exposure to pesticides or nitrates via this pathway has two major facets:

- Prediction of the fate of the chemical, after it is applied, as it is transported by water down through the crop root and soil vadose zones.
- Evaluation of the probability of the occurrence of contaminant concentrations of various magnitudes at various depths.

Several public domain models are capable of simulating the transport and transformation of chemicals in the subsurface and in the root zone of agricultural crops. However, none of these models had been linked together prior to PRZM-3, in such a way that a complete simulation package, that takes into account the effects of agricultural management practices on contaminant fate was available for use, either by the Agency or the agricultural chemical industry, to address groundwater contamination problems. Without such a scientifically credible modeling package, the decision maker must rely on modeling scenarios that are either incomplete or potentially incorrect. Each time a new scenario arose, recurring questions had to be answered:

- What models should be used?
- How should mass transfer between models be handled?

The resolution of these issues on a per-scenario basis is both expensive and time consuming. Furthermore, it precludes consistency of approach for the evaluation of contamination potential for across scenarios.

The modeling package described in this report seeks to overcome these problems by providing a consistent set of linked unsaturated zone models that have the flexibility to handle a wide variety of hydrogeological, soils, climate, and chemical scenarios. However, the formulation of the risk analysis problem requires more than a simple, deterministic evaluation of potential exposure concentrations. The inherent variability of force, capacitance and resistance in natural systems, combined with the inability to exactly describe these attributes of the system, suggests that exposure concentrations cannot be predicted with certainty. Therefore, the uncertainty associated with the

predictions must also be quantified. Consequently, this simulation package also seeks to provide this capability by utilizing Monte Carlo simulation techniques.

Stated more concisely, the objectives of this model development effort were to provide a simulation package that can:

- Simulate the transport and transformation of field-applied pesticides in the crop root zone and the underneath unsaturated zone, taking into account the effects of agricultural management practices
- Simulate the transport and transformation of nitrogen, introduced by atmospheric deposition and/or septic systems in the crop root zone and the underneath unsaturated zone
- Provide probabilistic estimates of potential exposure concentrations by taking into account the variability in natural system, population and processes, and the uncertainty in out ability to quantify these properties and processes.

Furthermore, it was desirable that the simulation package be easy to use and parameterize, and execute on IBM or IBM-compatible PCs and the Agency's DEC/VAX machines. As a result, considerable effort has gone into providing parameter guidance for both deterministic and probabilistic applications of the model, and on software development for facile model implementation.

1.2 Concept of Risk and Exposure Assessment

Exposure assessment, as defined for human impacts (U.S. Environmental Protection Agency 1984, 1992), is the estimation of the magnitude, frequency, duration, and route by which a quantity of a toxicant becomes available at certain exchange boundaries (i.e., lungs, gut, or skin) of a subject population over a specified time interval. Exposure assessment is a constitutive element of the larger problems of risk assessment and risk management, as illustrated in Figure 1.1. The concentration estimates generated during an exposure assessment must be combined with demographic and toxicological information to evaluate risk to a population – that can be used, in turn, to make policy decisions regarding the use or disposal of the chemical.

Major components of risk assessment are indicated in the following text. Of these, the first three constitute the important steps for exposure assessment and are discussed in detail here.

Characterization and quantification of chemical sources

1. Identification of exposure routes
2. Quantification of contaminant movement through the exposure routes to the receptor population/location
3. Characterization of the exposed population
4. Integration of quantified environmental concentrations with the characteristics of the exposed populations to yield exposure profiles

Characterization of sources(s) requires in a broad sense the estimation of the loading of a chemical into various environmental media. For the groundwater contamination problem, on a regional scale, this requires data on chemical sources/uses and distribution of those sources/uses (spatially and temporally). For pesticides, it also requires information on the crops being grown, registered or proposed chemical uses on those crops, and regional management practices. For a specific field-scale area, similar data would be needed to support an assessment; however, greater detail may be necessary.

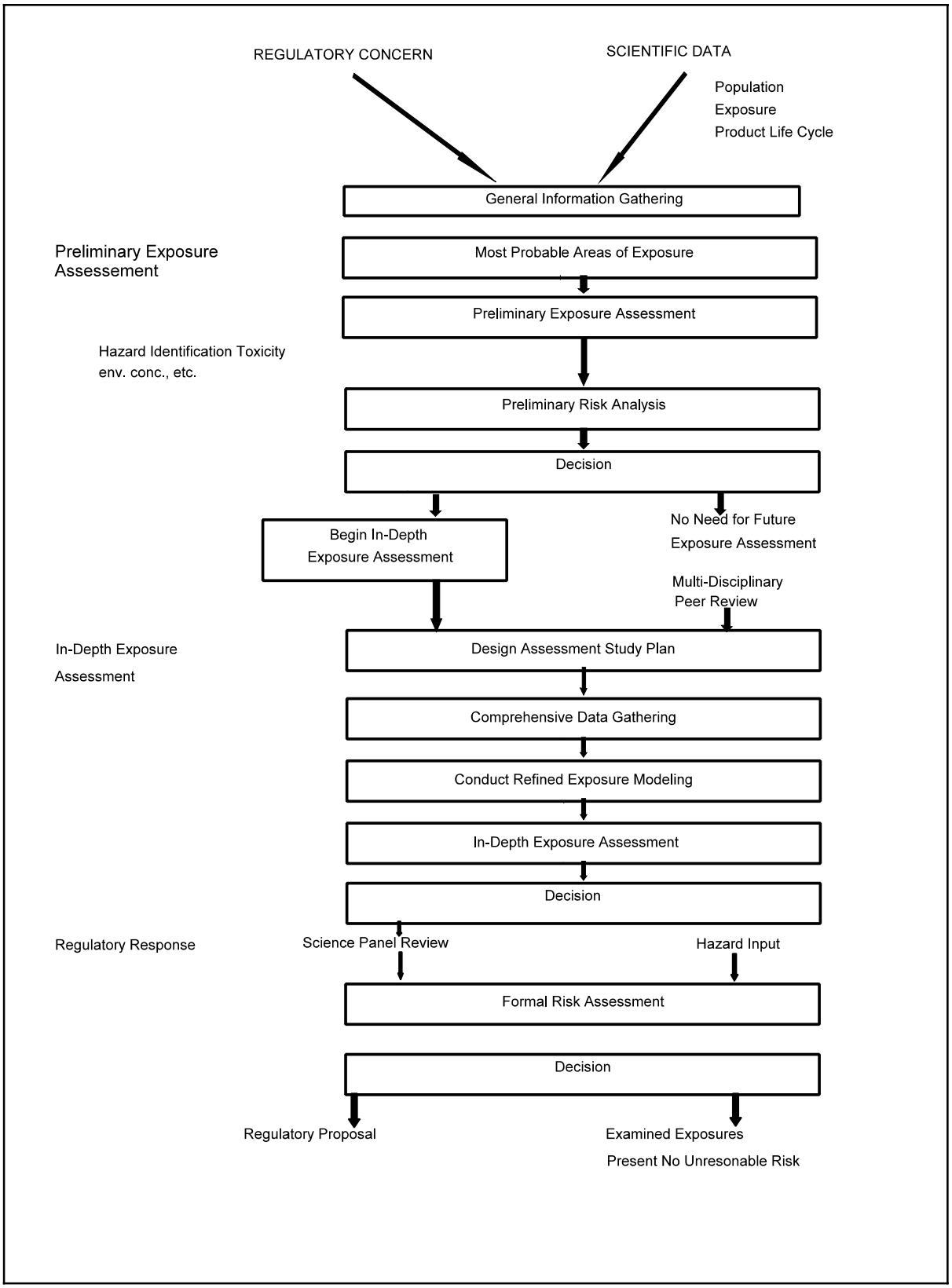


Figure 1.1 Decision path for risk assessment.

The identification of exposure pathways involves a qualitative (or semiquantitative) assessment of how the chemical is thought to move from the source to the exposed population. Important fate processes that may serve to reduce the concentration of the chemical(s) along various pathways in different environmental media are also identified. For the case of ingested groundwater exposure, important contaminant loading pathways and fate processes are predefined to a large extent in the models available for use. The quantification of contaminant concentrations in a medium, given the source strength, transport pathways, and attenuation mechanisms along each pathway, is the next step, and is the major benefit of using models such as PRZM-3. The guidelines are very specific in the requirement that concentrations be characterized by duration and frequency as well as magnitude. These characteristics can be determined through the analysis of time series exposure data generated by the model.

PRZM-3 produces time series of estimated toxicant concentrations, such as those in Figure 1.2. Each time series can be compared to a critical value of the concentration y. This type of analysis easily shows whether the criterion is exceeded and gives a qualitative feel for the severity of the exceedance state. If we determine how often a contaminant is at a particular level or within a specified range, a frequency distribution of the values of y (Figure 1.3) can be created. If, in addition, we choose any value of y in Figure 1.2 and determine the area under the curve to the right of that value, we can plot Figure 1.4, the cumulative frequency distribution of the toxicant concentration. The cumulative frequency distribution indicated the chance that any given value y that we select will be exceeded. If the example time series is long enough, then the "chance" approaches the true "probability" that y will be exceeded.

Thus far, only the concentration to which the organism will be exposed has been discussed, and nothing has been said concerning the duration of the event. If we take the same concentration time series and impose a window of length "t" on it at level y_c (Figure 1.5) and move that incrementally forward in time, we can make a statement concerning the toxicant concentration within the duration window. Normally, the average concentration within the window is used. The resulting cumulative frequency distribution indicates the chance that the moving average concentration duration t_c will exceed the critical value of y, y_c.

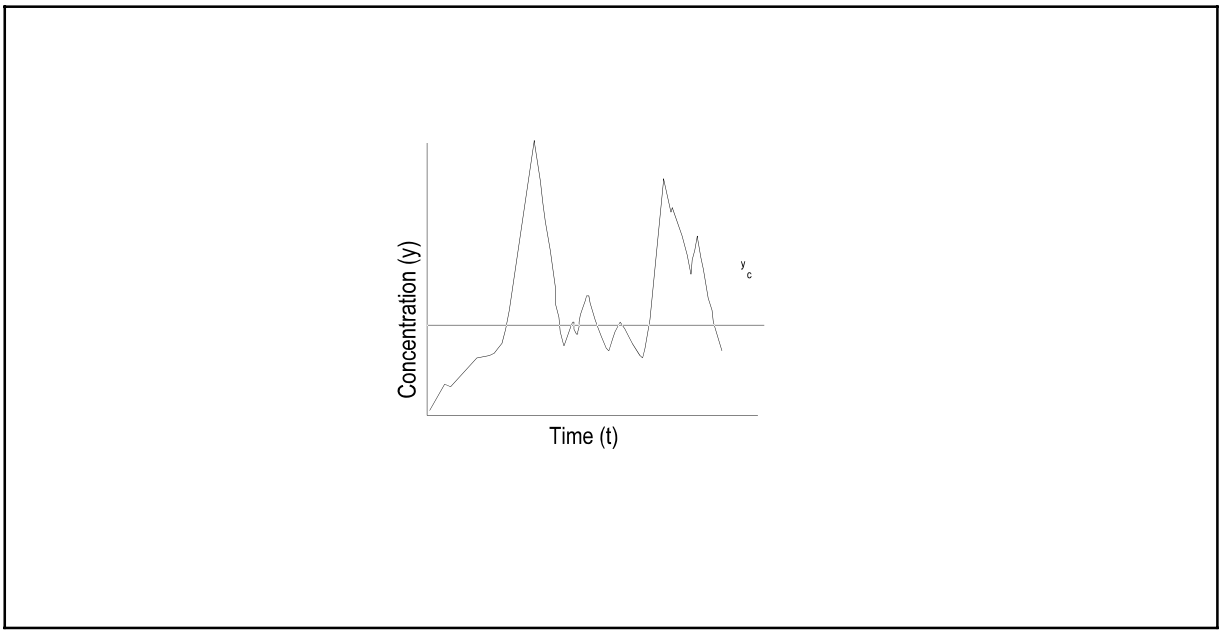


Figure 1.2 Time series plot of toxicant concentration.

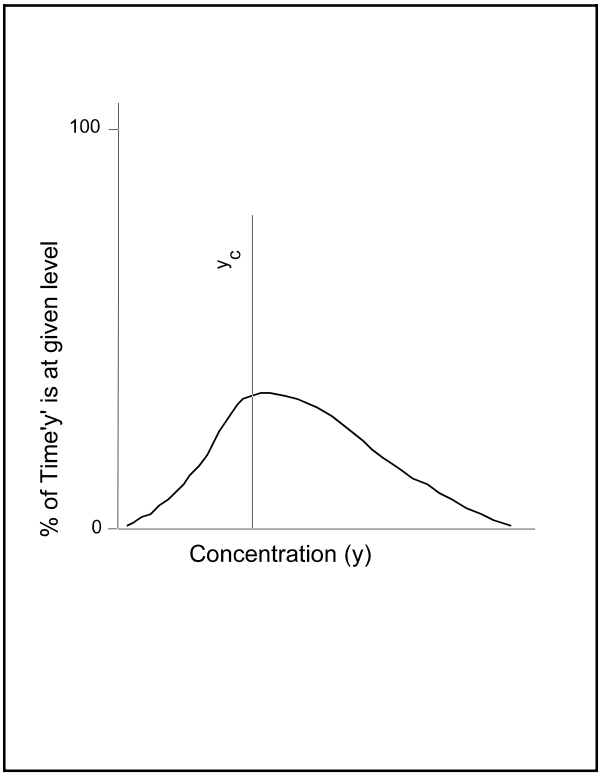


Figure 1.3 Frequency distribution of toxicant concentration.

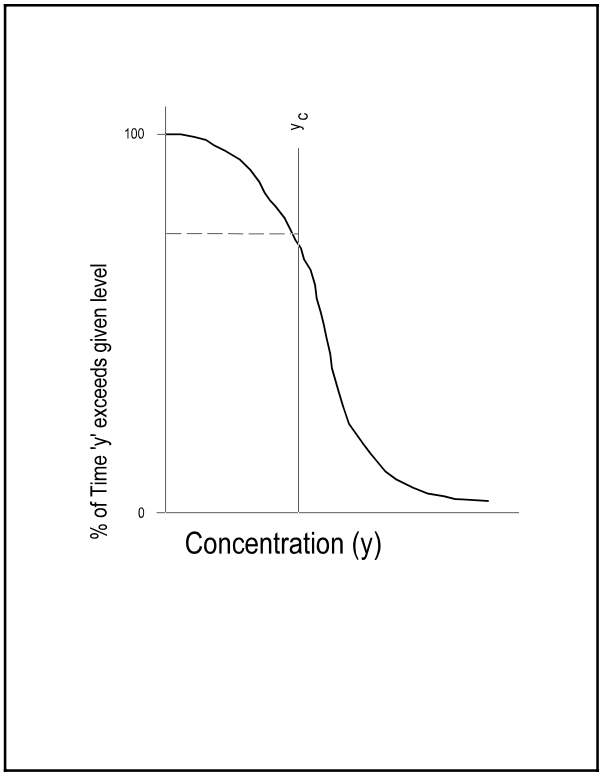


Figure 1.4 Cumulative frequency distribution of toxicant concentration.

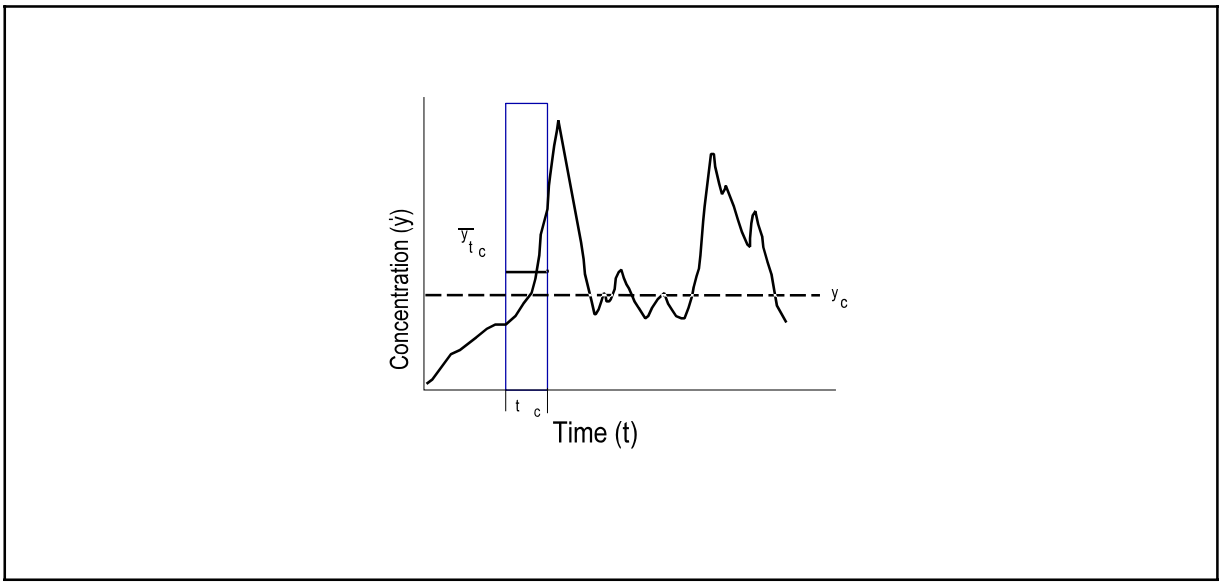


Figure 1.5 Time series of toxicant concentration with moving average concentration window of duration t_c.

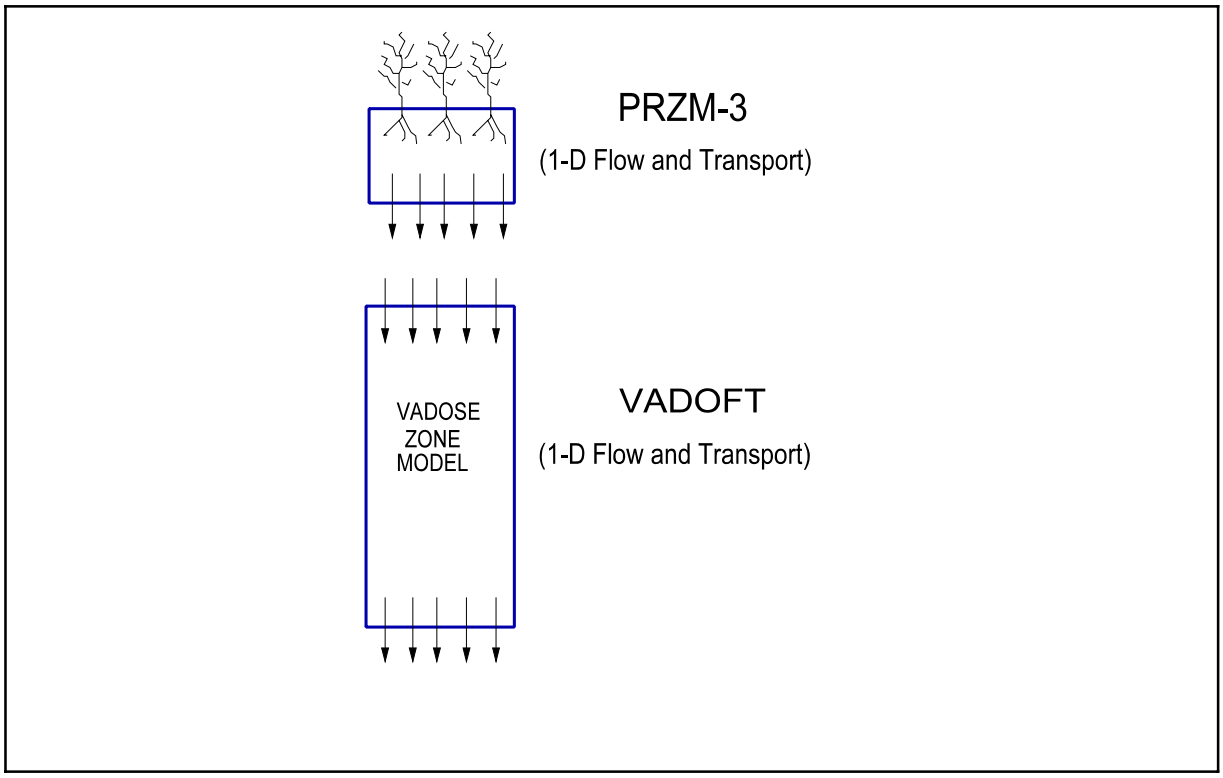


Figure 1.6 Linked modeling system configuration.

The moving average time window should be the same length as that specified for y_c. For instance, in the case of cancer risk, a 70-year (lifetime) window is normally used to average the data in the simulated time series. The use of the moving window for averaging the time series allows us to compare both the concentration and duration against the standard. The chance or probability that the moving average concentration exceeds the standard is the essence of the exposure assessment. This type of information provides a precursor to the estimates of risk involved using a given chemical under the conditions of the model simulation. The use of models like PRZM-3 that provide data the necessary data for environmental concentrations, duration and probability of occurrence ends here.

The next step in exposure assessment involves the characterization of the exposed population. Such factors as habits, age, sex, and location with respect to the source are of importance. The integration of the concentration estimates with population characteristics makes possible the counting of the conditional events of concentration in an environmental medium and the opportunity for the population to be exposed to these concentrations. The exposure assessment ends at this point. The actual intake of the chemicals, their fate within the human body (i.e., their pharmacokinetics), and their effects (i.e., toxicology) on the exposed population are not considered during exposure assessment.. These later issues, however, are also essential elements of risk assessment.

Although the concepts underlying an exposure assessment are relatively simple, the actual application of these concepts is complicated because of large variations in source-specific and environment-specific characteristics and the necessity to integrate specialized knowledge from a number of different fields. This variability underscores the need to use a model such as PRZM-3 in the evaluation of exposure concentrations.

1.3 Overview of PRZM-3

This section gives an overview of the PRZM-3 model, highlighting the features and limitations of the simulation package as a whole as well as those of the component models PRZM and VADOFT. The PRZM-3 code was designed to provide state-of-the-art deterministic simulation of the fate of pesticides, applied for agricultural purposes, both in the crop root zone and the underlying vadose zone. The model is capable of simulating multiple pesticides and/or parent/daughter relationships. The model is also capable of estimating the probabilities of concentrations or fluxes in or from the various media components for the purpose of performing exposure assessments.

To avoid writing an entirely new computer code, it was decided to make use of existing codes and software to the extent possible. Thus, due to its comprehensive treatment of important processes, its dynamic nature, and its widespread use and acceptability to the Agency and the agricultural chemical industry, the Pesticide Root Zone model (PRZM) (Carsel et al. 1985) was selected to simulate the crop root zone.

Having selected PRZM, two options were evaluated for developing a model to meet the objectives stated in Section 1.1. The first involved use of PRZM only. In this configuration, PRZM would be used to simulate both the root zone and the vadose zone. This option was rejected because the assumptions of the elementary soil hydraulics in PRZM (i.e., drainage of the entire soil column to field capacity in 1 day) were considered inadequate for simulating flow in a thick vadose zone. The second option involved PRZM linked to a to be determined unsaturated zone model. The option finally selected has been previously depicted in Figure 1.6. In this configuration, an enhanced version of PRZM was to be linked to a one-dimensional vadose zone flow and contaminant transport model. Both the vadose and PRZM models would simulate water flow and solute transport. Subsequently, a new code (VADOFT) was written to perform the necessary flow and chemical transport simulation in the vadose zone for this option.

1.3.1 Overview of PRZM

1.3.1.1 Features

The Pesticide Root Zone Model (PRZM) is a one-dimensional, dynamic, compartmental model that can be used to simulate chemical movement in unsaturated soil systems within and immediately below the plant root zone. It has two major components – hydrology (and hydraulics) and chemical transport. The hydrologic component for

calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Evapotranspiration is estimated either directly from pan evaporation data, or based on an empirical formula. Evapotranspiration is divided among evaporation from crop interception, evaporation from soil, and transpiration by the crop. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point, and saturation water content.

The chemical transport component can simulate pesticides and organic and inorganic nitrogen species. For pesticides, the transport component can simulate pesticide application on the soil or on the plant foliage. Biodegradation can be modeled in the root zone. Dissolved, adsorbed, and vapor-phase concentrations in the soil are estimated by simultaneously considering the processes of pesticide uptake by plants, surface runoff and erosion, decay/transformation, volatilization, foliar washoff, advection, dispersion, and retardation/sorption. For nitrogen, simulation of surface applications, atmospheric deposition, and septic effluent discharge can all be simulated. The nitrogen species of nitrate, ammonia, and four forms of organic nitrogen (i.e. particulate organic nitrogen (labile and refractory) and dissolved organic nitrogen (labile and refractory)) are represented. The soil nitrogen processes considered include plant uptake of nitrate and ammonium, return of plant nitrogen as organic nitrogen, denitrification or reduction of nitrate-nitrite, immobilization of nitrate-nitrite and ammonium, mineralization of organic nitrogen, fixation of atmospheric nitrogen, volatilization of ammonium, and the adsorption/desorption of ammonium and the organic forms.

Two options are available to solve the transport equations: (1) the original backwards-difference implicit scheme that can produce excessive numerical dispersion at high Peclet numbers; or (2) the method of characteristics algorithm that eliminates numerical dispersion, but slightly increases model execution time.

PRZM has the capability to simulate multiple zones. This allows PRZM and VADOFT to combine different root zone and vadose zone characteristics into a single simulation. Zones can be visualized as multiple vertical land segments joined together in a horizontal manner. There are three reasons a user may choose for implementing multiple zones:

(1) to simulate heterogenous PRZM root zones linked to a homogeneous vadose zone

(2) to simulate a homogeneous root zone linked to heterogenous vadose zones

(3) to simulate multiple homogeneous root zones linked to multiple homogeneous vadose zones

Weighing multiple zones together and their use are discussed in detail in Section 5.

Another feature for pesticide simulation is the ability to simulate as many as three chemicals simultaneously as either separate compounds or as a parent-daughter relationship. This gives the user the option to observe the behavior of multiple chemicals without making additional runs, or the ability to enter a mass transformation factor from a parent chemical to one or two daughter products and follow the behavior of all three.

Predictions are made on a daily basis. Output can be summarized for a daily, monthly, or annual period. Daily time series values of various fluxes or storages can be written to sequential files during program execution for subsequent analysis.

1.3.1.2 Limitations

There were significant limitations in the original (Release I) version of PRZM. A few were obvious to the developers; others were pointed-out subsequently by model users. These limitations are broken out into four categories:

- Hydrology
- Soil hydraulics

- Method of solution of the transport equation
- Deterministic nature of the model

Modifications made for PRZM-2 and PRZM-3 have overcome many of these limitations.

Hydrologic and hydraulic computations are still performed in PRZM on a daily time step even though, for some of the processes involved (evaporation, runoff, erosion), finer time steps might be used to ensure greater accuracy and realism. For instance, simulation of erosion by runoff depends upon the peak runoff rate, which is in turn dependent upon the time base of the runoff hydrograph. This depends to some extent upon the duration of the precipitation event. PRZM retains its daily time step primarily due to the relative availability of daily versus shorter time step meteorological data. This limitation has been mitigated, in part, by enhanced parameter guidance.

In PRZM, Release I, the soil hydraulics were simple–all drainage to field capacity water content was assumed to occur within 1 day. (An option to make drainage time dependent also was included, but there is little evidence to suggest that it was utilized by model users to any great extent.) This 1-day drainage assumption had the effect, especially in deeper soils, of inducing a greater-than-anticipated movement of chemical through the profile. While this representation of soil hydraulics has been retained in PRZM, the user now has the alternative of coupling PRZM to VADOFT. PRZM is then used to represent the root zone, while VADOFT, with a more rigorous representation of unsaturated flow, is used to simulate the thicker vadose zone. The VADOFT code is discussed in more detail in a subsequent section. For short distances from the soil surface to the water table, PRZM can be used to represent the entire vadose zone without invoking the use of VADOFT so long as no layers that would restrict drainage are present.

The addition of algorithms to simulate volatilization has brought into focus another limitation of the soil hydraulics representation. PRZM simulates only advective, downward movement of water and does not account for diffusive movement due to soil water gradients. This means that PRZM is unable to simulate the upward movement of water in response to gradients induced by evapotranspiration. This process has been identified by Jury et al. (1984)as an important one for simulating the effects of volatilization. However, the process would seem less likely to impact the movement of chemicals with high vapor pressures. For these chemicals, vapor diffusion would be a major process for renewing the chemical concentration in the surface soil.

Another limitation of the Release I model was the apparent inadequacy of the solution to the transport equation in advection-dominated systems. The backward difference formulation of the advection term tends to produce a high degree of numerical dispersion in such systems. This results in overprediction of downward movement due to smearing of the peak and subsequent overestimation of loadings to groundwater. In PRZM-2 and PRZM-3, an alternative formulation is available for advection-dominated systems. The advective terms are decoupled from the rest of the transport equation and solved separately using the method of characteristics (MOC). The remainder of the transport equation is then solved as before, using the fully implicit scheme. This approach effectively eliminates numerical dispersion with only a small increase in the computation time. In low-advection systems, the MOC approach reduces to the original PRZM solution scheme, which becomes exact as velocities approach zero.

The final limitation is the use of field-averaged water and chemical transport parameters to represent spatially heterogeneous soils. Several researchers have shown that this approach produces slower breakthrough times than are observed using stochastic approaches. This concern has been addressed by adding the capability to run PRZM-2 and PRZM-3 in a Monte Carlo framework. Thus, distributional, rather than field-averaged, values can be utilized as inputs that will produce distributional outputs of the relevant variables (e.g., flux to the water table).

The Special Actions option in PRZM-3 allows the user to output soil profile pesticide concentrations at user-specified times during the simulation period and to change selected model parameters to better represent chemical behavior and the impacts of agricultural management practices. The required input format and parameters are specified in Section 4.

By using the 'SNAPSHOT' capability of Special Actions, the user can output the pesticide concentration profile, i.e.,

the total concentration in each soil compartment, for any user-specified day during the simulation period. In this way, the user can run PRZM-3 with only monthly or annual output summaries and still obtain simulation results for selected days when field data were collected. There is no inherent limit to the number of SNAPSHOTs that can be requested in a single run. When more than one chemical is being simulated, the concentration profiles are provided by the order of the chemical number, i.e., NCHEM.

To better represent the expected behavior of the chemical being simulated, or the impacts of tillage or other agricultural practices, the following parameters can be reset to new values at any time during the simulation period:

Solution Decay Rate (DWRATE)
Sorbed Decay Rate (DSRATE)
Partition Coefficient (KD)
Bulk Density (BD)
Curve Number (CN)
USLE Cover Factor (USLEC)

Thus, for chemicals that demonstrate seasonal decay rates or partition coefficients, or different values for the period following application compared to later in the crop season, the appropriate parameters can be changed at user-specified times to mimic the observed, or expected, behavior of the compound.

Similarly, for agricultural practices or specific tillage operations that affect the soil bulk density, curve number, or cover factor, these parameter values can be altered during the simulation in an attempt to better represent their impacts. The parameter guidance in Section 5 may help the user in determining adjustments for these parameters. Users should note that adjustments to the bulk density, and possibly the partition coefficient, may affect the pesticide balance calculation.

1.3.2 Overview of the Vadose Zone Flow and Transport Model (VADOFT)

VADOFT is a finite-element code for simulating moisture movement and solute transport in the vadose zone. It is the second part of the two-component PRZM-3 model for predicting the movement of pesticides or nitrogen species within and below the plant root zone and assessing subsequent groundwater contamination. The VADOFT code uses Richards' equation to simulate one-dimensional, single-phase moisture and solute transport in unconfined, variably saturated porous media. Transport processes include hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. The code predicts infiltration or recharge rate and solute mass flux entering the saturated zone. The following description of VADOFT is adapted from Huyakorn et al.(1988).

1.3.2.1 Features

The code, which employs the Galerkin finite-element technique to approximate the governing equations for flow and transport, allows for a wide range of nonlinear flow conditions. Boundary conditions of the variably saturated flow problems may be specified in terms of prescribed pressure head or prescribed volumetric water flux per unit area. Boundary conditions of the solute transport problem may be specified in terms of prescribed concentration or prescribed solute mass flux per unit area. All boundary conditions may be time dependent. An important feature of the algorithm is the use of constitutive relationships for soil water characteristic curves based on soil texture.

1.3.2.2 Limitations

Major assumptions of the flow model are that the flow of the fluid phase is one-dimensional, isothermal and governed by Darcy's law and that the fluid is slightly compressible and homogeneous. Hysteresis effects in the constitutive relationships of relative permeability versus water saturation, and water saturation versus capillary pressure head, are assumed to be negligible.

Major assumptions of the solute transport model are that advection and dispersion are one-dimensional and that fluid

properties are independent of contaminant concentrations. Diffusive/dispersive transport in the porous-medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion. Adsorption and decay of the solute is described by a linear equilibrium isotherm and a lumped first-order decay constant. Parent/daughter chemical relationships may be simulated.

The code handles only single-phase flow (i.e., water) and ignores the presence of a second phase--i.e., air. The code does not take into account sorption nonlinearity or kinetic sorption effects that, in some instances, can be important. The code considers only single-porosity (granular) soil media. It does not simulate flow or transport in fractured porous media or structured soils.

1.3.3 Overview of the Monte Carlo Simulation Module

MCARLO performs all the functions necessary to execute a Monte Carlo simulation. It reads special data for parameters to be varied (e.g., distribution types and moments) and output variables to be observed, generates random numbers, correlates them and performs transformations, exchanges these generated values for PRZM-3 parameters, performs statistical analysis on the output variables, and writes out statistical summaries for the output variables.

The MCARLO module makes use of an input and output file. Inputs to the MCARLO module are discussed in Section 4. The user should be aware that many of the parameters entered in the Monte Carlo input file once designated as constants will be used in lieu of that same parameter value entered in the standard input file.

The final limitation is that only a small number of input variables may be changed at random by invoking the Monte Carlo routines. It is not difficult to add additional variables, however.

1.3.4 Model Linkage

One of the more challenging problems in this model development effort was the temporal and spatial linkage of the component models. In the section which follows, these linkages are discussed.

1.3.4.1 Temporal Model Linkage

The resolution of the temporal aspects of the two models was straightforward. PRZM runs on a daily time step. The time step in VADOFT is dependent upon the properties of soils and the magnitude of the water flux introduced at the top of the column. In order for the nonlinear Richards' equation to converge, VADOFT may sometimes require time steps on the order of minutes.

For the linkage of PRZM-3, through VADOFT the resolution of time scales is also straightforward. VADOFT is prescribed to simulate to a "marker" time value, specifically to the end of a day. The last computational time step taken by VADOFT is adjusted so that it coincides with the end of the day. PRZM's daily water fluxes are used as input to VADOFT. VADOFT utilizes this flux as a constant over the day and adjusts its internal computational time step in order to converge.

1.3.4.2 Spatial Linkages

The spatial linkages utilized for the models are more complex. The principal problem is the presence of a fluctuating water table. A second problem is that of the incompatibility between the hydraulics in PRZM and VADOFT. Of course, any linking scheme utilized must provide a realistic simulation of the flow of water and transport of solutes at the interfaces and must ensure mass balance.

The major problem with the interfacing of these two models is that while VADOFT solves the Richards' equation for water flow in a variably saturated medium, PRZM uses simple "drainage rules" to move water through the soil profile. Because of this incompatibility, there may be times when PRZM produces too much water for VADOFT to

accommodate within one day. This is very likely to happen in agricultural soils, where subsoils are typically of lower permeability than those of the root zone, which have been tilled and perforated by plant roots and soil biota. The result of this would be water ponded at the interface which would belong neither to PRZM or VADOFT.

The solution was to prescribe the flux from PRZM into VADOFT so that VADOFT accommodates all the water output by PRZM each day. This eliminates the problem of ponding at the interface. However, it does force more water into the vadose zone than might actually occur in a real system, given the same set of soil properties and meteorological conditions. The consequence is that water and solute are forced to move at higher velocities in the upper portions of the vadose zone. If the vadose zone is deep, then this condition probably has little impact on the solution. If it is shallow, however, it could overestimate loadings to groundwater, especially if chemical degradation rates are lower in the vadose zone than in the root zone.

1.3.5 Monte Carlo Processor

PRZM-3 can be run in a Monte Carlo mode so that probabilistic estimates of pesticide loadings to the saturated zone from the source area can be made. The input preprocessor allows the user to select distributions for key parameters from a variety of distributions; the Johnson family (which includes the normal and lognormal), uniform, exponential and empirical. If the user selects distributions from the Johnson family, he or she may also specify correlations between the input parameters. The Monte Carlo processor reads the standard deterministic input data sets for each model, then reads a Monte Carlo input file that specifies which parameters are to be allowed to vary, their distributions, the distribution parameters, and correlation matrix. The model then executes a prespecified number of runs.

The output processor is capable of preparing statistics of the specified output variables including mean, maximum values and quantiles of the output distribution. The output processor also can tabulate cumulative frequency histograms of the output variables and send them to a line printer for plotting.

1.3.6 Overview Summary

A modeling system (PRZM-3) has been developed for the U.S. Environmental Protection Agency that is capable of simulating the transport and transformation of pesticides, following application, down through the crop root zone and underlying vadose zone. The modeling system was designed to handle a variety of geometries likely to be encountered in performing evaluations for pesticide registration or special reviews. Recent enhancements have expanded modeling capabilities to include simulation of nitrogen species as well, enabling the model to be used for evaluation of subsurface nitrate contamination. A major objective was to keep the model simple and efficient enough so that it could be operated on an IBM-PC or IBM-compatible PC and used in a Monte Carlo mode to generate probabilistic estimates of pesticide loadings or water concentrations. The model consists of two major computational modules – PRZM, which performs pollutant fate calculations for the crop root zone and is capable of incorporating the effects of management practices, and VADOFT, which simulates one-dimensional transport and transformation within the vadose zone.

Linkage of these models is accomplished through the use of simple bridging algorithms that conserve water and solute mass.

SECTION 2
Model Development, Distribution, and Support

Refer to the README.TXT file for the most recent and detailed PRZM-3 model development, distribution, and support information. A copy of the README.TXT file is included in the distribution package or it can be viewed or downloaded from the Center for Exposure Assessment Modeling (CEAM) Internet site (Refer to Section 2.3, Obtaining a Copy of the PRZM-3 Model System).

2.1 Development and Testing

The distribution version of the PRZM-3 model system is built with the Lahey/Fujitsu Fortran 95 Pro compiler, version 7.1. Refer to Section 2.4.2 for specific hardware and software run time requirements for the host system for the PRZM-3 model system.

2.2 Distribution

The PRZM-3 model system and all support files and programs are available through the Internet from CEAM at no charge (Refer to Section 2.3, Obtaining a Copy of the PRZM-3 Model System).

Included in the distribution set are:

- an interactive installation program
- test input and output files for installation verification
- an executable task image file for the PRZM-3 model system
- Fortran source code files
- command and "make" files to compile, link, and run the task image file
- a PRZM-3 general execution and user support guide (README.TXT) file.

The README.TXT file contains a section entitled <u>File Name and Content</u> that provides a brief functional description of each PRZM-3 file by name or file name extension type. Other sections in this document contain further information about:

- system documentation
- installation procedure
- verifying installation
- development system
- code modification
- technical help contacts.

2.3 Obtaining a Copy of the PRZM-3 Model

2.3.1 Internet

PRZM-3 and other software, data, and documents can be downloaded from the Internet via the EPA Exposure Assessment Models Web site maintained by CEAM. The Exposure Assessment Models home page is located at the Uniform Resource Locator (URL):

http://www.epa.gov/ceampubl/

A complete list of software models, data, and documents distributed by CEAM is available at the URL:
http://www.epa.gov/ceampubl/products.htm

If you do not have access to the Internet, contact CEAM to request a copy of the model distribution package on disk. Refer to Section 2.8, Technical Help, for CEAM contact information.

2.4 General/minimum Hardware and Software Installation and Run Time Requirements

Refer to the README.TXT file for the most recent and complete information concerning hardware and software installation and run time requirements.

2.4.1 Installation Requirements

- CD-ROM drive (if installed from CD-ROM)
- approximately 6 MB available hard disk storage
- Windows 9x/NT/2K/XP operating system

2.4.2 Run Time Requirements

- DOS or operating system capable of emulating a DOS console (e.g., Win9x/NT/2K/XP)
- approximately 6 MB available hard disk storage

A Fortran compiler is not required to execute any portion of the model.

2.5 Installation

The PRZM-3 model system and related support files are distributed within an automated installation program which may be acquired either from the Internet or CD-ROM. In either case, the model and related support files are contained in the file Install_PRZM312.EXE. Save the installation program to a local disk before running the installation program.

To install PRZM-3:

- Close all applications
- Click on the installation program "Install_PRZM312.EXE"
- Follow the instructions presented by the installation program.

2.6 Installation Verification and Routine Execution

Refer to the following sections in the README.TXT file for complete instructions concerning installation verification and routine execution of the PRZM-3 model:

- File Name and Content
- Installation Verification

2.7 Code Modification

Included in the distribution file are:

- an executable task image file for the PRZM-3 model system
- Fortran source code files
- command and "make" files to compile, link, and run the task image file (PRZM3.EXE).

If the user wishes to modify the model or any other program, it will be up to him or her to supply or obtain:

- an appropriate text editor that saves files in ASCII (non-binary) text format

- Fortran development tools to recompile and link edit any portion of the model.

CEAM cannot support, maintain, or be responsible for modifications that change the function of any executable task image (*.EXE), DOS batch command (*.BAT), or "make" utility file(s) supplied with this model package.

2.8 Technical Help

For further information on installation and execution, refer to the Installation and Installation Verification sections of the README.TXT file. For questions or information concerning the distribution or installation of PRZM-3 software, documentation, or data please contact CEAM at:

- Phone: 706-355-8400
- Fax: 706-355-8104
- E-mail: ceam@epamail.epa.gov
- Mail:
  Center for Exposure Assessment Modeling (CEAM)
  National Exposure Research Laboratory - Ecosystems Research Division
  U.S. Environmental Protection Agency (U.S. EPA)
  960 College Station Road
  Athens, Georgia 30605-2700

CEAM operates and maintains a listserver system named CEAM-USERS. The CEAM-USERS listserver is an automated mailing list system which broadcasts up-to-date information concerning CEAM software product updates and releases as well as hints on software installation and use. Subscribers may broadcast messages to other list subscribers to ask and answer questions about exposure assessment modeling topics. Instructions for subscribing, posting messages, and managing membership setting are available on the CEAM Web site at the URL:

http://www.epa.gov/ceampubl/listserv.htm

2.9 Disclaimer

Mention of trade names or use of commercial products does not constitute endorsement or recommendation for use by the United States Environmental Protection Agency.

Execution of the PRZM-3 model system, and modifications to the DOS system configuration files (i.e., \CONFIG.SYS and \AUTOEXEC.BAT) must be used and/or made at the user's own risk. Neither the U.S. EPA nor the program authors can assume responsibility for model and/or program modification, content, output, interpretation, or usage.

The PRZM-3 program and files have been extensively tested and verified. However, as for all complex software products, the programs herein may not be completely free of errors and may not be applicable for all cases. In no event will the U.S. EPA be liable for direct, indirect, special, incidental, or consequential damages arising out of the use of the programs and/or associated documentation.

2.10 Trademarks

- LF95 is a registered trademark of Lahey Computer Systems, Inc. All other Lahey products are trademarks of Lahey Computer Systems, Inc.

SECTION 3
Modules and Logistics

The PRZM-3 model consists of four major modules. These are:

- EXESUP, which controls the simulation
- PRZM, which performs transport and transformation simulations for the root zone
- VADOFT, which performs transport and transformation simulations for the vadose zone
- MONTE CARLO, which performs sensitivity analysis by generating random inputs

In this section, Table 3.1 gives a listing of all subroutines and functions organized by module calling routines. Table 3.2 gives a listing of all parameter files and their dimensions. A brief description for each listing is also given.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
EXESUP		
	INIT	initializes common block CONST.INC
	ECHOF	echo names of files opened.
	ENDDAY	used to determine Julian day and simulation progress.
	FILOPN	opens and assigns file unit numbers.
	ECHOGD	echoes global data input.
	DONBAR	calculates percent complete bar.
	ADDSTR	add string to end of existing string.
	INPREA	reads and initializes program input.
	BMPCHR	converts character to uppercase.
	CENTER	centers string message on screen.
	COMRD	checks input for end of file.
	COMRD2	checks input for comment lines.
	COMRD3	checks input for END statement.
	DISPLAY	display data to echo file and screen.
	ECHORD	echoes line numbers read from input.
	ELPSE	add trailing string and fill middle.
	ERRCHK	write error messages.
	EXPCHK	check argument for exponential limits.
	FILCLO	closes open files.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	OPECHO	flags the printing utility.
	RELTST	checks argument as a real number.
	SQRCHK	gives square root with error checking.
	SUBIN	tracks entry into a subroutine.
	SUBOUT	tracks exit from a subroutine.
	TRCLIN	writes subroutine tracking to screen.
	SCREEN	controls display to screen.
	LFTJUS	left justifies a character string.
	LNCHK	takes natural log of a number.
	LNGSTR	returns length of a character string.
	LOGCHK	takes base 10 logarithm of a number with error checking provided.
	NAMFIX	left justifies and capitalizes a string.
	CLEAR	clears the display screen.
	FILCHK	checks that necessary files are open.
	EXESUP	controls calls to PRZM, VADOFT, and MONTE CARLO
	INITEM	determines global data.
	FILINI	initializes file unit numbers.
	PRZM3	controls model calling routines.
	LSUFIX	performs internal reads.
PRZM		
	BIODEG	perform time dependant solution for microbiodegradation.
	SLPST1	set up coefficient matrix for the solution of pesticide transport.
	PRZMRD	reads PRZM input file.
	HYDR2	perform soil hydraulic calculations.
	PLGROW	determines plant growth parameters for use in other subroutines.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	FARM	insures pesticide application is applied during adequate moisture conditions
	INIDAT	provides common block CMISC.INC values.
	TRDIA1	solves tridiagonal matrix.
	HYDROL	calculates snowmelt, crop interception, runoff, and infiltration.
	HFINTP	determines boundary for head, concentration or flux.
	PESTAP	computes amount of pesticide application.
	PLPEST	determines amount of pesticide which disappears by first order decay and pesticide washoff.
	SLPST0	sets up the matrix for transport of pesticide.
	CANOPY	calculates the overall vertical transport resistance.
	MOC	solves the advection component of the pesticide transport process.
	MASBAL	calculates mass balance error terms for both flow and transport.
	PSTLNK	provides linkage for transformation and source terms of parent/daughter.
	OUTCNC	prints daily, monthly, and annual pesticide concentration profiles.
	TRDIAG	solves tridiagonal matrix.
	OUTRPT	prints daily, monthly, and annual concentration profiles plus snapshots.
	VALDAT	checks simulation dates against calendar dates.
	XPRZM	performs PRZM execution calls.
	INITDK	initializes amount of pesticide decay each chemical which could have daughter products.
	OUTPST	prints daily, monthly, and annual pesticide flux profiles.
	INITL	initializes PRZM arrays.
	OUTTSR	prints daily, monthly, and annual time series data.
	OUTHYD	accumulates summaries for water flow.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	HYDR1	performs hydraulic calculations assuming a uniform soil profile.
	PRZECH	echoes PRZM input to files.
	RSTPUT	writes PRZM input to a restart file.
	RSTGET	reads PRZM input from a restart file.
	RSTPT1	writes PRZM input to a restart file.
	RCALC	function to compute biodegradation.
	RSTGT1	reads PRZM input from a restart file.
	PRZEXM	creates input file for EXAMS model.
	PRZDAY	transfers start and end dates to common block.
	THCALC	computes moisture for PRZM.
	INIACC	initializes PRZM storage arrays.
	KDCALC	computes KD.
	MCPRZ	computes MONTE CARLO inputs for PRZM.
	FNDCHM	function to find a chemical number.
	FNDHOR	function to find a horizon number.
	PZCHK	checks horizontal values for consistency.
	KHCORR	corrects Henry's law constant.
	ACTION	performs special actions.
	GETMET	reads in meteorological data.
	IRRIG	performs irrigation algorithm.
	FURROW	computes furrow irrigation.
	INFIL	computes Green-Ampt infiltration.
	EVPOTR	computes evapotranspiration.
	EROSN	computes erosion losses.
	SLTEMP	calculates soil temperatures.
	PRZM	performs calls to PRZM routines.
	TDCALC	calculates total days in a simulation.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	NITR	simulate nitrogen behavior in detail.
	NITRXN	perform reactions on all nitrogen forms.
	SV	calculate adsorption/desorption of nitrogen constituents using the single value freundlich method
	ITER	iterate until a sufficiently close approximation for the adsorbed and solution values on the freundlich isotherm is reached.
	FIRORD	calculate adsorption/desorption fluxes using temperature dependent first order kinetics.
	CRDYFR	determine number of days in month each crop is growing and fraction of monthly target plant uptake for each crop.
	YUPINI	calculate initial values of the daily plant uptake target on last day of previous month.
	CRPSEL	determine which, if any, of the current crop seasons includes the current day and month.
	YUPTGT	calculate daily yield-based plant uptake targets for each soil layer based on user-specified monthly fractions of the annual target and a trapezoidal function to interpolate between months.
	YUPLAY	calculate daily yield-based plant uptake targets for a soil layer based on user-specified monthly fractions of the annual target and a trapezoidal function to interpolate between months.
	LPYEAR	returns a leap year flag which is set to on if the year is a leap year
	PRZNRD	read nitrogen input parameters for PRZM nitrogen simulation
	OMSG	output an error or warning message from nitrogen simulation code.
	OMSINI	reset output message parameters for nitrogen simulation code.
	OMSTI	save an integer value to output with nitrogen simulation message.
	OMSTR	save a real value to output with nitrogen simulation message.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	OMSTC	save a character value to output with nitrogen simulation message.
	OMSTC	save a date to output with nitrogen simulation message.
	DAYVAL	linearly interpolate a value for this day, given values for the start of this month and next month.
	NITMOV	set up the coefficient matrix for the solution of the soil transport equation for nitrogen species.
	NITMOV	set up the coefficient matrix for the solution of the soil transport equation for nitrogen species, then call equation solver for the tridiagonal matrix.
	NITECH	echo user input nitrogen simulation parameters.
	OUTNIT	accumulate and output daily, monthly, and annual summaries for nitrogen species.
	WDTGET	retrieve buffer of time-series data from specified data set on WDM file.
	WDBSGR	retrieve real type attribute from specified data set on WDM file.
	VADOFT	
	VADCAL	calls relevant subroutines to compute nodal head and concentration.
	BALCHK	mass balance calculation.
	READTM	reads in HVTM, TMHV, QVTM from input.
	VADINP	reads in flow and transport input.
	TRIDIV	performs tridiagonal matrix solution.
	VADOFT	saves information between flow and transport.
	IRDVC	reads in integer vectors.
	VSWCOM	computes nodal values of water saturation and Darcy velocities.
	VADCHM	transfers chemical specific data to VADOFT variables.
	INTERP	performs linear interpolation using tabulated data of relative permeability versus water saturation.
	SWFUN	computes water saturation values for grid element.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	PKWFUN	computes relative permeability.
	DSWFUN	computes moisture capacity.
	XTRANS	controls transport calling routines.
	RDPINT	reads non-default nodes data.
	VARCAL	computes nodal head and concentration values.
	ASSEMF	assembly routine for flow.
	VADPUT	writes VADOFT input to restart file.
	VADGET	reads VADOFT input from a restart file.
	ASSEMT	assembly routine for transport.
	XFLOW	controls flow calling routines.
	MCVAD	determines MONTE CARLO variables for VADOFT.
	READVC	reads in vectors.
	CONVER	computes the limiting values of water saturation for each material.
	MTPV	calculates vectors.
	OUTPUT	write summary statistics.
	INITMC	initializes statistical summation arrays.
	DECOMP	decomposes the matrix BBT (N by N) into a lower triangular form.
	RANDOM	controls random numbers generation.
	NMB	generates normal (0-1) random numbers.
	UNIF	generates uniform random numbers.
	EXPRN	generates exponentially distributed random numbers.
	EMPCAL	generates values from empirical distributions.
	TRANSM	converts normally distributed correlated vectors to the parameter set returned to the model.
	TRANSB	transforms variables from normal space to SB space or vice-versa.
	OUTFOR	writes tables and plots of cumulative distribution.

Table 3.1 List of Subroutines and Functions and a Brief Description of Their Purpose

MODULE CALLING ROUTINE	SUBROUTINE or FUNCTION	PURPOSE
	STOUT	initializes the amount of pesticide decay.
	FRQTAB	prints tabular frequency output.
	FRQPLT	plots cumulative distributions.
MONTE CARLO		
	MCECHO	echoes MONTE CARLO input.
	READM	reads in MONTE CARLO input.
	MAXAVG	computes maximum daily average output.
	STATIS	performs summations for MONTE CARLO.

Table 3.2 List of All Parameters Files, Parameter Dimensions, and a Brief Description

FILE	PARAMETER	DESCRIPTION
CTRACE.INC	MAXSUB=50	maximum number of subroutines.
	MAXLIN=10	maximum number of lines for trace option.
PMXMAT.INC	MXMAT=5	maximum number of VADOFT materials.
PMXNLY.INC	MXNLAY=20	maximum number of layers in VADOFT.
PMXPRT.INC	MXPRT=100	maximum number of VADOFT observation nodes.
PMXTIM.INC	MXTIM=31	maximum number of VADOFT iterations allowed.
PMXTMV.INC	MXTMV=31	maximum number of VADOFT time interpolation values.
PMXVDT.INC	MXVDT=31	maximum number of VADOFT time steps.
PCMPLR.INC	REALMX=1.0D+30	maximum real number.
	REALMN=1.0D-30	minimum real number.
	MAXINT=2147483647	maximum integer value.
	MAXREC=512	maximum record length.
	EXNMX=-53.0	maximum negative exponential number.
	EXPMN=REALMN	minimum exponential real number.
	EXPMX=53.0	maximum positive exponential number.
	WINDOW=.TRUE.	allows screen window on or off.
	PCASCI=.TRUE.	allows attributes for PC's for displays.
	NONPC=.FALSE.	allows attributes for non-PC's for displays.
PMXNOD.INC	MXNOD=100	maximum number of VADOFT nodes allowed.
PMXZON.INC	MXZONE=10	maximum number of PRZM zones.
PPARM.INC	NCMPTS=100	maximum number of compartments in PRZM.
	NAPP=50	maximum number of applications in PRZM.
	NC=5	maximum number of crops allowed in PRZM.
	NPII=800	maximum number of PRZM particles in MOC.
	NCMPP2=NCMPTS+2	maximum number of compartments plus 2 for top and bottom ends.
	MXCPD=150	maximum number of cropping periods in PRZM.
PENANCE	KNOUT=6	screen unit number.

Table 3.2 List of All Parameters Files, Parameter Dimensions, and a Brief Description

FILE	PARAMETER	DESCRIPTION
	NMXFIL=99	maximum number of file units open.
	FILBAS=30	base file unit number.
PMXNSZ.INC	MXNSZO=10	maximum number of VADOFT zones allowed.
CMCRVR.INC	MCMAX=50	maximum number of random input variables.
	NMAX=10	maximum number of summary output variables.
	NCMAX=10	maximum number of CDF's.
	NRMAX=1000	maximum number of MONTE CARLO runs.
	NEMP=20	maximum number of empirical distributions.
	MCSUM = MCMAX+NMAX	maximum number of random input and output variables.
	NPMAX=5	maximum length of MONTE CARLO averaging periods.

SECTION 4
Input Parameters for PRZM-3.12

4.1 Input File Summary

PRZM-3 utilizes up to five input files, depending on the features and modules to be simulated:

- Execution Supervisor file (PRZM3.RUN). The Execution Supervisor file determines which modules are chosen for simulation; the number of zones used in a simulation; input, output, and scratch file names with optional path statements; the starting and ending date of a simulation; the number of chemicals (either separate or daughter); weighting parameters between PRZM and VADOFT zones; and global echo and trace levels during execution.

- PRZM parameter input file. The PRZM parameter input file specifies regional climatological information, hydrology and erosion parameters, crop characteristics including emergence and harvest dates, pesticide properties and application rates, and soil characteristics.

- Time-series files. Various time-series data are input via files specified in the execution supervisor. These include meteorological, nitrogen atmospheric deposition, and septic effluent data. Only the file containing meteorologic data is required for all PRZM-3 runs.

- VADOFT parameter input file. The VADOFT input file, containing soil horizon and chemical properties, is required if VADOFT or TRANSPORT SIMULATION are specified as “ON” in the execution supervisor (PRZM3.RUN) file.
- MONTE CARLO input file. This file is required when MONTE CARLO is specified as “ON” in the execution supervisor file. The file indicates parameter input values, distributions, and correlations.

All of these files, except for the time-series files, may have embedded comment lines. A comment line is any line beginning with three asterisks (***). These lines are ignored by the code during execution. To better understand record formats used in model input, an example record format statement appears below:

FORMAT 3I2,2X,F8.0,E10.3,1X,2(I5,1X,F8.0)

where input would look like:

```
010181    0.340    2.40E00    1    0.340    1    0.340
```

The format identifier, 3I2, specifies there are three integers with two columns each. The format identifier, 2X, specifies there are two blank spaces. The format identifier, F8.0, specifies there is one floating point field with eight columns and also a decimal point with no precision (although up to seven of these columns may be points of precision with the eighth column being the decimal point since this is a FORTRAN read statement). The format identifier, E10.3, specifies there is one field of ten columns that may include an exponential suffix. The format identifier, 2(I5,1X,F8.0), specifies that there are two sequential sets of I5,1X,F8.0 entered. All format specifiers should be right justified so that unused columns in a field are assumed to be zeros by the code.

Each of these module files along with their examples are discussed in the following pages. For further descriptions, see Section 4 on parameter estimation.

4.2 Time-series Files

The PRZM-3 model requires the input of various time-series data. These are input via files specified in the execution supervisor. The meteorological file is the only time-series file which is required for all PRZM-3 runs. The nitrogen

atmospheric deposition and septic effluent files are only required when nitrogen species are being simulated and atmospheric deposition and/or septic effluent is being considered.

4.2.1 Meteorological Data File

PRZM-3 requires the use of a meteorological file that is specified in the execution supervisor. Information on daily precipitation, pan evaporation, temperature, wind speed, and solar radiation is included in each record of the meteorological file. Data format requirements and an example input file are shown below:

Meteorological File Input Guide

RECORD FORMAT: 1X,3I2,5F10.0
READ STATEMENT: MM, MD, MY, PRECIP, PEVP, TEMP, WIND, SOLRAD

where

MM	=	meteorological month
MD	=	meteorological day
MY	=	meteorological year
PRECIP	=	precipitation (cm day^{-1})
PEVP	=	pan evaporation data (cm day^{-1})
TEMP	=	temperature (Celsius)
WIND	=	wind speed (cm sec^{-1})
SOLRAD	=	solar radiation (Langley)

Example Meteorological File

```
1 164    0.000    0.149   -0.278    388.925    225.597
1 264    0.000    0.242    8.611    388.925    226.408
1 364    0.000    0.227   13.611    388.925    227.280
1 464    1.041    0.164    9.444    388.925    228.211
1 564    0.203    0.211    9.722    388.925    229.200
1 664    1.143    0.186   10.278    388.925    230.248
1 764    0.000    0.181    6.389    388.925    231.353
1 864    3.048    0.216   12.222    388.925    232.515
1 964    0.000    0.229    7.778    388.925    233.733
1 1064   0.000    0.172    2.500    388.925    235.006
```

4.2.2 Atmospheric Deposition File

When nitrogen species are being simulated in PRZM-3, daily inputs of atmospheric deposition of nitrogen may be input using a file that is specified in the execution supervisor. Daily values for both dry and wet deposition of ammonia, nitrate, and organic N are included on each record of the file. Which dry and wet constituents being simulated are specified on record N4 of the PRZM input file (see Section 4.4.2.2) via a set of six flags (3 dry, 3 wet). Only the constituents with a flag value of -1 will be read from the atmospheric deposition file. Data format requirements and an example input file are shown below:

Atmospheric Deposition File Input Guide

RECORD FORMAT: 1X,3I2,6F10.0
READ STATEMENT: MM, MD, MY, AMMD, NITRD, ORGND, AMMW, NITRW, ORGNW

where

MM	=	calendar month
MD	=	calendar day
MY	=	calendar year
AMMD	=	ammonia concentration (g cm^{-1})
NITRD	=	nitrate concentration (g cm^{-1})
ORGND	=	organic N concentration (g cm^{-1})
AMMW	=	ammonia concentration (g cm^{-1})
NITRW	=	nitrate concentration (g cm^{-1})
ORGNW	=	organic N concentration (g cm^{-1})

Example Atmospheric Deposition File

```
1  182    .01    .005    0.0    0.0    0.0    0.0
1  282    .01    .005    0.0    0.0    0.0    0.0
1  382    .01    .005    0.0    0.0    0.0    0.0
1  482    .01    .005    0.0    0.0    0.0    0.0
1  582    .01    .005    0.0    0.0    0.0    0.0
1  682    .01    .005    0.0    0.0    0.0    0.0
1  782    .01    .005    0.0    0.0    0.0    0.0
1  882    .01    .005    0.0    0.0    0.0    0.0
1  982    .01    .005    0.0    0.0    0.0    0.0
1 1082    .01    .005    0.0    0.0    0.0    0.0
```

If daily time series of atmospheric deposition are not available, monthly values may be input on record N5 in the PRZM input file (see Section 4.4.2.2). This is indicated by entering flag values of -2 on record N4. The monthly values will be divided equally among the days in the respective months. Additionally, nitrogen applications with fertilizers or manure may be accomplished in a manner analogous to pesticide applications (see records N6 - N7 in Section 4.4.2.2).

4.2.3 Septic Effluent File

When nitrogen species from septic tank effluent are being simulated, PRZM-3 requires the use of a septic effluent file that is specified in the execution supervisor. Daily values for water, ammonia, nitrate, and organic nitrogen are included on each record of the file. These files are generated as output from the On-site Wastewater Disposal System (OSWDS) model (see Section 9.3). Data format requirements and an example input file are shown below:

Septic Effluent File Input Guide

RECORD FORMAT: 1X,3I2,4F10.0
READ STATEMENT: MM, MD, MY, INFLOW, AMMON, NITR, ORGN

where

MM	=	effluent month
MD	=	effluent day
MY	=	effluent year
INFLOW	=	amount of water (cm)
AMMON	=	ammonia concentration (g cm^{-1})
NITR	=	nitrate concentration (g cm^{-1})
ORGN	=	organic N concentration (g cm^{-1})

Example Septic Effluent File

```
  1  157    1.133    0.5101E-040.0000    0.1697E-04
  1  257    1.133    0.5101E-040.0000    0.1697E-04
  1  357    1.133    0.5101E-040.0000    0.1697E-04
  1  457    1.133    0.5101E-040.0000    0.1697E-04
  1  557    1.133    0.5101E-040.0000    0.1697E-04
  1  657    1.133    0.5101E-040.0000    0.1697E-04
  1  757    1.133    0.5101E-040.0000    0.1697E-04
  1  857    1.133    0.5101E-040.0000    0.1697E-04
  1  957    1.133    0.5101E-040.0000    0.1697E-04
  1 1057    1.133    0.5101E-040.0000    0.1697E-04
```

4.2.4 WDM Time-series File

Any of the time-series data described above may be accessed using the Watershed Data Management (WDM) utility (Lumb et al. 1990) instead of flat files. WDM is a robust data management tool which can maintain and compress large amounts of time-series data. It also allows faster input and output of time-series data than a flat file. WDM also comes with an interactive interface (ANNIE) which allows the user to perform detailed management and display of the time-series data on WDM files. Additional information about WDM and its acquisition may be found on the internet at “http://h2o.usgs.gov/software/lib.html”.

If any time-series data is to be input using a WDM file, the appropriate record is inserted in the execution supervisor file (see Section 4.3 for details) to specify the WDM file name. The actual time-series data to be read from the WDM file are specified on the appropriate records of the PRZM input file (see Section 4.4 for details). The location of the data on the WDM file is specified by the data-set number(s) provided on the PRZM input file record(s). If a WDM file is specified, but no data-set number is given for a specific time-series data, it is assumed that the data will come from a flat file (also specified in the execution supervisor file) or not be input at all. A brief summary of where various WDM time-series data sets are specified follows:

Time-series Data	PRZM Input File Location
Meteorological	Record 3, columns 49-68
Atmospheric Deposition	Record N4, columns 1-30
Septic Effluent	Record N2, columns 11-30

An additional method for retrieving pan evaporation data as monthly average values exists using WDM. Instead of placing the data-set number for pan evaporation in columns 54-58, a value of -1 may be used. This indicates that the monthly values for pan evaporation are found as attribute values on the data set for precipitation data (specified in columns 49-53). Thus, this method requires that precipitation time-series values are coming from WDM as well. The monthly values are divided equally among each day of corresponding month.

Output of time-series data may also be sent to a WDM file instead of a flat file in the same manner as input time series. On record 43 of the PRZM input file, a “W” is placed in column 40 and a data-set number is placed in columns 41-48. The results for the variable specified in columns 5-8 on that record will be output to this data set.

4.3 Execution Supervisor File (PRZM3.RUN)

The PRZM-3 model requires existence of a control file (PRZM3.RUN) also known as the execution supervisor file. This file specifies options by the user to control the overall (global) parameters during model execution. The file must always be resident in the current directory where the execution is performed.

4.3.1 Execution Supervisor Input Examples

The following pages contain examples of the execution supervisor input file. The first example demonstrates a run

with only one PRZM zone and one VADOFT zone. The second example demonstrates a run with two PRZM and two VADOFT zones with Monte Carlo capability in use. The third example demonstrates a run with only one PRZM zone with nitrogen simulation being performed and WDM capabilities in use.

4.3.1.1 Example Execution Supervisor (PRZM3.RUN) Input File: One Zone

```
*** option records
PRZM        ON
EXAMS       ON
VADOFT         ON
MONTE CARLO    OFF
TRANSPORT SIMULATION    ON
*** zone records
PRZM ZONES     1
EXAMS ENV.     1
VADOFT ZONES      1
ENDRUN
*** input file records
      PATH                    C:\PRZM3\INPUT\
      MCIN     MC.INP
      METEOROLOGY 1  MET.INP
      PRZM INPUT  1  PRZM3.INP
      EXAMS INPUT 1  EXAM3.EXA
      VADOFT INPUT   1  VADF3.INP
*** output file records
      PATH     C:\PRZM3\OUTPUT\
      TIME SERIES 1  PRZM.ZTS
      PRZM OUTPUT 1  PRZM.OUT
      EXAMS REPORT   1  EXAMS3.XMS
      EXAMS PLOT  1  EXAMS3.PEX
      VADOFT OUTPUT  1  VADF.OUT
      MCOUT    MC.OUT
      MCOUT2      MC2.OUT
*** scratch file records
      PATH     C:\PRZM3\OUTPUT
      PRZM RESTART   1  RESTART.PRZ
      VADOFT FLOW RS 1  VFLOW.RST
      VADOFT TRANS RST  1     VTRANS.RST
      VADOFT TAPE10  1  VADF.TAP
ENDFILES
*** global records
      START DATE     010181
      END DATE    311283
      NUMBER OF CHEMICALS           3
      PARENT OF 2    1
      PARENT OF 3    2
ENDDATA
*** display records
ECHO        4
TRACE       OFF
```

NOTE: Three asterisks (***) denote a comment line and are ignored by the program.

4.3.1.2 Example Execution Supervisor (PRZM3.RUN) Input File: Two Zones with Monte Carlo Option

```
***Options
PRZM        ON
EXAMS       OFF
```

```
VADOFT         ON
MONTE CARLO    ON
TRANSPORT SIMULATION    ON
PRZM ZONES     2
VADOFT ZONES      2
ENDRUN
***Input files
      MCIN     MC.INP
      METEOROLOGY 1  MET.INP
      METEOROLOGY 2  METx.INP
      PRZM INPUT  1  PRZM.INP
      PRZM INPUT  2  PRZMx.INP
      VADOFT INPUT   1  VADF.INP
      VADOFT INPUT   2  VADFx.INP
***Output files
      TIME SERIES 1  TIMES.OUT
      TIME SERIES 2  TIMESx.OUT
      PRZM OUTPUT 1  PRZM.OUT
      PRZM OUTPUT 2  PRZMx.OUT
      VADOFT OUTPUT  1  VADF.OUT
      VADOFT OUTPUT  2  VADFx.OUT
      MCOUT    MC.OUT
      MCOUT2      MC2.OUT
***Scratch files
      PRZM RESTART   1  RESTART.PRZ
      PRZM RESTART   2  RESTARTx.PRZ
      VADOFT FLOW RST   1     VFLOW.RST
      VADOFT FLOW RST   2     VFLOWx.RST
      VADOFT TRANS RST  1     VTRANS.RST
      VADOFT TRANS RST  2     VTRANSx.RST
      VADOFT TAPE10  1  VADF10.TAP
      VADOFT TAPE10  2  VADF10x.TAP
ENDFILES
      START DATE     010181
      END DATE    311281
      NUMBER OF CHEMICALS           3
      PARENT OF 2    1
      PARENT OF 3    2
      WEIGHTS
      1.0          0.0
      0.0          1.0
ENDDATA
ECHO        ON
TRACE       OFF
```

NOTE: Three asterisks (***) denote a comment line and are ignored by the program.

4.3.1.3 Example Execution Supervisor (PRZM3.RUN) Input File: One PRZM Zone with Nitrogen and WDM in Use

```
***Options
PRZM                    ON
EXAMS                   OFF
VADOFT                  OFF
MONTE CARLO             ON
TRANSPORT SIMULATION    OFF
NITROGEN SIMULATION     ON
***Zone records
```

```
PRZM ZONES                1
ENDRUN
***Input files
 PATH                    C:\PRZM3.0\INPUT\
 MCIN                    MCNIT.INP
***Met stations - all on main wdm file
 WDM FILE            1   PRECIP.WDM
 SEPTIC EFFLUENT     1   SEPTIC.INP
 PRZM INPUT          1   TESTNIT.INP
***Output files
 PATH                    C:\PRZM3.0\OUTPUT\
 TIME SERIES         1   TIMES.OUT
 PRZM OUTPUT         1   TESTNIT.OUT
 MCOUT                   MC.OUT
 MCOUT2                  MC2.OUT
***Scratch files
 PRZM RESTART        1   RESTART.PRZ
ENDFILES
***Global records
 START DATE              010157
 END DATE                311257
 NUMBER OF CHEMICALS     3
ENDDATA
***Display records
ECHO                     4
TRACE                    OFF
```

NOTE: Three asterisks (***) denote a comment line and are ignored by the program.

4.3.2 Execution Supervisor (PRZM3.RUN) Input Guide

RECORD 1 - OPTIONS	**FORMAT**	**A18,6X,A56**
LABEL (Col. 1-18)	**EXECUTION STATUS** (Col. 25-78)	
PRZM	ON or OFF	(the root zone model execution)
EXAMS	ON or OFF	(the aquatic exposure assessment model)
VADOFT	ON or OFF	(the vadose zone model execution)
MONTE CARLO	ON or OFF	(Monte Carlo execution)
TRANSPORT	ON or OFF	(vadose zone transport execution)
NITROGEN	ON or OFF	(nitrogen model execution)

RECORD 2 - ZONES	**FORMAT**	**A18,6X,I2**
LABEL (Col. 1-18)	**ZONE NUMBER** (Col. 25-78)	
PRZM ZONES	1 to 10	(total number of PRZM land zones)
EXAMS AQEs	1 to 10	(total number of EXAMS aquatic environments / PRZM run)
VADOFT ZONES	1 to 10	(total number of VADOFT land zones)
ENDRUN	-------	(specifies end of OPTIONS and ZONE records)

RECORD 3 - INPUT FILES	**FORMAT**	**A18,1X,I2,3X,A56**
LABEL (Col. 1-18)	**ZONE NUMBER** (Col. 20-21)	**NAME** (Col. 25-78)
PATH	-------	directory (optional)
METEOROLOGY	1 to 10	filename
PRZM INPUT	1 to 10	filename
EXAMS INPUT	1 to 10	filename
VADOFT INPUT	1 to 10	filename
MCIN	-------	filename
SEPTIC EFFLUENT	1 to 10	filename
NITROGEN DEPOSIT	1 to 10	filename
WDM FILE	--------	filename

RECORD 4 - OUTPUT FILES **FORMAT** **A18,1X,I2,3X,A56**

LABEL (Col. 1-18)	**ZONE NUMBER** (Col. 20-21)	**NAME** (Col. 25-78)
PATH	-------	directory (optional)
TIME SERIES	1 to 10	filename
PRZM OUTPUT	1 to 10	filename
EXAMS REPORT	1 to 10	filename
EXAMS PLOT	1 to 10	filename
VADOFT OUTPUT	1 to 10	filename
MCOUT	1 to 10	filename
MCOUT2	1 to 10	filename

RECORD 5 - SCRATCH FILES **FORMAT** **A18,1X,I2,3X,A56**

LABEL (Col. 1-18)	**ZONE NUMBER** (Col. 20-21)	**NAME** (Col. 25-78)
PATH	-------	directory (optional)
PRZM RESTART	1 to 10	filename
VADOFT FLOW RESTART	1 to 10	filename
VADOFT TRANS RESTART	1 to 10	filename
VADOFT TAPE	1 to 10	filename
ENDFILES	-------	(specifies end of file name records)

RECORD 6 - GLOBAL RECORDS **FORMAT** **A18,1X,3I2**

LABEL (Col. 1-18)	**VALUE** (Col. 20-25)	
START DATE	ddmmyy	(starting day, month, year)
END DATE	ddmmyy	(ending day, month, year)
NUMBER OF CHEMICALS	1 to 3	(number of chemicals)
PARENT OF 2	1	(parent of the second chemical if TRANSPORT=ON and if more than one chemical)
PARENT OF 3	1 or 2	(parent of third chemical if TRANSPORT=ON and if more than one chemical)
WEIGHTS	------	(indicates next values are weights)

NOTE: enter next lines only if PRZM or VADOFT have multiple zones. Enter a line for every increasing PRZM zone containing a fractional weight to each VADOFT zone. FORMAT: 10(F8.2)

1.0	0.0	(PRZM zone 1 weight to VADOFT zone 1 and 2)
0.0	1.0	(PRZM zone 2 weight to VADOFT zone 1 and 2)
ENDDATA	------	(specifies end of GLOBAL data)

RECORD 7 - DISPLAY RECORDS FORMAT A18,6X,A56

LABEL (Col. 1-18)	**VALUE** (Col. 25-78)	
ECHO	1 to 9	(amount output increasingly displayed to the screen and to files)
TRACE	ON or OFF	(tracking of subroutines for debugging)

EFFECT OF THE ECHO LEVEL ON MODEL OUTPUT

ECHO LEVEL	1	2	3	4	5	6	7	8	9
Percent bar graph	✓	✓	✓	✓	✓	✓	✓	✓	✓
Simulation status to screen		✓	✓	✓	✓	✓	✓	✓	✓
Simulation status to files			✓	✓	✓	✓	✓	✓	✓
Subroutine trace available				✓	✓	✓	✓	✓	✓
Warnings displayed					✓	✓	✓	✓	✓
Results of linkage routines						✓	✓	✓	✓
Detailed water/solute data							✓	✓	✓
Detailed head/concentration data							✓	✓	
Echo of line being read from input							✓	✓	
Echo of image being read from input								✓	

4.4 PRZM INPUT FILE

The PRZM-3 model requires a PRZM input file if the PRZM option is specified “ON” in the execution supervisor file.

4.4.1 Example PRZM Input Files

The following pages show three examples of PRZM input files. The first example shows an input sequence for pesticide simulation without erosion. The second example shows an input sequence for pesticide simulation with erosion. The third example shows an input sequence for nitrogen simulation.

4.4.1.1 Example PRZM Input File for PRZM-3: Pesticide Simulation–No erosion

```
PRZM3 Input File
3 chemicals, foliar application for chemical 1
   0.74    0.52       0    0.25       1       1
      0
      2
      1    0.25   60.00   80.00       3  86  80  86   0.00  100.00
      2    0.25   60.00   80.00       3  86  80  86   0.00  100.00
      2
  22 656  251056  261156       1
  22 657  251057  261157       2
Chemical Input Data:
      2       3       0       0
chem1-aerial        chem2-granular      chem3-injected
  11 756  0 2 0.00  1.00 0.95 0.01 4 2.00  0.50 1.00 0.00 8 4.00  0.75 1.00 0.00
  11 757  0 2 0.00  1.00 0.95 0.01 0 0.00  0.00 0.00 0.00 0 0.00  0.00 0.00 0.00
     0.       1     1.0       1     0.0       1     0.0
    0.0    .005     0.1
    0.0    .000     0.0
    0.0    .000     0.0
   0.00    0.00    0.00
Soil Series:        LEESBURG          OK185-3
  165.00          0   0   0   0   0   0   0   0   0
   0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00
      2
      1  10.000   1.400   0.462   0.000   0.000   0.000
         0.022   0.011   0.033   0.022   0.011   0.033   0.000   0.000   0.000
         0.100   0.462   0.100   0.725   5.000  81.000   0.600
         0.000   0.000   0.000   0.000   0.000   0.000
      2 155.000   1.400   0.462   0.000   0.000   0.000
         0.022   0.011   0.033   0.022   0.011   0.033   0.000   0.000   0.000
         1.000   0.462   0.100   0.725   5.000  81.000   0.600
         0.000   0.000   0.000   0.000   0.000   0.000
      0
   WATR    YEAR      10    PEST    YEAR      10    CONC    YEAR      10   1
      6
     11  -----
     12  -----
     13  -----
      4    DAY
   PRCP    TSER   0   0
   RUNF    TSER   0   0
   RFLX    TSER   0   0   1.E5
   RZFX    TSER   0   0   1.E5
```

4.4.1.2 Example PRZM Input File for PRZM-3: Pesticide Simulation–Erosion

```
PRZM3 Input File
3 chemicals, foliar application for chemical 1
   0.74    0.52       0    0.25       1       1
      4
   0.15    3.47    1.00   10.00              3    6.00   354.0
      2
      1    0.25   60.00   80.00       3              0.00  100.00
      2    0.25   60.00   80.00       3              0.00  100.00
      1       3
2206 2611 0101
0.42 0.42 0.42
0.17 0.17 0.17
  86   80   86
      2       3
2206 2611 0101
0.25 0.25 0.25
0.17 0.17 0.17
  86   80   86
      2
  220656  251056  261156       1
  220657  251057  261157       2
Chemical Input Data:
      2       3       0
chem1-aerial        chem2-granular      chem3-injected
  110756  0 2 0.00  1.00 0.95 0.05 4 2.00  0.50 1.00 0.00 8 4.00  0.75 1.00 0.00
  110757  0 2 0.00  1.00 0.95 0.05 0 0.00  0.00 0.00 0.00 0 0.00  0.00 0.00 0.00
     0.       1     1.0       1     0.0       1     0.0
    0.0    .005     0.1
    0.0    .000     0.0
    0.0    .000     0.0
   0.00    0.00    0.00
Soil Series:        LEESBURG          OK185-3
  165.00          0   0   0   0   0   0   0   0   0
   0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00
      2
      1  10.000   1.400   0.462   0.000   0.000   0.000
         0.022   0.011   0.033   0.022   0.011   0.033   0.000   0.000   0.000
         0.100   0.462   0.100   0.725   5.000  81.000   0.600
         0.000   0.000   0.000   0.000   0.000   0.000
      2 155.000   1.400   0.462   0.000   0.000   0.000
         0.022   0.011   0.033   0.022   0.011   0.033   0.000   0.000   0.000
         1.000   0.462   0.100   0.725   5.000  81.000   0.600
         0.000   0.000   0.000   0.000   0.000   0.000
      0
   WATR    YEAR      10    PEST    YEAR      10    CONC    YEAR      10   1
      6
     11  -----
     12  -----
     13  -----
      6   DAY
   PRCP    TSER   0   0
   RUNF    TSER   0   0
   ESLS    TSER   0   0   .1
```

```
   RFLX    TSER   0   0   1.E5
   EFLX    TSER   0   0   1.E5
   RZFX    TSER   0   0   1.E5
```

4.4.1.3 Example PRZM Input File for PRZM-3: Nitrogen Simulation

```
NITROGEN SIMULATION, TEMPERATURE CORRECTION, PRZM INPUT FOR LA PLATA, CO
SEPTIC SYSTEM, SOIL N CALIBRATION RUN #7
   0.75    0.44       0  15.000       1       2
      0
      1
      1    0.20    50.0  95.000       1  58  58  58                          0.0
      1
  020157  010557  011157       1
PESTICIDE TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
      1       1       0       0
Chem 1
  11 757  0 1 0.00  1.00 0.95 0.01
    0.0       1     0.0
SOILS PARAMETERS (HAPLOBOROLLS)
   250.0          0   0   0   0   0   0   1   1   0
   0.0E0  0.0E00  0.0E00
 0.60 0.60 0.45 0.16 0.25 0.25 0.25 0.25 0.25 0.25 0.18 0.16 0.97 10.0
 6.0  5.0  5.0  6.0  8.0 10.0 13.0 13.0 11.0  9.0  6.0  6.0
      5
      1     5.0    1.27    0.25     0.0     0.0
            0.0     0.0   0.000
            1.0    0.25    0.12    2.32     0.0
            5.0    50.0    23.0     0.0     0.0
      2    45.0    1.27    0.25     0.0     0.0
            0.0     0.0   0.000
            5.0    0.25    0.12    1.16     0.0
            7.0    50.0    23.0     0.0     0.0
      3    10.0    0.20    0.05     0.0     0.0
            0.0     0.0   0.000
            2.0    0.05    0.01    40.0     0.0
            7.0     5.0     2.0     0.0     0.0
      4    30.0     2.2    0.10     0.0     0.0
            0.0     0.0   0.000
            5.0    0.10    0.02    0.03     0.0
            7.5    30.0     5.0     0.0     0.0
      5   160.0    1.37    0.20     0.0     0.0
            0.0     0.0   0.000
           20.0    0.20    0.09    0.15     0.0
            8.0    52.0    22.0     0.0     0.0
      0       0
NITROGEN PARAMETERS
***septic effluent horizon, fract to refractory, effluent WDM datasets
   4   .7    0    0    0    0
***vnut fora imax nupt fixn amvo alpn vnpr
   0    1  100    1    0    1    1    0
*** deposition flags (AM  NO3  ORGN, 3 dry, 3 wet)
```

```
  -2   -2    0    0    0    0
 .01  .01  .01  .01  .01  .01  .01  .01  .01  .01  .01  .01
.005 .005 .005 .005 .005 .005 .005 .005 .005 .005 .005 .005
*** naps frmflg
   0    0
*** plant uptake target and max uptake ratio (nupt=1)
   60.0     2.0
*** fractions of total uptake
 .013  .03  .05  .07  .13  .19  .20  .15 .085  .05 .028 .004
*** horizon fractions of uptake
 .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05
 .85  .85  .85  .85  .85  .85  .85  .85  .85  .85  .85  .85
 .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05
 .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05  .05
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
*** above-ground plant uptake (vnut=0)
   0.45    0.45    0.45    0.45    0.45
*** general parameters
*** NOfr   NH3fr    plnt     des     ads  NO3imm     min  denitr    nitr NH3imm
    0.8     0.2    1.07    1.05    1.05    1.07    1.07    1.07    1.05    1.07
*** 1st order rates
***  ads     des  NO3imm     min   denit dni-thr   nitri  NH3imm
    0.0     0.0     0.0  0.0005     0.0     0.0     2.0     0.5
    0.0     0.0     0.0  0.0004     0.0     0.0     1.0     0.5
    0.0     0.0     0.0  0.0003     0.0     0.0     1.0     0.2
    0.0     0.0     0.3  0.0002     1.8     0.2     1.0     0.5
    0.0     0.0     0.5  0.0002     3.5     0.2     0.7     0.5
*** max solubility
  5000.0
***  xfix    kf      n1
    3.5     1.0     1.2
    3.5     1.0     1.2
    3.5     5.0     1.2
    5.0     0.5     1.0
    5.0     1.0     1.1
*** ammonia volatilization parameters
***theta   ref T     rates for each horizon
   1.05    25.0     0.3    0.03     0.1    0.05    0.05
***organic partitioning coeffs, conversion labile>refract, temp correct
  1000.0   5000.  0.0002    1.07
  1000.0   5000.  0.0002    1.07
  1000.0   5000.  0.0002    1.07
  1000.0   5000.  0.0002    1.07
  1000.0   5000.  0.0002    1.07
*** plant N return rates
*** BG return rates per horizon, fraction to refractory
   0.002   0.004   0.002   0.002     0.0     0.3
*** plant>litter rate, litter>soil return rate, fraction to refractory
  0.0007  0.0003     0.3
*** initial storages
*** LONP    LONS    RONP    RONS   AMSed   AMSol     NO3      BG
   300.0     0.0  1020.0     0.0    10.0     0.0     3.0     2.0
  1250.0     0.0  4600.0     0.0   150.0     0.0    15.0    16.0
```

```
  190.0     0.0   760.0     0.0    45.0     0.0     5.0     1.0
   34.0     0.0   137.0     0.0     8.0     0.0     1.0     1.0
  650.0     0.0  2280.0     0.0    50.0     0.0     7.0     0.0
*** AG-N   Litter N
    5.0     3.0
   WATR    YEAR      1    NITR    MNTH      1    CONC    YEAR      1
     6    YEAR

   RUNF    TSER   0   0
   STMP    TSER   5   5
   STMP    TSER  14  14
   STMP    TSER  19  19
   STMP    TSER  25  25
   STMP    TSER  33  33
```

4.4.2 PRZM Input Guide

The following pages describe the input records used by the PRZM input file. The input record descriptions are divided into two sections. The first section describes the records which are used for all PRZM simulations. The second section describes the additional records which are needed for nitrogen simulation in PRZM.

When performing nitrogen species simulation in PRZM, the nitrogen input records are to be inserted between records 40 and 41 of the PRZM input sequence described in the previous section. This keeps a logical order of specifying desired outputs after defining all other simulations. Record 41 contains the only modification to an existing PRZM input record. Output element ITEM2 is used to specify pesticide output summaries for a desired time interval and compartment frequency by entering PEST in its position. This element may now be set to NITR to achieve the same type of summary for nitrogen species output. As with pesticides, setting the element ITEM3 to CONC generates nitrogen storage output.

All required records in the PRZM-2 input sequence must be preserved in PRZM-3 input sequences. This means including record numbers 12 - 17 (or 12 - 16 if CAM on record 16 is set to 1) and elements of records 25, 33, 35, and 36 for pesticide parameters even though pesticides are not simulated when running nitrogen simulation. PRZM-2 requires at least one pesticide application (0 is not valid). Thus, to make an existing PRZM-2 input sequence upwardly compatible with PRZM-3, at least one "dummy" pesticide must be defined.

To minimize new input records, the existing cropping dates entered in the PRZM input sequence are used by the nitrogen module to define the crop growing periods. However, the nitrogen module requires a planting date and no planting date is entered in the PRZM input. It is thus assumed that the emergence date entered in the PRZM input will be used as the planting date in the nitrogen module. The cropping period for the crops being simulated must not vary from year to year as the nitrogen algorithm expects the same cropping periods each year. If the cropping period for a crop does vary in the input sequence, the first year's cropping period for that crop will be used throughout the simulation. Cropping periods may still wrap around the end of a year. However, the maximum number of cropping periods that the nitrogen module can simulate is three (versus the existing PRZM-2 limit of five).

Soil temperature must be simulated in PRZM-3 when running nitrogen simulation, as soil temperature values are used significantly in the nitrogen reaction algorithms. This requires ITFLAG to be set to 1 on record 19 and records 30, 31, and 39 to be defined.

4.4.2.1 PRZM Input Guide for All PRZM-3 Runs

RECORD 1 FORMAT A78

col: 1-78	TITLE:	label for simulation title.

RECORD 2 FORMAT A78

col: 1-78	HTITLE:	label for hydrology information title.

RECORD 3 FORMAT 2F8.0,I8,F8.0,2I8,5I4

col: 1-8	PFAC:	pan factor used to estimate daily evapotranspiration.
col: 9-16	SFAC:	snowmelt factor in cm/degrees Celsius above freezing.
col: 17-24	IPEIND:	pan factor flag. 0 = pan data read, 1 = temperature data read, 2 = either available used.
col: 25-32	ANETD:	minimum depth of which evaporation is extracted (cm).
col: 33-40	INICRP:	(INICRP is only used when ERFLAG=0.) Indicates the initial crop if the simulation date occurs before the emergence date of all cropping periods (see record 10). Value: • = 0 : no; • > 0 : its value designates the number of the crop whose data is to be used in the initialization, i.e., the conditions present before the first emergence date in the first simulation period. INICRP must be equal to one of the values of ICNCN (Record 9) and INCROP (Record 11).
col: 41-48	ISCOND:	surface condition of initial crop if INICRP>0. 1 = fallow, 2 = cropping, 3 = residue. ISCOND is ignored when ERFLAG > 0; In this case PRZM will determine the current crop conditions.
col: 49-52	DSN:	WDM data set number for precipitation data
col: 53-56	DSN:	WDM data set number for potential evaporation data
col: 57-60	DSN:	WDM data set number for temperature data
col: 61-64	DSN:	WDM data set number for wind speed data
col: 65-68	DSN:	WDM data set number for solar radiation data

RECORD 4 FORMAT 6F8.0
Only if IPEIND = 1 or 2 (see record 3).

col: 1-48	DT:	monthly daylight hours for January - June.

RECORD 5 FORMAT 6F8.0
Only if IPEIND = 1 or 2 (see record 3).

col: 1-48	DT:	monthly daylight hours for July - December.

RECORD 6 FORMAT I8

col: 1-8	ERFLAG:	flag to calculate erosion. ERFLAG=0, no erosion ERFLAG=1, not used (raises error condition) ERFLAG=2, MUSLE ERFLAG=3, MUST ERFLAG=4, MUSS

RECORD 7 FORMAT 4F8.0, 8X, I8, 2F8.0
Only if ERFLAG = 2, 3, 4 (see record 6).

col: 1-8	USLEK:	universal soil loss equation (K) of soil erodibility.
col: 9-16	USLELS:	universal soil loss equation (LS) topographic factor.
col: 17-24	USLEP:	universal soil loss equation (P) practice factor.
col: 25-32	AFIELD:	area of field or plot in hectares.
col: 40-48	IREG:	location of NRCS 24-hour hyetograph.
col: 49-56	SLP:	land slope (%)
col: 57-64	HL:	hydraulic length (m)

RECORD 8 FORMAT I8

col: 1-8	NDC:	number of different crops in the simulation ($1 \leq NDC \leq NC$).

RECORD 9 FORMAT I8,3F8.0,I8,3(1X,I3),2F8.0
Repeat this record up to NDC (see record 8).

col: 1-8	ICNCN:	crop number of the different crop.
col: 9-16	CINTCP:	maximum interception storage of the crop (cm).
col: 17-24	AMXDR:	maximum rooting depth of the crop (cm).
col: 25-32	COVMAX:	maximum areal coverage of the canopy (percent).
col: 33-40	ICNAH:	surface condition of the crop after harvest date (see record 11). 1 = fallow, 2 = cropping, 3 = residue. ICNAH is ignored when ERFLAG > 0; In this case PRZM will determine the current crop conditions.

col: 42-52	CN:	runoff curve numbers of antecedent moisture condition II for fallow, cropping, and residue (3 values). Only used if erosion flag is off (ERFLAG=0, see record 6), the which approach is deprecated, i.e., it is recommended that PRZM be run with ERFLAG>1. See record 9E for entry of CN when ERFLAG>1.
col: 53-60	WFMAX:	maximum dry weight of the crop at full canopy (kg m^{-2}). Required if CAM = 3 (see record 16) else set to 0.0 .
col: 61-68	HTMAX:	max. canopy height at maturation date (cm) (see record 11)

RECORD 9A FORMAT 2I8
Only if ERFLAG = 2, 3,or 4 (see record 6).
Repeat 9A-9E for each crop (see example input file)

col: 1-8	CROPNO:	crop number
col: 9-16	NUSLEC:	number of USLEC factors ($1 \leq$ NUSLEC ≤ 32).

RECORD 9B FORMAT 16(I2,I2,1X)
Only if ERFLAG = 2, 3,or 4 (see record 6).
Repeat 9B, 9C, and 9E if NUSLEC is >16 (see example input file)

col: variable	GDUSLEC:	day to start USLEC, Manning's N factor, and CN. The first date has to be the crop emergence date.
col: variable	GMUSLEC:	month to start USLEC, Manning's N factor, and CN. The first date has to be the crop emergence date.

RECORD 9C FORMAT 16(F4.0,1X)
Only if ERFLAG = 2, 3,or 4 (see record 6).

col: variable	USLEC:	universal soil loss cover management factors © value) for each NUSLEC.

RECORD 9D FORMAT 16(F4.0,1X)
Only if ERFLAG = 2, 3,or 4 (see record 6).

col: variable	MNGN:	Manning's N for each NUSLEC.

RECORD 9E FORMAT 16(I4,1X)
Only if ERFLAG = 2, 3,or 4 (see record 6).

col: variable	CN:	runoff curve number of antecedent moisture condition II for each NUSLEC.

RECORD 10 FORMAT I8

col: 1-8	NCPDS:	number of cropping periods (sum of NDC for all cropping dates in record 11). ($1 \leq$ NCPDS $\leq$ MXCPD)

RECORD 11 FORMAT 2X,3I2,2X,3I2,2X,3I2,I8
Repeat this record up to NCPDS (see record 10).

col: 3-4	EMD:	integer day of crop emergence.
col: 5-6	EMM:	integer month of crop emergence.
col: 7-8	IYREM:	integer year of crop emergence.
col: 11-12	MAD:	integer day of crop maturation.
col: 13-14	MAM:	integer month of crop maturation.
col: 15-16	IYRMAT:	integer year of crop maturation.
col: 19-20	HAD:	integer day of crop harvest.
col: 21-22	HAM:	integer month of crop harvest.
col: 23-24	IYRHAR:	integer year of crop harvest.
col: 25-32	INCROP:	crop number associated with NDC (see record 8).

RECORD 12 FORMAT A78

col: 1-80	PTITLE:	label for pesticide title.

RECORD 13 FORMAT 4I8

col: 1-8	NAPS:	total number of pesticide applications occurring at different dates (1 to 800). Note: if two or more pesticides are applied on the same date then NAPS = 1 for that day.
col: 9-16	NCHEM:	number of pesticide(s) in the simulation. This value should equal the number in the execution supervisor file (1 to 3).
col: 17-24	FRMFLG:	flag for testing of ideal soil moisture conditions for the application of pesticide(s) relative to the target date (see record 15 for target date information). 1, 2, and 3 = yes, 0 = no. 1 = check preceding days (WINDAY, record 16) after the target application date(APD, record 16) for ideal moisture conditions; 2 = check moisture conditions only on the target application date; 3 = check preceding days (WINDAY, record 16) after the target application date(APD, record 16) for ideal moisture conditions. Also, check soil moisture conditions on the target application date.

col: 25-32	DK2FLG	flag to allow input of bi-phasic half-life 1=yes, 0=no

RECORD 14 FORMAT 3(4X,2I2,I8))
Only if DKFLG2=1, Repeat for each chemical

col: variable	DKDAY:	day when first half-life begins.
col: variable	DKMNTH:	month when first half-life begins.
col: variable	DKNUM:	number of days after first half-life begins that half-life is changed to second half-life.

RECORD 15 FORMAT 3A20

col: 1-60	PSTNAM:	names of pesticide(s) for output titles.

RECORD 16 FORMAT 2X,3I2,I3,3(I2,F5.0,F6.0,F5.0,F5.0)
Repeat this record up to NAPS (see record 13).

col: 3-4	APD:	integer target application day.
col: 5-6	APM:	integer target application month.
col: 7-8	IAPYR:	integer target application year.
col: 9-11	WINDAY:	number of days in which to check soil moisture values following the target date for ideal pesticide(s) applications. Required if FRMFLG = 1, 2, or 3 else set to 0 (see record 13).

col: variable	CAM:	**C**hemical **A**pplication **M**ethod. 1 = soil applied, soil incorporation depth of 4 cm, linearly decreasing with depth; 2 = interception based on crop canopy, as a straight-line function of crop development; chemical reaching the soil surface is incorporated to 4 cm; 3 = interception based on crop canopy, the fraction captured increases exponentially as the crop develops; chemical reaching the soil surface is incorporated to 4 cm; 4 = soil applied, user-defined incorporation depth (DEPI), uniform with depth; 5 = soil applied, user-defined incorporation depth (DEPI), linearly increasing with depth; 6 = soil applied, user-defined incorporation depth (DEPI), linearly decreasing with depth; 7 = soil applied, T-Band granular application, user-defined incorporation depth (DEPI), use DRFT input variable to define fraction of chemical to be applied in top 2 cm, remainder of chemical will be uniformly incorporated between 2 cm and the user-defined depth; 8 = soil applied, chemical incorporated entirely into depth specified by user (DEPI) (modified CAM 1) 9 = linear foliar based on crop canopy, chemical reaching the soil surface incorporated to the depth given by DEPI (modified CAM 2); 10 = nonlinear foliar using exponential filtration, chemical reaching the soil surface incorporated to the depth given by DEPI (modified CAM 3); **NOTE:** DEPI must be set greater than 0.0 for CAM=4-10. If DEPI = 0, or DEPI < the depth of the first (top) surface soil layer, chemical reaching the soil surface is distributed into the first surface soil layer.
col: variable	DEPI:	depth of the pesticide(s) application (cm). Use with CAM=4-10. For CAM=2 or 3, chemical not intercepted by the crop foliage is incorporated to 4 cm. The default incorporation depth for CAM=2 or 3 can only be over-ridden by selecting CAM = 9 or 10 and entering a value >0.0 for DEPI. Should DEPI be zero, or a value less than the depth of the top soil compartment, chemical is distributed uniformly throughout the depth of the top soil compartment.
col: variable	TAPP:	target application rate of the pesticide(s) (kg ha^{-1}).
col: variable	APPEFF:	application efficiency (fraction). target application rate may be reduced to account for application inefficiencies
col: variable	DRFT:	spray drift (fraction). used for spray drift loading to EXAMS pond. However, (1-DRFT) should be >= to application efficiency. DRFT is also used when CAM=7 to represent fraction of chemical which is incorporated into top 2 cm (drift will be set to 0 for EXAMS pond loadings)

RECORD 17 FORMAT F8.0,3(I8,F8.0)

col: 1-8	FILTRA:	filtration parameter. Required if CAM = 3 else set to 0.0.

col: variable	IPSCND:	condition for disposition of foliar pesticide after harvest. 1 = surface applied, 2 = complete removal, 3 = left alone. Required if CAM=2 or 3.
col: variable	UPTKF:	plant uptake factor. 0 = no uptake is simulated. 1 = uptake is equal to transpiration * diss. phase concentration, 0.001 to 0.99 = uptake is a fraction of transpiration* dissolved phase concentration. **NOTE: Repeat IPSCND & UPTKF for each chemical (see example input file**.

RECORD 18 FORMAT 3F8.0
Only if CAM=2 or 3, repeat this record up to NCHEM.

col: 1-8	PLVKRT:	pesticide volatilization decay rate on plant foliage ($days^{-1}$).
col: 9-16	PLDKRT:	pesticide decay rate on plant foliage ($days^{-1}$).
col: 17-24	FEXTRC:	foliar extraction coefficient for pesticide washoff per centimeter of rainfall.

RECORD 18A FORMAT 3F8.0
Only if CAM=2 or 3, and NCHEM >1.

col: 1-8	PTRAN12:	foliar transformation rate for chemical 1-2
col: 9-16	PTRAN13:	foliar transformation rate for chemical 1-3
col: 17-24	PTRAN23:	foliar transformation rate for chemical 2-3

RECORD 19 FORMAT A78

col: 1-78	STITLE:	label for soil properties title.

RECORD 20 FORMAT F8.0,8X,9I4

col: 1-8	CORED:	total depth of soil core in cm. (must be sum of all horizons thicknesses (THKNS) in record 33 and at least as deep as the root depth in record 9).
col: 17-20	BDFLAG:	bulk density flag. 0 = apparent bulk density known and entered in record 33, 1 = mineral value entered
col: 21-24	THFLAG:	field capacity and wilting point flag. 0 = water contents are entered, 1 = calculated by the model

col: 25-28	KDFLAG:	soil/pesticide adsorption coefficient. 0 = KD value entered in record 37; 1 = KD value calculated by the model (see record 30); 2 = normalized Freundlich KD value entered in record 37 and the Freundlich exponent 1/n entered in record 30A; 3 = aged sorption is implemented with the Freundlich KD value entered in record 37. Compound specific aging factors are entered in records 30B and 30C.
col: 29-32	HSWZT:	drainage flag, 0 = free draining, 1 = restricted
col: 33-36	MOC:	method of characteristics flag. 1=yes, 0=no.
col: 37-40	IRFLAG:	irrigation flag. 0 = no irrigation simulated 1 = year round, 2 = during cropping period only.
col: 41-44	ITFLAG:	soil temperature simulation flag. 1 or 2 =yes, 0=no. Flag value must = 1 if nitrogen is being simulated. Flag value must = 2 if soil temperature is simulated with the use of temperature and moisture corrected degradation (record 32A).
col: 45-48	IDFLAG:	thermal conductivity and heat capacity flag. 1=yes, 0=no
col: 49-52	BIOFLG:	biodegradation flag. 1=yes, 0=no.

RECORD 21 FORMAT 5F8.0
Only if BIOFLG = 1 (see record 20)

col: 1-8	AM:	maintenance coef. of metabolizing X_m population (day^{-1})
col: 9-16	AC:	maintenance coef. of co-metabolizing X_c population (day-1).
col: 17-24	AS:	maintenance coef. of sensitive X_s population (day^{-1}).
col: 25-32	AR:	maintenance coef. of non-sensitive X_r population (day^{-1}).
col: 33-40	KE:	average enzyme content of the X_c population (dimensionless).

RECORD 22 FORMAT 7F8.0
Only if BIOFLG = 1 (see record 20).

col: 1-8	KSM:	saturation constant of the metabolizing X_m population with respect to pesticide concentration.
col: 9-16	KCM:	saturation constant of the metabolizing X_m population with respect to carbon concentration.
col: 17-24	KC:	saturation constant of the co-metabolizing X_c population.
col: 25-32	MKS:	saturation constant of the sensitive X_s population.

col: 33-40	KR:	saturation constant of the non-sensitive X_r population.
col: 41-48	KIN:	inhibition constant (mg g^{-1} dry soil).
col: 49-56	KSK:	carbon solubilization constant (day^{-1}).

RECORD 23 FORMAT 6F8.0
Only if BIOFLG =1 (see record 20).

col: 1-8	KLDM:	death rate of metabolizing X_m population (day^{-1}).
col: 9-16	KLDC:	death rate of co-metabolizing X_c population(day^{-1}).
col: 17-24	KLDS:	death rate of sensitive X_s population (day^{-1}).
col: 25-32	KLDR:	death rate of non-sensitive X_r population (day^{-1}).
col: 33-40	KL1:	second order death rate of X_s population (mg g^{-1} day^{-1}).
col: 41-48	KL2:	dissociation constant of enzyme substrate complex (day^{-1}).

RECORD 24 FORMAT 5F8.0
Only if BIOFLG = 1 (see record 20).

col: 1-8	USM:	growth rate of metabolizing X_m population with respect to pesticide concentration (day^{-1}).
col: 9-16	UCM:	specific growth rate of metabolizing X_m population with respect to carbon concentration (day^{-1}).
col: 17-24	MUC:	specific growth rate of co-metabolizing X_c population (day^{-1}).
col: 25-32	US:	specific growth rate of sensitive X_s population (day^{-1}).
col: 33-40	UR:	specific growth rate of non-sensitive X_r population (day^{-1}).

RECORD 25 FORMAT 5F8.0
Only if BIOFLG = 1 (see record 20).

col: 1-8	YSM:	true growth yield of the metabolizing X_m population with respect to pesticide concentration (mg(dry wt.)/mg).
col: 9-16	YCM:	true growth yield of the metabolizing X_m population with respect to carbon concentration (mg(dry wt.)/mg).
col: 17-24	YC:	true growth yield of the co-metabolizing X_c population (mg(dry wt.)/mg).
col: 25-32	YS:	true growth yield of the sensitive X_s population (mg(dry wt.)/mg).
col: 33-40	YR:	true growth yield of the non-sensitive X_r population (mg(dry wt.)/mg).

RECORD 26 FORMAT 9F8.0

col: variable	DAIR:	diffusion coefficient for the pesticide(s) in the air (cm^2 day^{-1}). Only required if HENRYK is greater than 0 else set to 0.0 for each NCHEM
col: variable	HENRYK:	Henry's law constant of the pesticide(s) for each NCHEM (dimensionless).
col: variable	ENPY:	enthalpy of vaporization of the pesticide(s) for each NCHEM (kcal $mole^{-1}$).

RECORD 27 FORMAT I8,3F8.0
Only if IRFLAG = 1 or 2 (see record 20).

col: 1-8	IRTYP:	type of irrigation: 1 = flood irrigation, 2 = furrow, 3 = over canopy (may generate runoff), 4 = under canopy sprinkler (may generate runoff), 5 = over canopy without runoff generation, 6 = over canopy, user-defined rates, with runoff generation, 7 = over canopy, user-defined rates, without runoff generation.
col: 9-16	FLEACH:	leaching factor as a fraction of irrigation water depth.
col: 17-24	PCDEPL:	fraction of available water capacity at which irrigation is applied. Usually ~0.45 – 0.55; PRZM accepts values between 0.0 and 0.9
col: 25-32	RATEAP:	maximum rate at which irrigation is applied (cm hr^{-1}).

RECORD 28 FORMAT 7F8.0
Only if IRFLAG = 1 or 2 and IRTYP = 2 (see record 20).

col: 1-8	Q0:	flow rate of water entering heads of individual furrows (m^3 s^{-1}).
col: 9-16	BT:	bottom width of the furrows (m).
col: 17-24	ZRS:	slope of the furrow channel walls (horizontal/vertical).
col: 25-32	SF:	slope of the furrow channel bottom (vertical/horizontal).
col: 33-40	EN:	Manning's roughness coefficient for the furrow.
col: 41-48	X2:	length of the furrow (m).
col: 49-56	XFRAC:	location in furrow where PRZM infiltration calculations are performed, as a fraction of the furrow length (X2). If XFRAC = -1, average depths are used in PRZM.

RECORD 29 FORMAT 2F8.0
Only if IRFLAG = 1 or 2 and IRTYP = 2 (see record 20).

col: 1-8	KS:	saturated hydraulic conductivity of the soil in which furrows are dug ($m\ s^{-1}$).
col: 9-16	HF:	green-amp infiltration suction parameter (m).

RECORD 30 FORMAT I8,3F8.0
Only if KDFLAG = 1 (see record 20).

col: 1-8	PCMC:	flag to select which model is used to estimate KD (see record 36). 1 = mole fraction, 2 = mg $liter^{-1}$, 3 = micromoles $liter^{-1}$, 4 = KOC entered (dimensionless).
col: variable	SOL:	pesticide(s) solubility entered according to PCMC flag above for each NCHEM.

RECORD 30A FORMAT 3F8.0
Only if KDFLAG = 2 or 3 (see record 20).

col: variable	FRNDCF:	Freundlich exponent 1/n (dimensionless) for each NCHEM.

RECORD 30B FORMAT 15I5
Only if KDFLAG = 3 (see record 20).

col: variable	BAKD:	Days for the definition of the aging factors VAKD (record 30C) for each NCHEM. Expressed as off-sets from the application date. Although most sensible for single applications, PRZM restarts the sequence at the date of additional pesticide applications. Up to 5 values**.** The first day must be 0 (zero), so that the sequence will start at the application date.

RECORD 30C FORMAT 15F5.0
Only if KDFLAG = 3 (see record 20).

col: variable	VAKD:	time dependent factor changing on days BAKD (record 30B) to calculate an aged sorption (dimensionless) for each NCHEM**.** Up to 5 values.

RECORD 31 FORMAT 14F5.0
Only if ITFLAG = 1 or 2 (see record 20).

col: 1-60	ALBEDO:	monthly values of soil surface albedo (12 values).
col: 61-65	EMMISS:	reflectivity of soil surface to longwave radiation (fraction).

col: 66-70	ZWIND:	height of wind speed measurement above the soil surface (m)

RECORD 32 FORMAT 12F5.0
Only if ITFLAG = 1 or 2 (see record 20).

col: 1-60	BBT:	average monthly values of bottom boundary soil temperatures in °C (12 values).

RECORD 32A FORMAT 6F8.0 (I.e., QFAC(1) .. QFAC(Nchem) TBASE(1) .. TBASE(Nchem))
Only if ITFLAG = 1 or 2 (see record 20).

col: variable	QFAC:	factor for rate increase when temperature increases by 10°C. (If QFAC is set equal to zero, PRZM will not simulate degradation change with temperature.)
col: variable	TBASE:	temperature during the test of biodegradation.

RECORD 32B FORMAT 3(I8,2F8.0)
Only if ITFLAG = 2 (see record 20). One set (MSFLG, MSEFF, MSLAB) for each NCHEM.

col: variable	MSFLG:	flag to select moisture corrected degradation: = 1 : reference soil moisture is absolute to field capacity (FC), = 2 : reference soil moisture is relative to FC.
col: variable	MSEFF:	exponent of moisture corrected degradation (moisture relationship according to WALKER).
col: variable	MSLAB:	reference soil moisture.

RECORD 33 FORMAT I8

col: 1-8	NHORIZ:	total number of horizons (minimum of 1).

RECORD 34 FORMAT I8,7F8.0
Repeat records 34-38 in data sets up to NHORIZ.

col: 1-8	HORIZN:	horizon number in relation to NHORIZ.
col: 9-16	THKNS:	thickness of the horizon.
col: 17-24	BD:	bulk density if BDFLAG=0 or mineral density if BDFLAG=1.
col: 25-32	THETO:	initial soil water content in the horizon (cm^3 cm^{-3}).
col: 33-40	AD:	soil drainage parameter if HSWZT = 1, else set to 0.0 (day^{-1}).
col: 41-variable	DISP:	pesticide(s) hydrodynamic solute dispersion coefficient for each NCHEM.

col: variaable	ADL:	lateral soil drainage parameter if HSWZT = 1

RECORD 35 FORMAT 8X,5F8.0
Only if BIOFLG = 1 (see record 20).

col: 9-16	Q:	average carbon content of the population. (dimensionless).
col: 17-24	CM1:	mineralizable carbon (mg g^{-1}).
col: 25-32	Y1:	conc. of metabolizing microbial population (mg g^{-1}).
col: 33-40	Y2:	conc. of co-metabolizing microbial population (mg g^{-1}).
col: 41-48	Y3:	conc. of sensitive microbial population (mg g^{-1}).
col: 49-56	Y4:	conc. of non-sensitive microbial population (mg g^{-1}).

RECORD 36 FORMAT 8X,9F8.0
(i.e., DWRATE(1) .. DWRATE(Nchem) DSRATE(1) .. DSRATE(Nchem) DGRATE(1) .. DGRATE(Nchem))
Only if DKFLG2=0 (see record 13).
Note: set DWRATE and DSRATE equal to simulate lumped first-order degradation.

col: variable	DWRATE:	dissolved phase pesticide(s) decay rate for each NCHEM (day^{-1}).
col: variable	DSRATE:	adsorbed phase pesticide(s) decay rate for each NCHEM (day^{-1}).
col: variable	DGRATE:	vapor phase pesticide(s)decay rate for each NCHEM (day^{-1}).

RECORD 36 FORMAT 8X,9F8.0
Only if DKFLG2=1 (see record 13).

col: variable	DWRAT1:	dissolved phase pesticide(s) decay rate for first phase of bi-phase reaction for each NCHEM (day^{-1}).
col: variable	DSRAT1:	adsorbed phase pesticide(s) decay rate for first phase of bi-phase reaction for each NCHEM (day^{-1}).
col: variable	DGRAT1:	vapor phase pesticide(s)decay rate for first phase of bi-phase reaction for each NCHEM (day^{-1}).

RECORD 36A FORMAT 8X,9F8.0
Only if DKFLG2=1 (see record 13).

col: variable	DWRAT2:	dissolved phase pesticide(s) decay rate for second phase of bi-phase reaction for each NCHEM (day^{-1}).
col: variable	DSRAT2:	adsorbed phase pesticide(s) decay rate for second phase of bi-phase reaction for each NCHEM (day^{-1}).

col: variable	DGRAT2:	vapor phase pesticide(s)decay rate for second phase of bi-phase reaction for each NCHEM (day^{-1}).

RECORD 37 FORMAT 8X,7F8.0

col: 9-16	DPN:	thickness of compartments in the horizon (cm).
col: 17-24	THEFC:	field capacity in the horizon (cm^3 cm^{-3}).
col: 25-32	THEWP:	wilting point in the horizon (cm^3 cm^{-3}).
col: 33-40	OC:	organic carbon in the horizon (percent).
col: variable	KD:	pesticide(s) partition coefficient for each NCHEM. Required if KDFLAG = 0, 2, or 3 (see record 20), else set to 0.0 (cm^{-3} g^{-1}).

RECORD 38 FORMAT 8X,5F8.0
Only if ITFLAG = 1or 2 (see record 20).

col: 9-16	SPT:	initial temp. of the horizon (Celsius).
col: 17-24	SAND:	sand content in the horizon. Required if THFLAG = 1, else set to 0.0 (percent).
col: 25-32	CLAY:	clay content in the horizon. Required if THFLAG = 1, else set to 0.0 (percent).
col: 33-40	THCOND:	thermal conductivity of the horizon (cm^{-1} day^{-1}). Required if IDFLAG = 0, else set to 0.0.
col: 41-48	VHTCAP:	heat capacity per unit volume of the soil horizon (cm^{-3} $Celsius^{-1}$). Required if IDFLAG = 0, else set to 0.0.

RECORD 39 FORMAT 8X,6F8.0
Only if DKFLG2=0 and NCHEM>1 (see record 13). Note: this record is used for parent/daughter relationship. Set to zero for simulating independent parent chemicals.

col: 9-16	DKRW12:	dissolved transformation fraction for chemical 1 to 2.
col: 17-24	DKRW13:	dissolved transformation fraction for chemical 1 to 3. If NCHEM = 2, set to 0.0 .
col: 25-32	DKRW23:	dissolved phase transformation fraction for chemical 2 to 3. If NCHEM = 2, set to 0.0 .
col: 33-40	DKRS12:	sorbed phase transformation fraction for chemical 1 to 2.
col: 41-48	DKRS13:	sorbed phase transformation fraction for chemical 1 to 3. If NCHEM = 2, set to 0.0 .
col: 49-56	DKRS23:	sorbed phase transformation fraction for chemical 2 to 3. If NCHEM = 2, set to 0.0.

RECORD 39 FORMAT 8X,3F8.0
Only if DKFLG2=1 and NCHEM >1 (see record 13).
Note: this record is used for parent/daughter relationship.
Set to zero for simulating independent parent chemicals.

col: 9-16	DKW112:	dissolved phase transformation fraction for first phase of bi-phase transformation for chemical 1 to 2.
col: 17-24	DKW113:	dissolved phase transformation fraction for first phase of bi-phase transformation for chemical 1 to 3. If NCHEM = 2, set to 0.0.
col: 25-32	DKW123:	dissolved phase transformation fraction for first phase of bi-phase transformation for chemical 2 to 3. If NCHEM = 2, set to 0.0 .
col: 33-40	DKS112:	sorbed phase transformation fraction for first phase of bi-phase transformation for chemical 1 to 2.
col: 41-48	DKS113:	sorbed phase transformation fraction for first phase of bi-phase transformation for chemical 1 to 3. If NCHEM = 2, set to 0.0
col: 49-56	DKS123:	sorbed phase transformation fraction for first phase of bi-phase transformation for chemical 2 to 3. If NCHEM = 2, set to 0.0**.**

RECORD 39A FORMAT 8X,3F8.0
Only if DKFLG2=1 and NCHEM >1 (see record 13).
Note: this record is used for parent/daughter relationship.
Set to zero for simulating independent parent chemicals.

col: 9-16	DKW212:	dissolved phase transformation fraction for second phase of bi-phase transformation for chemical 1 to 2.
col: 17-24	DKW213:	dissolved transformation fraction for second phase of bi-phase transformation for chemical 1 to 3. If NCHEM = 2, set to 0.0.
col: 25-32	DKW223:	dissolved phase transformation fraction for second phase of bi-phase transformation for chemical 2 to 3. If NCHEM = 2, set to 0.0.
col: 33-40	DKS212:	sorbed phase transformation fraction for second phase of bi-phase transformation for chemical 1 to 2.
col: 41-48	DKS213:	sorbed phase transformation fraction for second phase of bi-phase transformation for chemical 1 to 3. If NCHEM = 2, set to 0.0.
col: 49-56	DKS223:	sorbed phase transformation fraction for second phase of bi-phase transformation for chemical 2 to 3. If NCHEM = 2, set to 0.0.

RECORD 40 FORMAT 2I8

col: 1-8	ILP:	flag for initial pesticide(s) levels before simulation start date. 1 = yes, 0 = no.

col: 9-16	CFLAG:	conversion flag for initial pesticide(s) levels. 0 = mg/kg^{-1}, 1 = kg/ha^{-1}. Leave blank if ILP = 0.

RECORD 41 FORMAT 8F8.0
Only if ILP = 1 (see record 40).
NOTE: number of lines = THKNS(I) divided by DPN(I) where I = HORIZN.
Maximum of 8 values per line. Enter this record in data sets for each NCHEM.

col: 1-80	PESTR:	initial pesticide(s) levels.

RECORD 42 FORMAT 3(4X,A4,4X,A4,I8),I4

col: 5-8	ITEM1:	hydrologic hardcopy output flag. WATR is inserted or leave blank.
col: 13-16	STEP1:	time step of hydrologic output. DAY = daily, MNTH = monthly, YEAR = yearly.
col: 17-24	LFREQ1:	frequency of hydrologic output given by a specific compartment number.
col: 29-32	ITEM2:	pesticide flux output flag. PEST is inserted or leave blank.
col: 37-40	STEP2:	same as STEP1.
col: 41-48	LFREQ2:	same as LFREQ1.
col: 53-56	ITEM3:	pesticide concentration output flag. CONC is inserted or leave blank.
col: 61-64	STEP3:	same as STEP1.
col: 65-72	LFREQ3:	same as LFREQ1.
col: 73-76	EXMFLG:	flag for reporting output to file for EXAMS model. 1 = yes, 0 = no. If ERFLAG=0, EXMFLG is automatically set to 0

RECORD 43 FORMAT I8
Only if EXMFLG = 1 (see record 42)

col: 1-8	EXMENV:	EXAMS environment catalog number

RECORD 44 FORMAT I8,A16,2I8,F8.0
Only if EXMFLG = 1 (see record 42), repeat RECORD 44 for each chemical

col: 1-8	EXMCHM:	EXAMS chemical catalog number
col: 9-24	CASSNO:	chemical CASS Number (optional)
col: 24-32	NPROC:	signals the type of process transforming parent to metabolite in EXAMS. (see Burns 2000, Section 6)

col: 33-40	RFORM	gives the reactive molecular form from the transformation of parent to metabolite in EXAMS. (see Burns 2000, Section 6)
col: 41-48	YIELD	product yield from the transformation pathway dimensions of mole of transformation product produced per mole of parent compound reacted

RECORD 45 FORMAT I8,4X,A4

col: 1-8	NPLOTS:	number of times series plots (max. of 12).
col: 13-16	STEP4:	output time step. This option outputs pesticide runoff and erosion flux and pesticide leaching below core depth. Three options are available: DAY for daily, MNTH for monthly, YEAR for yearly.

RECORD 46 FORMAT 4X,A4,A1,3X,A4,1X,I3,1X,I3,F8.0,7X,A1,I8
Only if NPLOTS > 0 (see record 45) and ECHO > 2. (Echo level is set in PRZM3.RUN file).
NOTE: repeat this record up to NPLOTS.

col: 5-8	PLNAME:	name of plotting variable (see Table 4.1).
col: 9-9	INDX:	index to identify which pesticide if applicable. 1 = first chemical, 2 = second chemical, 3 = third chemical.
col: 13-16	MODE:	plotting mode. TSER (daily), TCUM (cumulative), TAVE (daily average over multiple compartments), TSUM (daily sum over multiple compartments)
col: 18-20	IARG:	argument value for PLNAME (see Table 4.1).
col: 22-24	IARG2:	argument value for PLNAME (see Table 4.1). (If TSER or TCUM enter same value as IARG
col: 25-32	CONST:	constant with which to multiply for unit conversion. Leave blank for default to 1.0 .
col: 40-40	PLTYP:	input W for WDM file, P for printer (not required unless running PATRIOT)
col: 41-48	PLTDSN:	WDM data set number for the output time series (Not required unless running PATRIOT)

RECORD 47 FORMAT A78
Only if special actions are desired (see record 48).

col: 1-78	ATITLE:	label for special actions title.

RECORD 48 FORMAT 2X,3I2,1X,A8,1X,I3,3F8.0
Only if special actions are desired.
Repeat this record for each special action required (up to 12).

col: 3-4	SADAY:	day of special action.
col: 5-6	SAMON:	month of special action.
col: 7-8	SAYR:	year of special action.
col: 10-17	SPACT:	special action variable (see below).
col: 19-21	NACTS:	horizon or crop number affected by special actions (see below).
col: variable	SPACTS:	new value(s) for the special action

SPACT	NACTS	SPACTS	Format
BD	HORIZON NO.	NEW VALUE(S)	(F8.0)
CN	CROP NO.	NEW VALUES	(3I8)
DSRATE	HORIZON NO.	NEW VALUE(S)	(3F8.0)
DWRATE	HORIZON NO.	NEW VALUE(S)	(3F8.0)
KD	HORIZON NO.	NEW VALUE(S)	(3F8.0)
SNAPSHOT*	----------	----------	
USLEC	CROP NO.	NEW VALUE(S)	(3F8.0)
* Used to display pesticide concentration profile.			

4.4.2.2 PRZM Input Guide for PRZM-3 Nitrogen Simulation Records

RECORD N1 FORMAT A78

col: 1-78	NTITLE:	title for nitrogen simulation.

RECORD N2 FORMAT I5,F5.0,4I5

col: 1-5	SEPHZN:	horizon number into which septic effluent is introduced.
col: 6-10	ORGFRC:	fraction of organic nitrogen in septic effluent which is refractory (the rest becomes labile).
col: 11-30	SEPDSN:	data-set numbers from WDM file (if in use) for septic effluent values in the following order: water, ammonia, nitrate, organic N.

RECORD N3 FORMAT 8I5

col: 1-5	VNUTFG:	flag to allow plant uptake parameters to vary throughout the year. 1 = yes, 0 = no.

col: 6-10	FORAFG:	method for simulating adsorption and desorption of ammonium. 0 = first-order kinetics, 1 = single value Freundlich.
col: 11-15	ITMAXA:	maximum number of iterations to be attempted in solving Freundlich equation (only needed if FORAFG = 1).
col: 16-20	NUPTFG:	method for simulating plant uptake of nitrogen. 0 = first-order kinetics, 1 = yield-based algorithm.
col: 21-25	FIXNFG:	flag to simulate nitrogen fixation. 1 = yes, 0 = no. (If FIXNFG = 1, NUPTFG must be 1 also).
col: 26-30	AMVOFG:	flag to simulate ammonia volatilization. 1 = yes, 0 = no.
col: 31-35	ALPNFG:	flag to simulate above-ground and litter compartments for plant nitrogen. 1 = yes, 0 = no.
col: 36-40	VNPRFG:	flag to allow plant return parameters to vary throughout the year. 1 = yes, 0 = no.

RECORD N4 FORMAT 6I5

col: 1-30	NIADFG:	array of flags indicating the source of atmospheric deposition data for nitrogen species (ammonia, nitrate, organic N). Three flags for dry deposition are followed by three flags for wet deposition. 0 = no deposition for this species, -2 = monthly values entered on ensuing record (N5), -1 = deposition values come from file specified in execution supervisor, > 0 = values come from this data-set number on WDM file.

RECORD N5 FORMAT 12F5.0

Repeat this record for each occurrence of NIADFG=-2 in record N4.

col: 1-60	NIAFXM/NIACNM:	monthly values for nitrogen

atmospheric deposition (NIAFXM = dry deposition, NIACNM = wet deposition).

RECORD N6 FORMAT 2I5

col: 1-5	NNAPS:	total number of agricultural nitrogen applications occurring at different dates (0 to 50).
col: 6-10	NFRMFG:	flag for testing of ideal soil moisture conditions for the agricultural nitrogen application relative to target dates (see record N6 for target dates information). 1 = yes, 0 = no.

RECORD N7 FORMAT 2X,3I2,I8,5F8.0
Repeat this record up to NNAPS (see record N5).
Not required if NAPS=0.

col: 3-4	NAPD:	integer target application day.
col: 5-6	NAPM:	integer target application month.
col: 7-8	NAPYR:	integer target application year.
col: 9-16	NWNDAY:	number of days in which to check soil moisture values following the target dates for ideal nitrogen applications. Required if NFRMFG=1, else set to 0.
col: 17-24	NDEPI:	depth of the nitrogen application (cm).
col: 25-48	NTAPP:	total application of the nitrogen species (kg ha^{-1}) in the following order: ammonia, nitrate, organic N.
col: 49-56	NAPFRC:	fraction of organic N applied which becomes refractory (the rest becomes labile).

RECORD N8 FORMAT 8F8.0
Only if NUPTFG = 0 and VNUTFG = 0 (see record N5).
NOTE: number of lines = (NHORIZ divided by 8) plus 1
Maximum of 8 values per line.

col: 1-64	KPLN:	plant nitrogen uptake reaction rate parameters for each soil horizon (/day).

RECORD N9 FORMAT 12F5.0
Only if NUPTFG = 0 and VNUTFG = 1 (see record N5).
Repeat this record up to NHORIZ.

col: 1-60	KPLNM:	monthly plant nitrogen uptake reaction rate parameters for each soil horizon (/day).

RECORD N10 FORMAT 2F8.0
Only if NUPTFG = 1 (see record N5).

col: 1-8	NUPTGT:	total annual target for plant uptake of nitrogen for all soil layers and all crops during the calendar year (kg/ha/yr).
col: 9-16	NMXRAT:	ratio of the maximum uptake rate to the optimum (target) rate when the crop is making up a deficit in nitrogen uptake.

RECORD N11 FORMAT 12F5.0
Only if NUPTFG = 1 (see record N5).

col: 1-60	NUPTFM:	monthly fractions of the total annual nitrogen plant uptake target (see record 52) applied to each month (total of values must sum to 1.0).

RECORD N12 FORMAT 12F5.0
Only if NUPTFG = 1 (see record N5).
Repeat this record up to NHORIZ.

col: 1-60	NUPTM:	fractions of the monthly nitrogen plant uptake target applied to each soil horizon (values across soil horizons must sum to 1.0 for each month).

RECORD N13 FORMAT 8F8.0
Only if ALPNFG = 1 and VNUTFG = 0 (see record N5).
NOTE: number of lines = (NHORIZ divided by 8) plus 1
Maximum of 8 values per line.

col: 1-64	ANUTF:	above-ground plant uptake fractions for each soil horizon.

RECORD N14 FORMAT 12F5.0
Only if ALPNFG = 1 and VNUTFG = 1 (see record N5).
Repeat this record up to NHORIZ.

col: 1-60	ANUFM:	monthly fractions of plant uptake which go to above-ground plant N storage.

RECORD N15 FORMAT 10F8.0

col: 1-8	GNPM(1):	fraction of nitrogen uptake which comes from nitrate (GNPM(1) and GNPM(2) must sum to 1.0).
col: 9-16	GNPM(2):	fraction of nitrogen uptake which comes from ammonium (GNPM(1) and GNPM(2) must sum to 1.0).
col: 17-24	GNPM(3):	temperature coefficient for plant uptake (only needed if NUPTFG = 0).
col: 25-32	GNPM(4):	temperature coefficient for ammonium desorption (only needed if FORAFG = 0).
col: 33-40	GNPM(5):	temperature coefficient for ammonium adsorption (only needed if FORAFG = 0).
col: 41-48	GNPM(6):	temperature coefficient for nitrate immobilization.
col: 49-56	GNPM(7):	temperature coefficient for organic N ammonification.
col: 57-64	GNPM(8):	temperature coefficient for NO3 denitrification.
col: 65-72	GNPM(9):	temperature coefficient for nitrification.
col: 73-80	GNPM(10):	temperature coefficient for ammonium immobilization.

RECORD N16 FORMAT 8F8.0
Repeat this record up to NHORIZ.

col: 1-8	NPM(1):	first-order reaction rate for ammonium desorption for each soil horizon (only needed if FORAFG = 0) (/day).
col: 9-16	NPM(2):	first-order reaction rate for ammonium adsorption for each soil horizon (only needed if FORAFG = 0) (/day).
col: 17-24	NPM(3):	first-order reaction rate for nitrate immobilization for each soil horizon (/day).
col: 25-32	NPM(4):	first-order reaction rate for organic N ammonification for each soil horizon (/day).
col: 33-40	NPM(5):	first-order reaction rate for denitrification for each soil horizon (/day).
col: 41-48	DNTHRS:	fraction of saturated water content at which denitrification begins to occur.
col: 49-56	NPM(6):	first-order reaction rate for nitrification for each soil horizon (/day).
col: 57-64	NPM(7):	first-order reaction rate for ammonium immobilization (/day).

RECORD N17 FORMAT F8.0
Only if FORAFG = 1 (see record N5).

col: 1-8	GNPM(11):	maximum solubility of ammonium in water (ppm).

RECORD N18 FORMAT 3F8.0
Only if FORAFG = 1 (see record N5).
Repeat this record up to NHORIZ.

col: 1-8	NPM(8):	maximum concentration (on the soil) of ammonium which is permanently fixed to the soil for each soil horizon (ppm).
col: 9-16	NPM(10):	coefficient parameter for the Freundlich adsorption/desorption equation for each soil horizon (-).
col: 17-24	NPM(11):	exponent parameter for the Freundlich adsorption/desorption equation for each soil horizon.

RECORD N19 FORMAT 8F8.0
Only if AMVOFG = 1 (see record N5)
NOTE: number of lines = (NHORIZ+2 divided by 8) plus 1
Maximum of 8 values per line.

col: 1-8	THVOL:	temperature correction coefficient for ammonia volatilization (needed on first record only).
col: 9-16	TRFVOL:	reference temperature for the correction (needed on first record only) (deg C).

col: 17-64	KVOL:	ammonia volatilization rates for each soil horizon (/day).

Note: ammonia volatilization is performed in the nitrogen simulation code (i.e., not in the volatilization portion of the PRZM pesticide code) using these parameters.

RECORD N20 FORMAT 4F8.0
Repeat this record up to NHORIZ.

col: 1-8	ORNPM(1):	particulate/soluble partitioning coefficient for labile organic N.
col: 9-16	ORNPM(2):	particulate/soluble partitioning coefficient for refractory organic N.
col: 17-24	ORNPM(3):	first-order conversion rate of labile to refractory particulate organic N (/day).
col: 25-32	ORNPM(4):	associated temperature correction coefficient.

RECORD N21 FORMAT 8F8.0
Only if VNPRFG = 0 (see record N5)
NOTE: number of lines = (NHORIZ+1 divided by 8) plus 1
Maximum of 8 values per line.

col: var*	KRETBN:	first-order return rates of below-ground plant N to organic N storage for each soil horizon.

* column locations depend on # of horizons

col: var**	BGNPRF:	fraction of plant N return that becomes particulate refractory organic N (the rest becomes particulate labile).

** column location depends on # of fields filled by values for KRETBN; BGNPRF value location follows last KRETB value

RECORD N22 FORMAT 3F8.0
Only if ALPNFG = 1 and VNPRFG = 0 (see record N5).

col: 1-8	AGKPRN:	first-order fall rate of above-ground plant N to litter N (/day).
col: var*	KRETAN:	first-order return rates of litter N to organic N storage in the top soil horizon (/day).

* column locations depend on # of horizons

col: var**	LINPRF:	fraction of litter N return that becomes particulate refractory organic N (the rest becomes particulate labile).

** column location depends on # of fields filled by values for KRETBN; BGNPRF value location follows last KRETB value

RECORD N23 FORMAT 12F5.0
Only if VNPRFG = 1 (see record N5).
Repeat this record up to NHORIZ.

col: 1-60	KRBNM:	monthly first-order return rates of below-ground plant N to organic N for each soil horizon (/day).

RECORD N24 FORMAT 12F5.0
Only if VNPRFG = 1 (see record N5).

col: 1-60	BNPRFM:	monthly fractions of below-ground plant N return which becomes particulate refractory organic N (the rest becomes particulate labile).

RECORD N25 FORMAT 12F5.0
Only if ALPNFG = 1 and VNPRFG = 1 (see record N5).

col: 1-60	KRANM:	monthly first-order return rate of above-ground plant N to litter N (/day).

RECORD N26 FORMAT 12F5.0
Only if ALPNFG = 1 and VNPRFG = 1 (see record N5).

col: 1-60	KRLNM:	monthly return rates of litter plant N to particulate labile organic N for the top soil horizon (/day).

RECORD N27 FORMAT 12F5.0
Only if ALPNFG = 1 and VNPRFG = 1 (see record N5).

col: 1-60	LNPRFM:	monthly fractions of litter N return which becomes particulate refractory organic N (the rest becomes particulate labile).

RECORD N28 FORMAT 8F8.0
Repeat this record up to NHORIZ.

col: 1-8	NIT(1):	initial storage of particulate labile organic N in each soil horizon (in kg/ha).
col: 9-16	NIT(2):	initial storage of adsorbed ammonium in each soil horizon (kg/ha).
col: 17-24	NIT(3):	initial storage of solution ammonium in each soil horizon (kg/ha).
col: 25-32	NIT(4):	initial storage of nitrate in each soil horizon (kg/ha).
col: 33-40	NIT(5):	initial storage of plant N in each soil horizon (kg/ha).
col: 41-48	NIT(6):	initial storage of particulate refractory organic N in each soil horizon (kg/ha).
col: 49-56	NIT(7):	initial storage of solution labile organic N in each soil horizon (kg/ha).

col: 57-64	NIT(8):	initial storage of solution refractory organic N in each soil horizon (kg/ha).

RECORD N29 FORMAT 2F8.0
Only if ALPNFG = 1 (see record N5).

col: 1-8	AGPLTN:	initial storage of above-ground plant N (kg/ha).
col: 9-16	LITTRN:	initial storage of litter N (kg/ha).

Table 4.1 Variable Designations for Plotting Files

Variable Designation (PLNAME)	Fortran Variable	Description	Units	Arguments Required (IARG)
Water Storage				
INTS	CINT	Interception storage on canopy	cm	None
SWTR	SW	Soil water storage	cm	1-NCOM2
SNOP	SNOW	Snow pack storage	cm	None
THET	THETN	Soil water content	cm cm^{-1}	1-NCOM2
Water Fluxes				
PRCP	PRECIP	Precipitation	cm day^{-1}	None
SNOF	SNOWFL	Snowfall	cm day^{-1}	None
THRF	THRUFL	Canopy throughfall	cm day^{-1}	None
INFL	AINF	Percolation into each compartment	cm day^{-1}	1-NCOM2
RUNF	RUNOF	Runoff depth	cm day^{-1}	None
CEVP	CEVAP	Canopy evaporation	cm day^{-1}	None
SLET	ET	Actual evapotranspiration from each compartment	cm day^{-1}	1-NCOM2
TETD	TDET	Total daily actual evapotranspiration	cm day^{-1}	None
OUTF	OUTFL	Lateral water outflow	cm day^{-1}	None
IRRG	IRRR	Applied irrigation	cm day^{-1}	None
Sediment Flux				
ESLS	SEDL	Event soil loss	Tonnes day^{-1}	None
Pesticide Storages				
FPST	FOLPST	Foliar pesticide storage	g cm^{-2}	None
TPST	PESTR	Total soil pesticide storage in each soil compartment	g cm^{-2}	1-NCOM2
SPST	SPESTR	Dissolved pesticide storage in each soil compartment	g cm^{-2}	1-NCOM2
Pesticide Fluxes				
TPAP	TAPP	Total pesticide application	g cm^{-2} day^{-1}	None

Table 4.1 Variable Designations for Plotting Files

Variable Designation (PLNAME)	Fortran Variable	Description	Units	Arguments Required (IARG)
FPDL	FPDLOS	Foliar pesticide decay loss	g cm^{-2} day^{-1}	None
WFLX	WOFLUX	Foliar pesticide washoff flux	g cm^{-2} day^{-1}	None
DFLX	DFFLUX	Individual soil compartment pesticide net diffusive flux	g cm^{-2} day^{-1}	1-NCOM2
AFLX	ADFLUX	Pesticide advective flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
DKFX	DKFLUX	Pesticide decay flux in each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
DWRT	DWRATE	Dissolved decay rate from each soil compartment	day^{-1}	1-NCOM2
DSRT	DSRATE	Sorbed decay rate from each soil compartment	day^{-1}	1-NCOM2
UFLX	UPFLUX	Pesticide uptake flux from each soil compartment	g cm^{-2} day^{-1}	1-NCOM2
RFLX	ROFLUX	Pesticide runoff flux	g cm^{-2} day^{-1}	None
EFLX	ERFLUX	Pesticide erosion flux	g cm^{-2} day^{-1}	None
RZFX	RZFLUX	Net pesticide flux past the maximum root depth	g cm^{-2} day^{-1}	None
LTFX	LATFLX	Lateral pesticide outflow	g cm^{-2} day^{-1}	None
COFX	DCOFLX	Pesticide outflow below soil core	g cm^{-2} day^{-1}	None
TUPX	SUPFLX	Total pesticide uptake flux from entire soil profile	g cm^{-2} day^{-1}	None
TDKF	SDKFLX	Total pesticide decay flux from entire profile	g cm^{-2} day^{-1}	None
PCNC	TCNC	Pesticide concentration in canopy	g cm^{-3}	None
VFLX	PVFLUX	Soil pesticide volatilization flux	g cm^{-2} day^{-1}	None
FPVL	FPVLOS	Foliar pesticide volatilization flux Soil Temperature	g cm^{-2} day^{-1}	None
STMP	SPT	Soil temperature in each soil compartment	°C	1-NCOM2
KDFR	KD	KD for each soil compartment	cm^3 g^{-1}	1-NCOM2
Canopy Height				

Table 4.1 Variable Designations for Plotting Files

Variable Designation (PLNAME)	Fortran Variable	Description	Units	Arguments Required (IARG)
CHGT	HEIGHT	Canopy height	cm	None
Curve Number				
CURV	CVNUM	Curve number	none	None
Soil Concentration*				
TCON	TCON	Total soil concentration	mg/kg	1-NCOM2
ACON	ACON	Adsorbed soil concentration	mg/kg	1-NCOM2
GCON	GCON	Gas soil concentration	mg/l	1-NCOM2
DLYS	DLYS	Dissolved soil concentration weighted for sphere of influence	mg/l	1-NCOM2
DCON	DCON	Dissolved soil concentration	mg/l	1-NCOM2
*Default concentration units may be converted using multiplication factor				
Nitrogen Storages				
PLON	NIT(I,1)	Particulate labile organic N	kg ha^{-1}	1-NCOM2
AMAD	NIT(I,2)	Adsorbed ammonium	kg ha^{-1}	1-NCOM2
AMSU	NIT(I,3)	Solution ammonium	kg ha^{-1}	1-NCOM2
NO3	NIT(I,4)	Nitrate	kg ha^{-1}	1-NCOM2
PLTN	NIT(I,5)	Plant nitrogen	kg ha^{-1}	1-NCOM2
SLON	NIT(I,6)	Solution labileorganic N	kg ha^{-1}	1-NCOM2
PRON	NIT(I,7)	Particulate refractory organic N	kg ha^{-1}	1-NCOM2
SRON	NIT(I,8)	Solution refractory organic N	kg ha^{-1}	1-NCOM2
AGPN	AGPLTN	Above ground plant nitrogen	kg ha^{-1}	None
LITN	LITTRN	Litter nitrogen	kg ha^{-1}	None
Nitrogen Fluxes				
ELON	SEDN(1)	Labile organic N erosion loss	kg ha^{-1} day^{-1}	None
EAMA	SEDN(2)	Adsorbed ammonium erosion loss	kg ha^{-1} day^{-1}	None
ERON	SEDN(3)	Refractory organic N erosion loss	kg ha^{-1} day^{-1}	None
RAMA	RON(1)	Solution ammonium runoff loss	kg ha^{-1} day^{-1}	None

Table 4.1 Variable Designations for Plotting Files

Variable Designation (PLNAME)	Fortran Variable	Description	Units	Arguments Required (IARG)
RNO3	RON(2)	Nitrate runoff loss	kg ha^{-1} day^{-1}	None
RLON	RON(3)	Labile organic N runoff loss	kg ha^{-1} day^{-1}	None
RRON	RON(4)	Refractory organic N runoff loss	kg ha^{-1} day^{-1}	None
PSAM	PSAMS	Solution ammonium flux from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
OSAM	OSAMS	Solution ammonium lateral outflow from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
PSNI	PSNO3	Nitrate flux from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
OSNI	OSNO3	Nitrate lateral outflow from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
DENI	DENIF	Denitrification	kg ha^{-1} day^{-1}	1-NCOM2
AMNI	AMNIT	Ammonia nitrification	kg ha^{-1} day^{-1}	1-NCOM2
AMIM	AMIMB	Ammonia immobilization	kg ha^{-1} day^{-1}	1-NCOM2
ONMNZ	ORNMN	Organic nitrogen mineralization	kg ha^{-1} day^{-1}	1-NCOM2
DDAM	NIADDR(1)	Dry atmospheric deposition of ammonia	kg ha^{-1} day^{-1}	1-NCOM2
DDNI	NIADDR(2)	Dry atmospheric deposition of nitrate	kg ha^{-1} day^{-1}	1-NCOM2
DDON	NIADDR(3)	Dry atmospheric deposition of organic N	kg ha^{-1} day^{-1}	1-NCOM2
WDAM	NIADWT(1)	Wet atmospheric deposition of ammonia	kg ha^{-1} day^{-1}	1-NCOM2
WDNI	NIADWT(2)	Wet atmospheric deposition of nitrate	kg ha^{-1} day^{-1}	1-NCOM2
WDON	NIADWT(3)	Wet atmospheric deposition of organic N	kg ha^{-1} day^{-1}	1-NCOM2
NFIX	NFIXFX	Nitrogen fixation	kg ha^{-1} day^{-1}	1-NCOM2
PSLN	PSSLN	Labile organic N flux from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
OSLN	OSSLN	Labile organic N lateral outflow from each compartment	kg ha^{-1} day^{-1}	1-NCOM2

Table 4.1 Variable Designations for Plotting Files				
Variable Designation (PLNAME)	**Fortran Variable**	**Description**	**Units**	**Arguments Required (IARG)**
PSRN	PSSRN	Refractory organic N flux from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
OSRN	OSSRN	Refractory organic N lateral outflow from each compartment	kg ha^{-1} day^{-1}	1-NCOM2
NIIM	NIIMB	Nitrate immobilization	kg ha^{-1} day^{-1}	1-NCOM2
AMVO	AMVOL	Ammonia volatilization	kg ha^{-1} day^{-1}	1-NCOM2
LARF	REFRON	Labile to refractory conversion	kg ha^{-1} day^{-1}	1-NCOM2
ANIU	NIUPA	Above-ground nitrate plant uptake	kg ha^{-1} day^{-1}	1-NCOM2
AAMU	AMUPA	Above-ground ammonia plant uptake	kg ha^{-1} day^{-1}	1-NCOM2
BNIU	NIUPB	Below-ground nitrate plant uptake	kg ha^{-1} day^{-1}	1-NCOM2
BAMU	AMUPB	Below-ground ammonia plant uptake	kg ha^{-1} day^{-1}	1-NCOM2
REAG	RETAGN	Plant return to litter	kg ha^{-1} day^{-1}	1-NCOM2
ARLN	RTLLN	Litter return to labile organic N	kg ha^{-1} day^{-1}	1-NCOM2
ARRN	RTRLN	Litter return to refractory organic N	kg ha^{-1} day^{-1}	1-NCOM2
BRLN	RTLBN	Below-ground return to labile organic N	kg ha^{-1} day^{-1}	1-NCOM2
BRRN	RTRBN	Below-ground return to refractory organic N	kg ha^{-1} day^{-1}	1-NCOM2

4.5 VADOFT Input File

PRZM-3 requires a VADOFT flow input file if VADOFT is specified "ON" in the execution supervisor (PRZM3.RUN) file. Also if TRANSPORT SIMULATION is specified "ON", VADOFT transport input must follow.

When nitrogen simulation is being performed, VADOFT simulates the three nitrogen constituents as if they were three chemicals. Thus, a VADOFT input sequence for modeling nitrogen must contain parameters for all three species. This effects records 11, 14, 20, and 22 of VADOFT input for transport (see Section 4.5.3). Output from VADOFT is still reported by chemical number. Thus, chemical number one is ammonia, chemical number two is nitrate, and chemical number 3 is total organics.

4.5.1 Example VADOFT Input File

```
**********************************FLOW*************************************
3 CHEMICAL, 2 HORIZON, 1 MATERIAL, VADOSE ZONE FLOW SIMULATION FOR ZONE 1
        61      1   1   1   1   1       1       1       0       0
        20      2   1       .01
        1       1   1   1   0   1       2       1       0
                0.0     1.0     1.0             1.0
        1           0.0     1.0
        2
        1       20  1       50.0
        2       40  1       80.0
        0.0E00  0
        0       1       0.0     0.0E00  0       0       0       0
        7.12E02         .43E00  0.0E00  0.0E00
        0.045E00        -1.0E00 0.145E00        2.68E00 0.626E00                5   10
YEAR
**********************************TRANSPORT********************************
3 CHEMICAL, 2 HORIZON, 1 MATERIAL, VADOSE TRANSPORT SIMULATION FOR ZONE 1
        61      1   1   1   0   1
        0       1   1   0   0   1       2       1
                0.0     1.0     1.0             1.0
 1      0.0             1.0
        2
        1       20  1   50.0
        2       40  1   80.0
        0.0E00  0   0.0E00  0   0.0E00  0
        0       0       0.0     0.0     0       0       0       0
        1.30E01 .43E00
        1.00E00 1.01E00 1.00E00 0.0E00  0.0E00  0.0E00
        1           0.0     1.0         0.0E00
        1       2.000E-2    0.00E00     7.00E-3 0.00E00 2.30E-2 0.0E00
        1       1
 5      10
 YEAR
```

4.5.2 VADOFT Input Guide for Flow

RECORD 1 FORMAT A80

col: 1-80	TITLE:	label for flow simulation title.

RECORD 2 FORMAT 10I5

col: 1-5	NP:	total number of VADOFT nodal points (max of 100).
col: 6-10	NMAT:	total number of different porous materials (maximum of 5).
col: 11-15	NONU:	flag to indicate if initial condition is non-uniform. 1 = yes, 0 = no.

col: 16-20	ITRANS:	flag to indicate if running in transient or steady-state. Must be set to 1 if PRZM is ON. 1 = transient, 0 = steady-state.
col: 21-25	IMODL:	flag to indicate if running flow or transport model. 1 = flow, 0 = transport. Set to 1 here.
col: 26-30	IKALL:	time stepping index. 1 = backward difference, 0 = central difference. This flag is automatically set to 1 in FLOW.
col: 31-35	IMBAL:	flag to indicate if mass balance computation is required. 1 = yes, 0 = no.
col: 36-40	INTSPC:	flag to indicate initial conditions for head values. 1 = hydraulic head, 0 = pressure head.
col: 41-45	IHORIZ:	flag to indicate if flow direction is horizontal. 1 = yes, 0 = no. Set to 0 if PRZM is ON.
col: 46-50	ICHAIN:	flag to indicate if daughter products are used. 1 = yes, 0 = no. Automatically set to 0 for flow.

RECORD 3 FORMAT 3I5,E10.3

col: 1-5	NITMAX:	maximum number of iterations per time step. Suggested value of 20.
col: 6-10	INEWT:	flag to indicate nonlinear iterative procedure for solving saturated flow equation. 0 = Picard, 1 = standard Newton-Raphson, 2 = modified Newton-Raphson. Suggested value of 2 if PRZM is ON.
col: 11-15	IRESOL:	maximum number of refinements each time step if solution does not converge. Suggested value of 1.
col: 16-25	HTOL:	head tolerance for the nonlinear solution (length). Suggested value of 0.01.

RECORD 4 FORMAT 8I5

col: 1-5	KPROP:	flag to indicate relationship between relative permeability versus saturation and pressure head versus saturation. 1 = functional parameters supplied in record 15, 0 = model calculated.
col: 6-10	ITSGN:	flag to indicate if output time values are to be model calculated. 1 = yes, 0 = no.
col: 11-15	ITMARK:	flag to indicate if output time values differ from computational time values (see records 6 and 7). 1 = yes, 0 = no.
col: 16-20	NSTEP:	value of which time step to output nodal values from. When NSTEP = n, then output is printed. Must be from 1 up to 31 (days).
col: 21-25	NVPR:	value of which time step to output nodal velocities. When NVPR = n, then output is printed. Must be from 1 up to 31 (days).

col: 26-30	IOBSND:	flag to indicate if values are printed at certain observation nodes. 1 = yes, 0 = no. NOTE: Echo level must be greater than or equal to 6 in PRZM3.RUN file.
col: 31-35	NOBSND:	number of observation node(s) to be printed. NOBSND must not be greater than NP (see record 2). If IOBSND = 0 then set NOBSND = 0.
col: 36-40	IPRCHK:	flag to indicate if detailed information is generated in the flow matrix. 1 = yes, 0 = no.

RECORD 5 FORMAT 4E10.3
Only if ITRANS = 1 (see record 2).

col: 1-10	TIMA:	initial time value (t). Suggested value if PRZM is ON: 0.0
col: 11-20	TIN:	initial time step value(t). Suggested value if PRZM is ON: 1.0. Omit if ITSGN = 0.
col: 21-30	TFAC:	time step multiplier. Suggested value if PRZM is ON: 1.0. Omit if ITSGN = 0.
col: 31-40	TMAX:	maximum time step value allowed (t). Suggested value if PRZM is ON: 1.0 Omit if ITSGN = 0.

RECORD 6 FORMAT 8E10.3
Only if ITGSN = 0 (see record 4) and ITRANS = 1.

col: 1-80	TMVEC(I):	time values corresponding to the number of time steps where I = 1...31 (t). Input up to 8 values per line.

RECORD 7 FORMAT I5,2E10.3
Only if ITMARK = 1 and ITRANS = 1.

col: 1-5	ITMGEN:	flag to indicate if backup file marker time values are used. 1 = yes, 0 = no.
col: 6-15	STMARK:	starting marker time value (t). If PRZM and TRANSPORT are ON, set to 0.0.
col: 16-25	DTMARK:	marker time value increment (t). If PRZM and TRANSPORT are ON, set to 1.0.

RECORD 8 FORMAT 8E10.3
Only if ITRANS = 1, ITMARK = 1 and ITMGEN = 0.

col: 1-80	TMFOMT:	output marker file time values (t) corresponding to TMVEC(I) (see record 6). Input up to 8 values per line.

RECORD 9 FORMAT I5

col: 1-5	NLAYRG:	number of soil horizons to be discretized.

RECORD 10 FORMAT 3I5,E10.3
Repeat this record up to NLAYRG (see record 9).

col: 1-5	ILAYR:	horizon number in relation to NLAYRG.
col: 6-10	NELM:	number of finite elements in ILAYR.
col: 11-15	IMATL:	porous material number related to NMAT (see record 2) in ILAYR.
col: 16-25	THL:	thickness of the horizon (ILAYR).

RECORD 11 FORMAT E10.3,I5

col: 1-10	CHINV:	default initial values of pressure (l) or hydraulic head (m l^3) for nodes in the matrix.
col: 11-15	CNPIN:	number of non-default nodes in the matrix related to the default initial values (CHINV) if NONU = 1 (see record 2), else set to 0.

RECORD 12 FORMAT 2I5,2E10.3,2I5,2E10.3

col: 1-5	IBTND1:	type of boundary condition for the first node. 1 = pressure head, 0 = water flux.
col: 6-10	IBTNDN:	type of boundary condition for the last node. 1 = pressure head, 0 = water flux.
col: 11-20	VALND1:	value of the pressure head or water flux at the first node. The value should be positive for influx and negative for efflux. Set to 0.0 if PRZM is ON.
col: 21-30	VALNDN:	value of the pressure head or water flux at the last node. The value should be positive for influx and negative for efflux. Set to 0.0 if fluid is exiting the last node.
col: 31-35	ITCND1:	flag to indicate if the boundary condition at the first node is transient. 1 = yes, 0 = no. Automatically set to 0 if PRZM is ON.
col: 36-40	ITCNDN:	flag to indicate if the boundary condition at the last node is transient. 1 = yes, 0 = no. Automatically set to 0 if PRZM is ON.
col: 41-50	FLX1:	fluid flux injected into the first node (l^3 t). Automatically set to 0.0 for FLOW if PRZM is ON.
col: 51-60	FLXN:	fluid flux injected into the last node (l^3 t). Automatically set to 0.0 for FLOW if PRZM is ON.

RECORD 13 FORMAT 4E10.3
Repeat this record up to NMAT (see record 2).

col: 1-10	PROP1:	saturated hydraulic conductivity of the material (use cm day^{-1} if PRZM is ON).
col: 11-20	PROP2:	effective porosity of the material.
col: 21-30	PROP3:	specific storage of the material. For unsaturated flow, set to 0.0.
col: 31-40	PROP4:	air entry pressure head of the material.

RECORD 14 Omit for FLOW simulation.

RECORD 15 FORMAT 5E10.3
Repeat this record up to NMAT if KPROP = 1.

col: 1-10	FVAL1:	residual water phase saturation of the material (residual water content / saturated water content).
col: 11-20	FVAL2:	parameter n of the relative permeability versus saturation relationship. Suggested value of 0.0 or negative value.
col: 21-30	FVAL3:	leading coefficient of the saturation versus capillary head relationship (alpha).
col: 31-40	FVAL4:	power index of the saturation versus capillary head relationship (beta).
col: 41-50	FVAL5:	power index of the saturation versus capillary head relationship (gamma). Suggested value of 1.0 - (1.0/FVAL4).

RECORD 16 FORMAT I5
Repeat records 16-19 in data sets up to NMAT if KPROP = 0.

col: 1-5	NUMK:	number of entry pairs of relative permeability and saturation of the material.

RECORD 17 FORMAT 8E10.3
Only if KPROP = 0.

col: 1-10	SMV1:	value of water phase saturation for point 1 of the entry pairs related to NUMK.
col: 11-20	PKRW1:	value of relative permeability (l^2) for point 1 of the entry pairs related to NUMK.
col: 21-30	SMV2:	etc.
col: 31-40	PKRW2:	etc.

RECORD 18 FORMAT I5
Only if KPROP = 0.

col: 1-5	NUMP:	number of entry pairs of pressure head versus saturation values for the material.

RECORD 19 FORMAT 8E10.3
Only if KPROP = 0.

col: 1-10	SSWV1:	value of water phase saturation for point 1 of the entry pairs related to NUMP.
col: 11-20	HCAP1:	value of the pressure head (l) for point 1 of the entry pairs related to NUMP.
col: 21-30	SSWV2:	etc.
col: 31-40	HCAP2:	etc.

RECORD 20 FORMAT 5(I5,E10.3)
Only if NONU = 1.
NOTE: enter next two variables sequentially for every non-default node (CNPIN).

col: 1-5	N:	non-default node number relative to CNPIN (see record 11).
col: 6-15	PINT:	non-default initial value of pressure head (l) or hydraulic head (m l^3) of the node number (n).

RECORD 21 Omit for FLOW simulation.

RECORD 22 Omit for FLOW simulation.

RECORD 23 Omit for FLOW simulation.

RECORD 24 FORMAT I5
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-5	NTSNDH1:	number of selected time values of pressure head or water flux for transient simulation at first node.

RECORD 25 FORMAT 8E10.3
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-80	TMHV1:	time values in relation to NTSNDH1 at the first node for pressure head or water flux (t). Enter up to 8 values per line up to NTSNDH1 lines.

RECORD 26 FORMAT 8E10.3
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-80	HVTM1:	values of pressure head or water flux corresponding to TMHV1 at the first node (length). Enter up to 8 values per line up to NTSNDH1 lines.

RECORD 27 Omit for FLOW simulation.

RECORD 28 FORMAT I5
Only if ITCNDN =1 and PRZM is OFF.

col: 1-5	NTSNDH2:	number of selected time values of pressure head or water flux for transient simulation at the last node.

RECORD 29 FORMAT 8E10.3
Only if ITCNDN = 1 and PRZM is OFF.

col: 1-80	TMHV2:	time values in relation to NTSNDH2 at the last node for pressure head or water flux (t). Enter up to 8 values per line up to NTSNDH2 lines.

RECORD 30 FORMAT 8E10.3
Only if ITCNDN = 1 and PRZM is OFF.

col: 1-80	HVTM2:	values of pressure head or water flux corresponding to TMHV2 at the last node (length). Enter up to 8 values per line up to NTSNDH2 lines.

RECORD 31 Omit for FLOW simulation.

RECORD 32 FORMAT 16I5
Only if IOBSND = 1.

col: 1-80	NDOBS:	increasing sequential numbers of observation nodes. Enter up to 16 per line up to NOBSND (see record 4).

RECORD 33 FORMAT A4

col: 1-4	OUTF:	output time step for printing. Enter DAY for daily, MNTH for monthly, YEAR for yearly.

4.5.3 VADOFT Input Guide for Transport

RECORD 1 FORMAT A80

col: 1-80	TITLE:	label for transport simulation title.

RECORD 2 FORMAT 10I5

col: 1-5	NP:	total number of VADOFT nodal points.
col: 6-10	NMAT:	total number of different porous materials (maximum of 5).
col: 11-15	NONU:	flag to indicate if initial condition is non-uniform. 1 = yes, 0 = no.
col: 16-20	ITRANS:	flag to indicate if running in transient or steady-state. Must be set to 1 if PRZM is ON. 1 = transient, 0 = steady-state.
col: 21-25	IMODL:	flag to indicate if running flow or transport model. 1 = flow, 0 = transport. Set to 0 here.
col: 26-30	KALL:	time stepping index. 1 = backward difference, 0 = central difference. This flag is automatically set to 1 for steady-state simulation.
col: 31-35	IMBAL:	flag to indicate if mass balance computation is required. 1 = yes, 0 = no.
col: 36-40	INTSPC:	flag to indicate initial conditions for head values. 1 = hydraulic head, 0 = pressure head. Automatically set to 0 for transport.
col: 41-45	IHORIZ:	flag to indicate if flow direction is horizontal. 1 = yes, 0 = no. Set to 0 if PRZM is ON.
col: 46-50	ICHAIN:	flag to indicate if daughter products are used. 1 = yes, 0 = no.

RECORD 3 Omit for transport simulation.

RECORD 4 FORMAT 8I5

col: 1-5	KPROP:	flag to indicate relationship between relative permeability versus saturation and pressure head versus saturation. Set to 0 for Transport simulation.
col: 6-10	ITSGN:	flag to indicate if output time values are to be model calculated. 1 = yes, 0 = no.
col: 11-15	ITMARK:	flag to indicate if output time values differ from computational time values (see records 6 and 7). 1 = yes, 0 = no.
col: 16-20	NSTEP:	value of which time step to output nodal values from. When NSTEP = n, then output is printed. Must be from 1 up to 31 (days).
col: 21-25	NVPR:	value of which time step to output nodal velocities. When NVPR = n, then output is printed. Must be from 1 up to 31 (days).

col: 26-30	IOBSND:	flag to indicate if values are printed at certain observation nodes. 1 = yes, 0 = no. NOTE: Echo level must be greater than or equal to 6 in PRZM3.RUN file.
col: 31-35	NOBSND:	number of observation node(s) to be printed. NOBSND must not be greater than NP (see record 2). If IOBSND = 0 then set NOBSND = 0.
col: 36-40	IPRCHK:	flag to indicate if detailed information is generated in the flow matrix. 1 = yes, 0 = no.

RECORD 5 FORMAT 4E10.3
Only if ITRANS = 1 (see record 2).

col: 1-10	TIMA:	initial time value (t). Suggested value if PRZM is ON: 0.0
col: 11-20	TIN:	initial time step value(t). Suggested value if PRZM is ON: 1.0. Omit if ITSGN = 0.
col: 21-30	TFAC:	time step multiplier. Suggested value if PRZM is ON: 1.0. Omit if ITSGN = 0.
col: 31-40	TMAX:	maximum time step value allowed (t). Suggested value if PRZM is ON: 1.0 Omit if ITSGN = 0.

RECORD 6 FORMAT 8E10.3
Only if ITGSN = 0 (see record 4) and ITRANS = 1.

col: 1-80	TMVEC(I):	time values corresponding to the number of time steps where I = 1...31 (t). Input up to 8 values per line.

RECORD 7 FORMAT I5,2E10.3
Only if ITMARK = 1 and ITRANS = 1.

col: 1-5	ITMGEN:	flag to indicate if backup file marker time values are used. 1 = yes, 0 = no.
col: 6-15	STMARK:	starting marker time value (t). If PRZM and TRANSPORT are ON, set to 0.0.
col: 16-25	DTMARK:	marker time value increment (t). If PRZM and TRANSPORT are ON, set to 1.0.

RECORD 8 FORMAT 8E10.3
Only if ITRANS = 1, ITMARK = 1 and ITMGEN = 0.

col: 1-80	TMFOMT:	output marker file time values (t) corresponding to TMVEC(I) (see record 6). Input up to 8 values per line.

RECORD 9 FORMAT I5

col: 1-5	NLAYRG:	number of soil horizons to be discretized.

RECORD 10 FORMAT 3I5,E10.3
Repeat this record up to NLAYRG (see record 9).

col: 1-5	ILAYR:	horizon number in relation to NLAYRG.
col: 6-10	NELM:	number of finite elements in ILAYR.
col: 11-15	IMATL:	porous material number related to NMAT (see record 2) in ILAYR.
col: 16-25	THL:	thickness of the horizon (ILAYR).

RECORD 11 FORMAT E10.3,I5
Repeat for each NCHEM.

col: 1-10	CHINV:	default initial values of concentration (m l^3) for nodes in the matrix.
col: 11-15	CNPIN:	number of non-default nodes in the matrix related to the default initial values (CHINV) if NONU = 1 (see record 2), else set to 0.

RECORD 12 FORMAT 2I5,2E10.3,2I5,2E10.3

col: 1-5	IBTND1:	type of boundary condition for the first node. 1 = concentration, 0 = solute flux.
col: 6-10	IBTNDN:	type of boundary condition for the last node. 1 = concentration, 0 = solute flux.
col: 11-20	VALND1:	value of the concentration or solute flux at the first node. The value should be positive for influx and negative for efflux. Set to 0.0 if PRZM is ON.
col: 21-30	VALNDN:	value of the concentration or solute flux at the last node. The value should be positive for influx and negative for efflux. Set to 0.0 if fluid is exiting the last node.
col: 31-35	ITCND1:	flag to indicate if the boundary condition at the first node is transient. 1 = yes, 0 = no. Automatically set to 0 if PRZM is ON.
col: 36-40	ITCNDN:	flag to indicate if the boundary condition at the last node is transient. 1 = yes, 0 = no. Automatically set to 0 if PRZM is ON.
col: 41-50	FLX1:	fluid flux injected into the first node (l^3 t). Automatically set to 0.0 if PRZM is ON.
col: 51-60	FLXN:	fluid flux injected into the last node (l^3 t). Automatically set to 0.0 if PRZM is ON.

RECORD 13 FORMAT 2E10.3
Repeat records 13-14 in data sets up to NMAT.

col: 1-10	CPROP1:	longitudinal dispersivity of the material.
col: 11-20	CPROP2:	effective porosity of the material.

RECORD 14 FORMAT 3(2E10.3)

col: variable	CPROP3:	retardation coefficient for the material. Enter this value up to NCHEM.
col: variable	CPROP4:	molecular diffusion for the material. Enter this value up to NCHEM.

RECORD 15 Omit for TRANSPORT

RECORD 16 Omit for TRANSPORT

RECORD 17 Omit for TRANSPORT

RECORD 18 Omit for TRANSPORT

RECORD 19 Omit for TRANSPORT

RECORD 20 FORMAT 5(I5,E10.3)
Only if NONU = 1. Repeat this record up to NCHEM.
NOTE: enter next two variables sequentially for every non-default node (CNPIN).

col: 1-5	N:	non-default node number relative to CNPIN (see record 11).
col: 6-15	PINT:	non-default initial value of concentration (m l^3) of the node number (n).

RECORD 21 FORMAT I5,3E10.3
Repeat records 21-22 in data sets up to NMAT.

col: 1-5	I:	porous material number in relation to NMAT.
col: 6-15	VDFI:	default value of darcy velocity.
col: 16-25	SWDFI:	default value of water saturation.
col: 26-35	UWFI:	value of upstream weighting factor. Set to 0.0 if no upstream weighting is desired.

RECORD 22 FORMAT I5,6E10.3

col: 1-5	I:	porous material number in relation to NMAT.
col: variable	CLAMDI:	decay coefficient of the material. Enter this value up to NCHEM.
col: variable	CRACMP:	transformation mass fraction of the material. Enter this value up to NCHEM.

RECORD 23 FORMAT 2I5

col: 1-5	NVREAD:	flag to indicate if darcy velocities will be read from internal scratch files. If PRZM and TRANSPORT are ON, but not FLOW, then NVREAD is set to 1. 1 = yes, 0 = no.
col: 6-10	IVSTED:	flag to indicate if the velocities are at steady-state. This implies steady-state within each day, not the entire simulation. 1 = yes , 0 = no. If PRZM is ON then IVSTED is set to 1.

RECORD 24 FORMAT I5
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-5	NTSNDH1:	number of selected time values of concentration or solute flux for transient simulation at first node.

RECORD 25 FORMAT 8E10.3
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-80	TMHV1:	time values in relation to NTSNDH1 at the first node for pressure head or water flux (t). Enter up to 8 values per line up to NTSNDH1 lines.

RECORD 26 FORMAT 8E10.3
Only if ITCND1 = 1 and PRZM is OFF.

col: 1-80	HVTM1:	values of concentration or solute flux corresponding to TMHV1 at the first node (length). Enter up to 8 values per line up to NTSNDH1 lines.

RECORD 27 FORMAT 8E10.3
Only if IBTND1 = 0 and PRZM is OFF.

col: 1-80	QVTM1:	volumetric fluxes corresponding to TMHV1 at the first node. Enter 8 values per line up to NTSNDH1.

RECORD 28 FORMAT I5
Only if ITCNDN =1 and PRZM is OFF.

col: 1-5	NTSNDH2:	number of selected time values of concentration or solute flux for transient simulation at the last node.

RECORD 29 FORMAT 8E10.3
Only if ITCNDN = 1 and PRZM is OFF.

col: 1-80	TMHV2:	time values in relation to NTSNDH2 at the last node for concentration or solute flux (t). Enter up to 8 values per line up to NTSNDH2 lines.

RECORD 30 FORMAT 8E10.3
Only if ITCNDN = 1 and PRZM is OFF.

col: 1-80	HVTM2:	values of pressure head or water flux corresponding to TMHV2 at the last node (length). Enter up to 8 values per line up to NTSNDH2 lines.

RECORD 31 FORMAT 8E10.3
Only if ITCNDN = 1 and PRZM is OFF.

col: 1-80	QVTM2:	volumetric fluxes corresponding to TMHV2 at the last node. Enter 8 values per line up to NTSNDH2.

RECORD 32 FORMAT 16I5
Only if IOBSND = 1.

col: 1-80	NDOBS:	increasing sequential numbers of observation nodes. Enter up to 16 per line up to NOBSND (see record 4).

RECORD 33 FORMAT A4

col: 1-4	OUTT:	output time step for printing. Enter DAY for daily, MNTH for monthly, YEAR for yearly.

4.6 MONTE CARLO INPUT FILE

PRZM-3 requires a Monte Carlo input file when MONTE CARLO is specified "ON" in the execution supervisor file. The following is an example Monte Carlo input file.

4.6.1 Example MONTE CARLO Input File

```
***Title
MONTE CARLO TEST INPUT
***Number of runs and confidence level
 100                 90.0
***Monte Carlo inputs
KOC 1                 1        800. 1400.              10.10000.        1.
```

```
FIELD CAPACITY      1   1   .316    .130          0.05    0.60    5.
WILTING POINT       1   1   .150    .066          0.03    0.30    5.
ORGANIC CARBON      1   1   1.30    .870          0.01    5.00    1.
FIELD CAPACITY      2   1   .288    .110          0.04    .540    5.
WILTING POINT       2   1   .143    .076          0.03    .030    5.
ORGANIC CARBON      2   1   .110    .070          0.01    1.00    1.
DISPERSION 1    1   1   50.0        15.0          10.0    90.0    7.
***Empirical Distribution Data
 4
 89.7        0.10
 82.9        0.20
 76.1        0.30
 69.3        0.40
***Monte Carlo outputs
INFILTRATION    1   1           CDF         WRITE       1
DISPERSION 1    1   1           CDF         WRITE       1
END
***Correlations
FIELD CAPACITY  1   1   WILTING POINT       1           1       0.757
FIELD CAPACITY  1   1   ORGANIC CARBON              1           1       0.609
FIELD CAPACITY  2   1   WILTING POINT       2           1       0.757
FIELD CAPACITY  2   1   ORGANIC CARBON              2           1       0.170
END
```

NOTE: The above Monte Carlo input file contains lines beginning with three asterisks (***). These are considered comment lines and will be ignored by the program.

4.6.2 MONTE CARLO Input Guide

RECORD 1 FORMAT A80

col: 1-80	TITLE:	label for Monte Carlo simulation title.

RECORD 2 FORMAT I5,F10.0

col: 1-5	NRUN:	number of Monte Carlo runs (1 to 1000).
col: 6-15	PALPH:	confidence level for percentile confidence bounds. Entered as a percent(%). Default of 90.

RECORD 3 FORMAT A20,2I5,5F10.0
Repeat this record for number of inputs desired up to 50 records.

col: 1-20	PNAME:	Monte Carlo input variable name (up to 20 characters). See Table 4.2.
col: 21-25	IND1:	integer index for horizon, application, or material. See Table 4.2.
col: 26-30	INDZ:	zone number (1 to 10).

col: 31-40	VAR1:	the mean value of the distribution variable.
col: 41-50	VAR2:	the standard deviation of the distribution variable.
col: 51-60	VAR3:	the minimum value for the variable.
col: 61-70	VAR4:	the maximum value for the variable.
col: 71-80	VAR5:	flag to indicate the type of the variable distribution. 0 = constant, 1 = normal, 2 = log-normal, 3 = exponential, 4 = uniform, 5 = Johnson SU, 6 = Johnson SB, 7 = empirical, entered in record 4, 8 = triangular

RECORD 4 FORMAT A3

col: 1-3	ENDIT:	enter "END" to indicate end of record 3

RECORD 5 FORMAT I5
only if VAR5 = 7 (see record 3).

col: 1-5	NDAT:	number of data pairs in empirical cumulative distribution (1 to 20).

RECORD 6 FORMAT 2F10.0
only if VAR5 = 7 (see record 3).
Note: repeat record 5 for every time VAR5 =7.

col: 1-10	DIST1:	value of quantile for data pair I where I = 1....NDAT.
col: 11-20	DIST2:	cumulative probability for data pair I where I = 1....NDAT.

RECORD 7 FORMAT A20,2I5,2(A20),I5
repeat this record for number of outputs desired up to 10 records.

col: 1-20	SNAME:	Monte Carlo output variable name. See Table 4.2.
col: 21-25	IND1:	integer index for horizon, application, or material number. See Table 4.2.
col: 26-30	INDZ:	zone number (1 to 10).
col: 31-50	SNAME2:	enter "CDF" to indicate if cumulative distributions are plotted.
col: 51-70	SNAME3:	enter "WRITE" to indicate if values are written as output for each Monte Carlo run (NRUN).

col: 71-75 NAVG: length of the averaging period (in days) for output variables (1 to 5).

RECORD 8 FORMAT A3

col: 1-3 ENDIT: enter "END" to indicate end of output variables.

RECORD 9 FORMAT A20,2I5,A20,2I5,F10.0
only if VAR5 = 1, 2, 5, or 6
Note: this record may be repeated up to half of the number of inputs in record 3 if correlation is desired.

col: 1-20 NAME1: variable (PNAME) in record 3 to be correlated.

col: 21-25 IND1: integer index for horizon, application, or material number (1 to 10).

col: 26-30 INDZ: zone number (1 to 10).

col: 31-50 NAME2: variable (PNAME) in record 3 to be correlated with NAME1.

col: 51-55 IND1: same as IND1 above.

col: 56-60 INDZ: same as INDZ above.

col: 61-70 CORR: the value of the correlation coefficient for NAME1 and NAME2.

RECORD 10 FORMAT A3

col: 1-3 ENDIT: enter "END" to indicate end of correlation inputs.

Table 4.2 Monte Carlo Input and Output Labels

Parameter	**Monte Carlo Label**	**Index**
Random PRZM Model Inputs		
Soil Bulk Density (g/cm^3)	BULK DENSITY	Horizon
Wilting Point (cm^3/cm^3)	WILTING POINT	Horizon
Field Capacity (cm^3/cm^3)	FIELD CAPACITY	Horizon
Organic Carbon Content (%)	ORGANIC CARBON	Horizon
Application Mass, Chem 1(kg/ha)	APPLICATION 1	App.
Application Mass, Chem 2(kg/ha)	APPLICATION 2	App.
Application Mass, Chem 3(kg/ha)	APPLICATION 3	App.
Dispersion Coeff., Chem 1(cm^2/day)	DISPERSION 1	Horizon
Dispersion Coeff., Chem 2(cm^2/day)	DISPERSION 2	Horizon

Table 4.2 Monte Carlo Input and Output Labels

Parameter	Monte Carlo Label	Index
Dispersion Coeff., Chem 3(cm^2/day)	DISPERSION 3	Horizon
Decay Rate in Water, Chem 1($days^{-1}$)	WATER DECAY 1	Horizon
Decay Rate in Water, Chem 2($days^{-1}$)	WATER DECAY 2	Horizon
Decay Rate in Water, Chem 3($days^{-1}$)	WATER DECAY 3	Horizon
Decay Rate in Vapor, Chem 1($days^{-1}$)	VAPOR DECAY 1	Horizon
Decay Rate in Vapor, Chem 2($days^{-1}$)	VAPOR DECAY 2	Horizon
Decay Rate in Vapor, Chem 3($days^{-1}$)	VAPOR DECAY 3	Horizon
Decay Rate of Sorbed, Chem 1($days^{-1}$)	SORBED DECAY 1	Horizon
Decay Rate of Sorbed, Chem 2($days^{-1}$)	SORBED DECAY 2	Horizon
Decay Rate of Sorbed, Chem 3($days^{-1}$)	SORBED DECAY 3	Horizon
Henry's Constant, Chem 1	HENRY'S CONSTANT 1	-----
Henry's Constant, Chem 2	HENRY'S CONSTANT 2	-----
Henry's Constant, Chem 3	HENRY'S CONSTANT 3	-----
Irrigation Moisture Level (Fraction)	IRRIG LEVEL	-----
Application Year	APP YEAR	App.
Julian Application Year	APP DAY	App.
Soil Water Content (cm^3/cm^3)	THETA	Comp.
Total Soil Pesticide, Chem 1(kg/ha)	SOIL PESTICIDE 1	Comp.
Total Soil Pesticide, Chem 2(kg/ha)	SOIL PESTICIDE 2	Comp.
Total Soil Pesticide, Chem 3(kg/ha)	SOIL PESTICIDE 3	Comp.
Infiltration Depth (cm)	INFILTRATION	-----
Runoff Depth (cm)	RUNOFF	-----
Precipitation (cm)	PRECIPITATION	-----
Evapotranspiration	EVAPOTRANSPIRATION	Comp.
Flood or Furrow Irrigation Depth	IRREG DEPTH	-----
Nitrate Application (kg/ha)	NO3 APPLICATION	App.
Ammonia Application (kg/ha)	NH3 APPLICATION	App.
Organic N Application (kg/ha)	ORGN APPLICATION	App.

Table 4.2 Monte Carlo Input and Output Labels

Parameter	Monte Carlo Label	Index
Plant N Uptake Rate (/day)	PLANTN UPTAKE	Horizon
Below-Ground Plant N Return Rate (/day)	BG PLANT N RETURN	Horizon
Above-Ground Plant N Return Rate (/day)	AG PLANT N RETURN	Horizon
Ammonium Desorption Rate (/day)	NH4 DESORPTION	Horizon
Ammonium Adsorption Rate (/day)	NH4 ADSORPTION	Horizon
Nitrate Immobilization Rate (/day)	NO3 IMMOBILIZATION	Horizon
Organic N Ammonification Rate (/day)	AMMONIFICATION	Horizon
Denitrification Rate (/day)	DENITRIFICATION	Horizon
Nitrification Rate (/day)	NITRIFICATION	Horizon
Ammonium Immobilization Rate (/day)	NH4 IMMOBILIZATION	Horizon
Ammonia Volatilization Rate (/day)	NH3 VOLATILIZATION	Horizon
Random PRZM Model Outputs		
Runoff Flux, Chem 1 (kg/ha/day)	RUNOFF FLUX 1	-----
Runoff Flux, Chem 2 (kg/ha/day)	RUNOFF FLUX 2	-----
Runoff Flux, Chem 3 (kg/ha/day)	RUNOFF FLUX 3	-----
Erosion Flux, Chem 1 (kg/ha/day)	EROSION FLUX 1	-----
Erosion Flux, Chem 2 (kg/ha/day)	EROSION FLUX 2	-----
Erosion Flux, Chem 3 (kg/ha/day)	EROSION FLUX 3	-----
Decay Flux, Chem 1 (kg/ha/day)	DECAY FLUX 1	-----
Decay Flux, Chem 2 (kg/ha/day)	DECAY FLUX 2	-----
Decay Flux, Chem 3 (kg/ha/day)	DECAY FLUX 3	-----
Volat. Flux, Chem 1 (kg/ha/day)	VOLAT. FLUX 1	-----
Volat. Flux, Chem 2 (kg/ha/day)	VOLAT. FLUX 2	-----
Runoff Flux, Ammonia	RUNOFF FLUX NH3	-----
Runoff Flux, Nitrate	RUNOFF FLUX NO3	-----
Runoff Flux, Organic N	RUNOFF FLUX ORGN	-----
Erosion Flux, Ammonia	EROSION FLUX NH3	-----

Table 4.2 Monte Carlo Input and Output Labels

Parameter	Monte Carlo Label	Index
Erosion Flux, Organic N	EROSION FLUX ORGN	-----
Groundwater Flux, Ammonia	GW FLUX NH3	-----
Groundwater Flux, Nitrate	GW FLUX NO3	-----
Groundwater Flux, Organic N	GW FLUX ORGN	-----
Groundwater Flux, Total N	GW FLUX TOTN	-----
Plant Uptake Flux, Ammonia	UPTAKE FLUX NH3	-----
Plant Uptake Flux, Nitrate	UPTAKE FLUX NO3	-----
Plant Uptake Flux, (NH3 + NO3)	UPTAKE FLUX TOTN	-----
Plant Return Flux, Organic N	RETURN FLUX ORGN	-----
Immobilization Flux, Ammonium	IMMOBIL. FLUX NH4	-----
Immobilization Flux, Nitrate	IMMOBIL. FLUX NO3	-----
Immobilization Flux, (NH4 + NO3)	IMMOBIL. FLUX TOTN	-----
Volatilization Flux, Ammonia	VOLATIL. FLUX	-----
Denitrification Flux	DENIT. FLUX	-----
Nitrification Flux	NITRIFICATION FLUX	-----
Ammonification Flux	AMMONIFIC. FLUX	-----
Random VADOFT Model Inputs		
Volat. Flux, Chem 3 (kg/ha/day)	VOLAT. FLUX 3	-----
Plant Flux, Chem 1 (kg/ha/day)	PLANT FLUX 1	Comp.
Plant Flux, Chem 2 (kg/ha/day)	PLANT FLUX 2	Comp.
Plant Flux, Chem 3 (kg/ha/day)	PLANT FLUX 3	Comp.
Root Zone Flux, Chem 1 (kg/ha/day)	ROOT FLUX 1	-----
Root Zone Flux, Chem 2 (kg/ha/day)	ROOT FLUX 2	-----
Root Zone Flux, Chem 3 (kg/ha/day)	ROOT FLUX 3	-----
Hydraulic Conductivity	HYDRAULIC CONDUC	Material
Residual Saturation	RESIDUAL SATURATION	Material
Van-Genuchten Alpha	V-G ALPHA	Material

Table 4.2 Monte Carlo Input and Output Labels

Parameter	Monte Carlo Label	Index
Van-Genuchten N	V-G POWER N	Material
Decay Rate Chemical 1	VADOFT DECAY 1	Material
Decay Rate Chemical 2	VADOFT DECAY 2	Material
Decay Rate Chemical 3	VADOFT DECAY 3	Material
Dispersion Coefficient, Chemical 1	VAD DISPC 1	Material
Dispersion Coefficient, Chemical 2	VAD DISPC 2	Material
Dispersion Coefficient, Chemical 3	VAD DISPC 3	Material
Retardation, Chemical 1	VAD RETARD 1	Material
Retardation, Chemical 2	VAD RETARD 2	Material
Retardation, Chemical 3	VAD RETARD 3	Material
Random VADOFT Model Outputs		
Total Water Flux	VAD WATER FLUX	-----
Advection Flux, Chemical 1	VAD ADVECTION 1	-----
Advection Flux, Chemical 2	VAD ADVECTION 2	-----
Advection Flux, Chemical 3	VAD ADVECTION 3	-----
Dispersion Flux, Chemical 1	VAD DISPERSION 1	-----
Dispersion Flux, Chemical 2	VAD DISPERSION 2	-----
Dispersion Flux, Chemical 3	VAD DISPERSION 3	-----
Decay Flux, Chemical 1	VAD DECAY FLUX 1	-----
Decay Flux, Chemical 2	VAD DECAY FLUX 2	-----
Decay Flux, Chemical 3	VAD DECAY FLUX 3	-----
Concentration, Chemical 1	VAD CONC 1	Node
Concentration, Chemical 2	VAD CONC 2	Node
Concentration, Chemical 3	VAD CONC 3	Node

NOTE: Monte Carlo output of nitrogen constituents is achieved by using the existing VADOFT Model Outputs, with Chemical 1 being equivalent to Ammonia, Chemical 2 being equivalent to Nitrate, and Chemical 3 being equivalent to Total Organics (see Section 4.5).

SECTION 5
Parameter Estimation

This section describes estimation the values of those parameters identified in Section 2 to order to aid the user with an aid in constructing the required records for EXESUP, PRZM, and VADOFT modules. For convenience to the user, all variables (or parameters) from Section 4 are categorized by module name and alphabetized to ensure quick reference.

5.1 EXESUP (Execution Supervisor)

The Execution Supervisor generally consists of labels and options; therefore, only parameters with obscure definitions are defined.

ECHO - This value can be entered as an integer value (1-9) to control the amount of display sent to the screen and output files. Also entering "ON" or "OFF", rather than an integer value, defaults the echo level to 5 (ON) or a minimal display of 1 (OFF). For MONTE CARLO simulations, the echo level defaults to 1 automatically to prevent excessive output.

ENDDATE - A valid calendar date that specifies the day at which all of the simulation processes stop. The user must choose this date with respect to meteorological file dates to ensure adequate weather data exist for the total elapsed time (STARTDATE to ENDDATE) of the simulation.

NUMBER OF CHEMICALS - This value (1-3) controls the number of pesticides being simulated. As many as three separate chemicals are allowed per simulation. Whether these multiple chemicals have a parent-daughter relationship depends upon transformation mass fractions entered in the PRZM and VADOFT input files.

PARENT OF 2 - This value implies the NUMBER OF CHEMICALS is greater than 1 and that a possible parent-daughter relationship exists.

PARENT OF 3 - This value implies the NUMBER OF CHEMICALS is greater than 2 and that a possible parent-daughter relationship exists.

PATH - A computer-specific drive and directory statement allowing any proceeding file names to be read or written in this area.

STARTDATE - A valid calendar date that specifies the day at which all simulation processes begin. The user must choose this date with respect to meteorological file dates to ensure adequate weather data exists from this date forward to the ENDDATE.

TRACE - Primarily a tool for code debugging. By entering "ON" or "OFF", the user has the option to track subroutine calling processes during a simulation.

WEIGHTS - Values entered that specify a fractional percent of fluxes between PRZM and VADOFT zones. These values are ordered into a matrix with a sum of 1.0 for each PRZM zone.

5.2 PRZM (Pesticide Root Zone Model)

AC - Maintenance coefficient of the co-metabolizing X_c population. This value specifies the amount of energy required to maintain co-metabolizing (inhibited growth) microorganisms.

AD - Soil water drainage rate. This value is required if HSWZT = 1. It is an empirical constant, dependent on both soil type and the number of compartments (DPN(I)/THKNS(I), where I = number of horizons) to be simulated. Although there is limited experience using this option, three soils were evaluated for testing AD. The analysis was

performed by comparing the storage of water in the soil profile following the infiltration output from SUMATRA-1 (van Genuchten 1978). Each soil had a profile depth of 125 cm. The amount of water moving out of the profile changed by only 1 to 2% over the range of compartments (15-40) used in the simulation. Calibrating PRZM by comparison was accomplished and estimates of AD calculated. Suggested values of AD for clay loam, loamy sand, and sand as a function of the number of compartments are given in **Figure 5.1**.

AFIELD - This is the erosion area or plot size in hectares.

ALBEDO - Soil surface albedo. To simulate soil temperatures, ALBEDO values for each must be specified for each month. As the surface condition changes, the ALBEDO values change accordingly. Values for some natural surface conditions are provided in Table 5.21.

AM - Maintenance coefficient of the metabolizing X_m population. This parameter is used in biodegradation processes to express the amount of energy required to maintain metabolizing (enhanced) microorganism growth rates.

AMXDR - The maximum active rooting depth of crops. PRZM requires this parameter in centimeters to estimate the actual root depth from the land surface. For ranges of specific root depths, consult the USDA Handbook No. 283 (Usual Planting and Harvesting Dates), or the local Cooperative Extension Service. For general information, Table 5.9 shows the ranges for major crops.

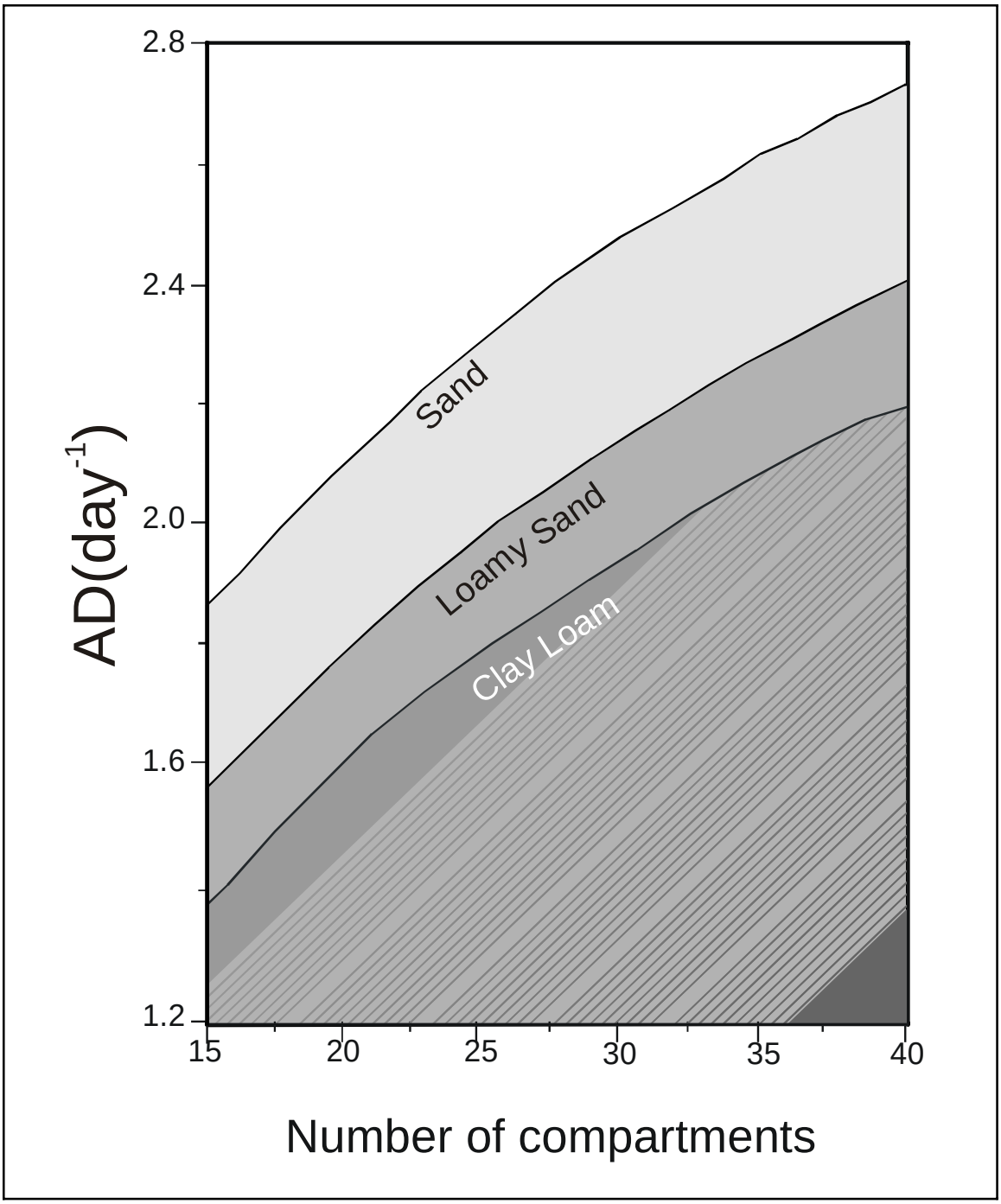


Figure 5.1 Estimation of drainage rate AD (day^{-1}) versus number of compartments.

ANETD - This value represents soil evaporation moisture loss during a fallow, dormant period. Evaporation is initially assumed to occur in the top 10 cm of soil with remaining moisture losses occurring below 10 cm up to the maximum rooting depth. Values for ANETD apply when there is no growing season, allowing a reduced level of moisture loss through evaporation. For soils with limited drainage, set ANETD to 10 cm. Values for free drainage soils are shown in **Figure 5.2**.

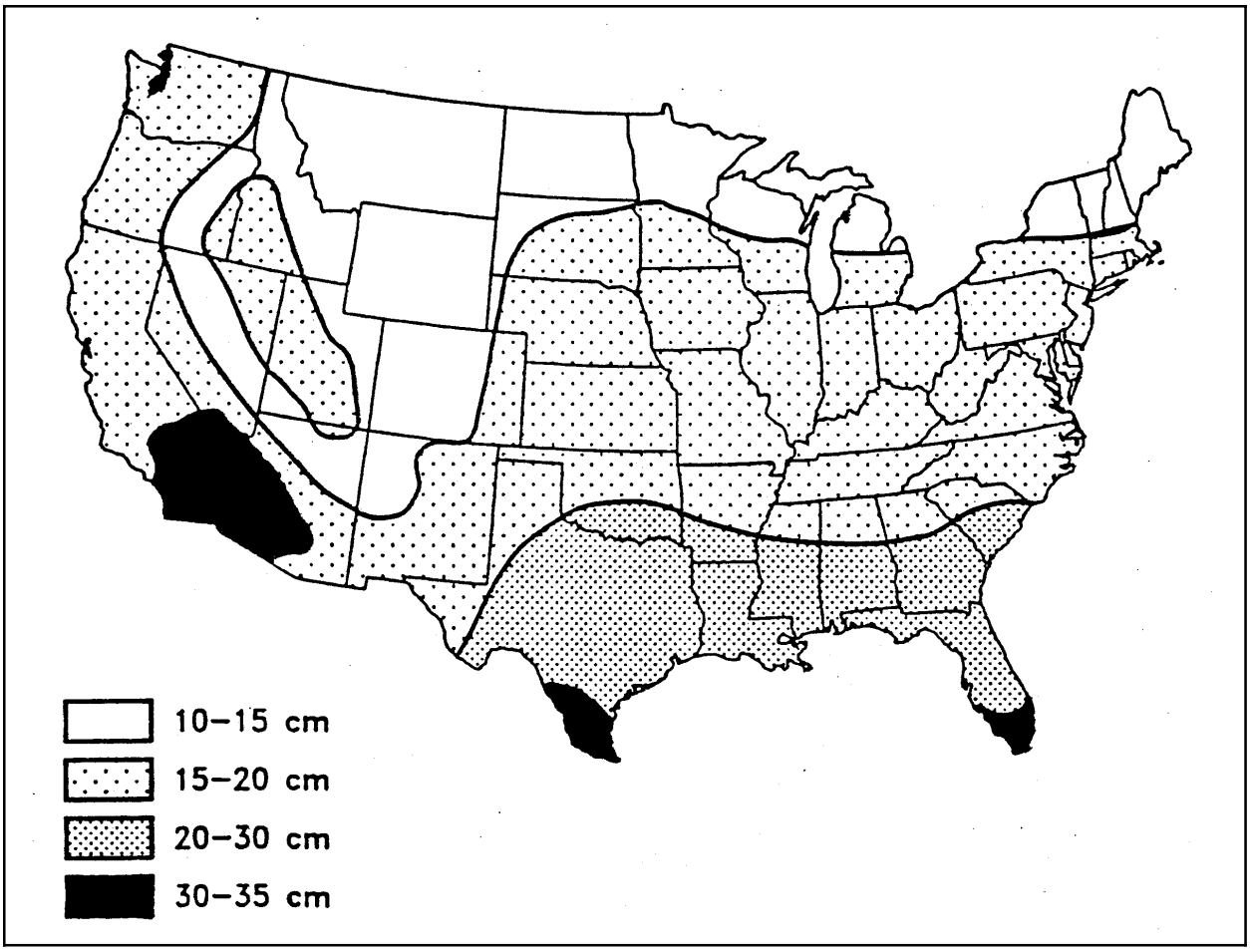


Figure 5.2 Diagram for estimating soil evaporation loss.

APPEFF - Application efficiency of pesticide application (TAPP). TAPPis multiplied by APPEFF to calculate effective rate of application.

AR - Maintenance coefficient of the non-sensitive X_r microbial population. This parameter specifies the energy required to sustain non-sensitive (indifferent) microorganisms.

AS - Maintenance coefficient of the sensitive X_s population. This parameter specifies the energy required to sustain sensitive (lethally affected) microorganisms.

BD - Soil bulk density. This value is required in the basic chemical transport equations of PRZM, and is also used to estimate moisture saturation values. Two methods are provided for estimating BD if site data are not available. Method one requires percent sand, clay and organic matter. The procedure of Rawls (1983) is used to estimate BD via Equation 5.1:

Method 1

$$BD = \frac{100}{\frac{\%OM}{OMBD} + \frac{100 - \%OM}{MBD}} \qquad \textbf{(5.1)}$$

where

BD = soil bulk density, g cm^{-3}

OM = organic matter content of the soil, (percent)
OMBD = organic matter bulk density of the soil, g cm^{-3}
MBD = mineral bulk density, g cm^{-3}

Step 1. Locate the percent sand along bottom of **Figure 5.3**.
Step 2. Locate the percent clay along side of **Figure 5.3**.
Step 3. Locate the intersection point of the two values and read the mineral bulk density.
Step 4. Solve the Rawls equation for BD.

Method 2

Step 1. Use Table 5.29 to locate the textural class.
Step 2. Read mean BD for the general soil texture.

Table 5.30 shows distributional properties of BD information.

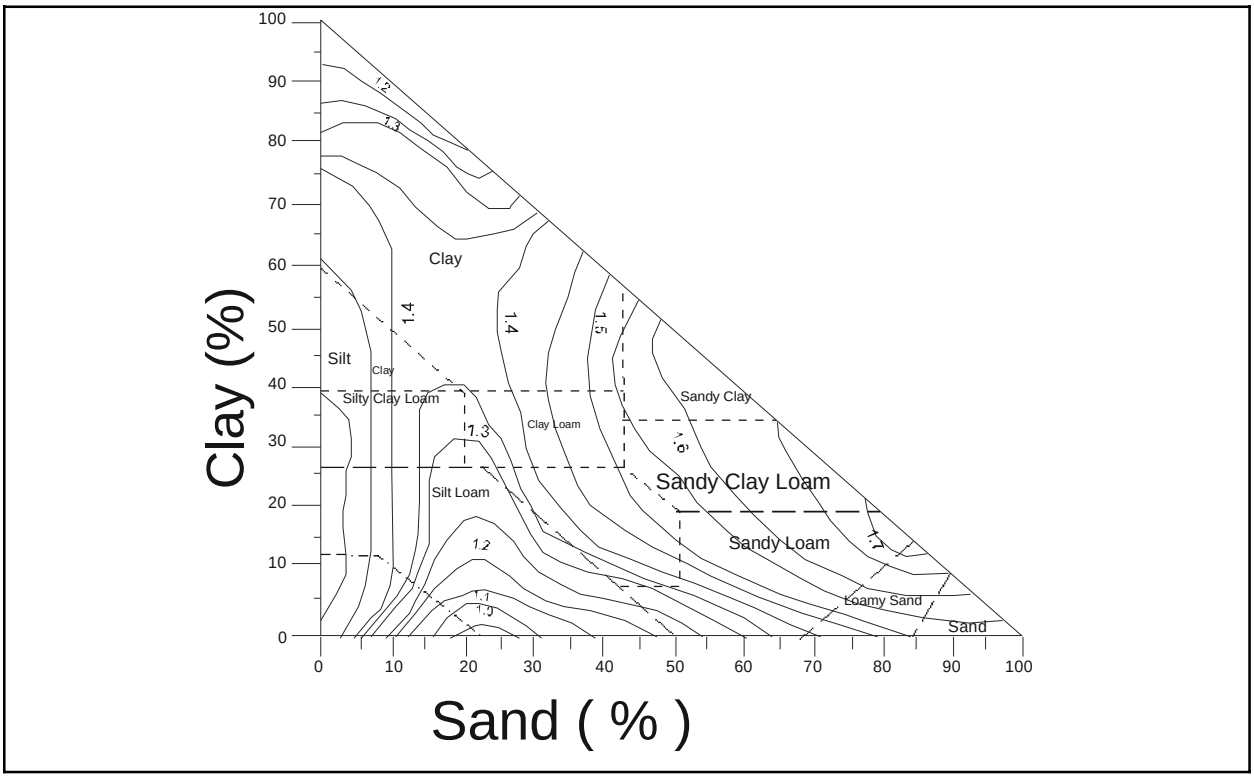


Figure 5.3 Mineral bulk density (g cm^{-3}).

Figure 5.3 provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville Maryland.

BBT - Bottom boundary soil temperatures. BBT values for each month must be specified. The BBT soil temperature for shallow core depths will vary significantly with time throughout the year. For deep cores, BBT will be relatively constant. BBT can be estimated from NOAA data reports, Department of Commerce. Depending on core depth used in the simulation, the average temperature of shallow groundwater, as shown in **Figure 5.4**, can be used to estimate BBT.

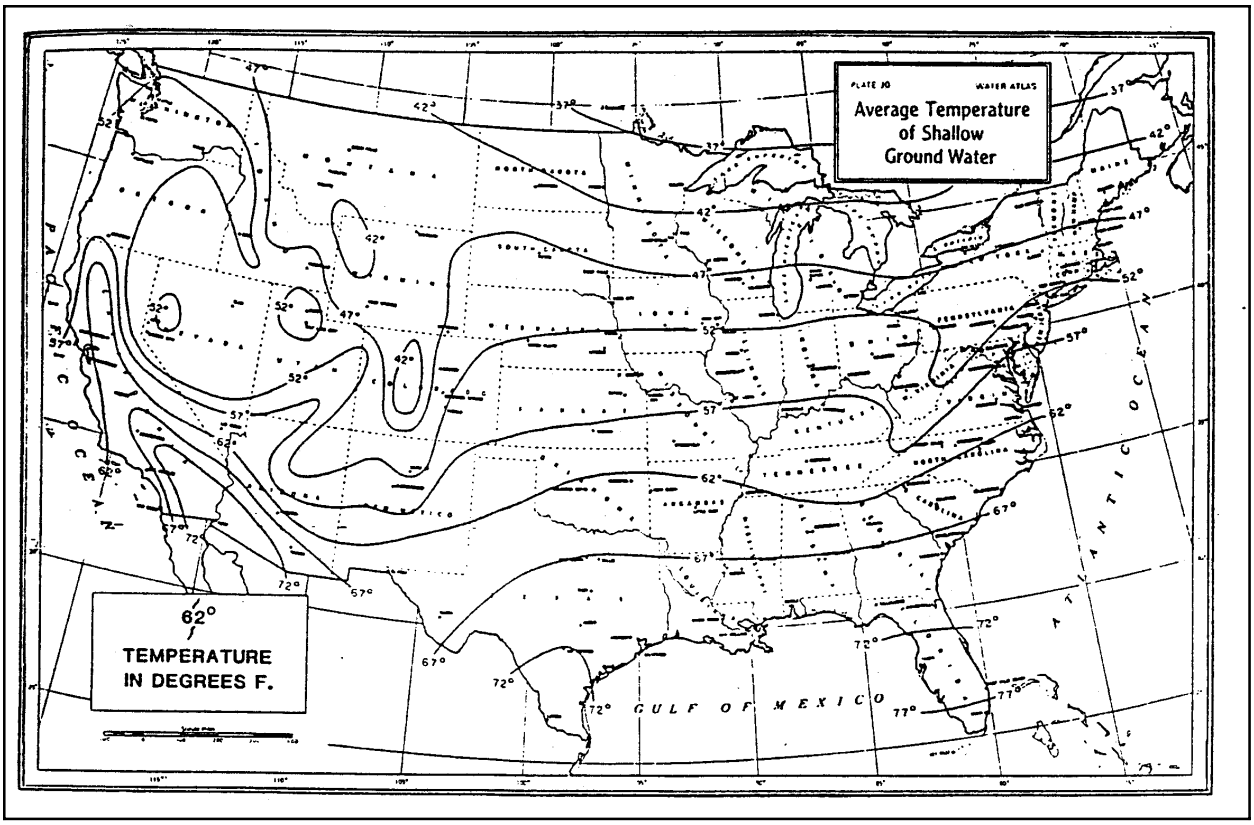


Figure 5.4 Average temperature of shallow groundwater.

BDFLAG - Flag to indicate bulk density calculation.

BIOFLG - Biodegradation flag. This flag allows the user to simulate the degradation of pesticides by microorganisms in the root zone. Parameters associated with biodegradation are very specific and can be difficult to obtain for specific soil conditions. As an alternative, estimates of biological parameters can be found in literature on the kinetics of microbial growth in liquid culture.

BT - Bottom width of the furrows. BT will depend mostly upon the type of equipment used to dig the furrow channels and the spacing between the furrows.

CAM - Chemical application model flag. This flag specifies how the pesticide is applied to soil or foliage. CAM = 1 should be used for surface-applied chemicals and results in a linearly decreasing concentration distribution in the soil to a depth of 4 cm. CAM = 2 results in linear interception by the crop foliage based on the degree of crop canopy development. CAM = 3 results in nonlinear interception by the crop foliage, i.e., the fraction of pesticide captured by the foliage increases exponentially as the crop canopy matures. CAM = 4 is used for uniform incorporation into the soil to a depth specified by the user. CAM = 5 results in linearly increasing incorporation to a user-defined depth. CAM = 6 results in linearly decreasing incorporation to a depth specified by the user. CAM = 7 approximates T-Band application to a user-defined incorporation depth. The variable DRFT is used to define the fraction of chemical to be applied in the top 2 cm. The remainder of the chemical is uniformly incorporated between 2 cm and the user-defined depth. CAM = 8 incorporates chemical directly to the depth specified by the user (modification of CAM 1). CAM = 9 is a modification of CAM 2 allowing a user-specified depth (DEPI) of incorporation of chemical not intercepted by the foliage. CAM = 10 is a modification of CAM 3 allowing a user-specified depth (DEPI) of incorporation of chemical not intercepted by the foliage.

CFLAG - Conversion flag for initial pesticide levels. This flag is valid when ILP = 1. If CFLAG = 0, then initial

pesticide levels (PESTR) are in units of mg kg^{-1}. If CFLAG = 1, then initial pesticide levels (PESTR) are in units of kg ha^{-1}. Leave CFLAG blank if ILP = 0.

CINTCP - The maximum rainfall interception storage of the crop (cm). This parameter estimates the amount of rainfall that is intercepted by a fully developed plant canopy and retained on the plant surface. A range of 0.1 to 0.3 for a dense crop canopy is reported by USDA (Knisel 1980). Values for several major crops are provided in Table 5.4.

CM - Mineralizable carbon (mg g^{-1}). This value represents the carbon substrate in the soil solution originating from a fraction of the carbon compounds of the solid phase.

CN - Runoff curve numbers at antecedent moisture condition II. The interaction of soil hydrologic groups (**Figure 5.5**) and land use treatment (cover) is accounted-for by assigning a runoff curve number (CN) for the average soil moisture condition (AMC II) to important soil-cover complexes for fallow, cropping, and residue parts of a growing season. Tables 5.10 through 5.14 can be used to help estimate the correct curve numbers.

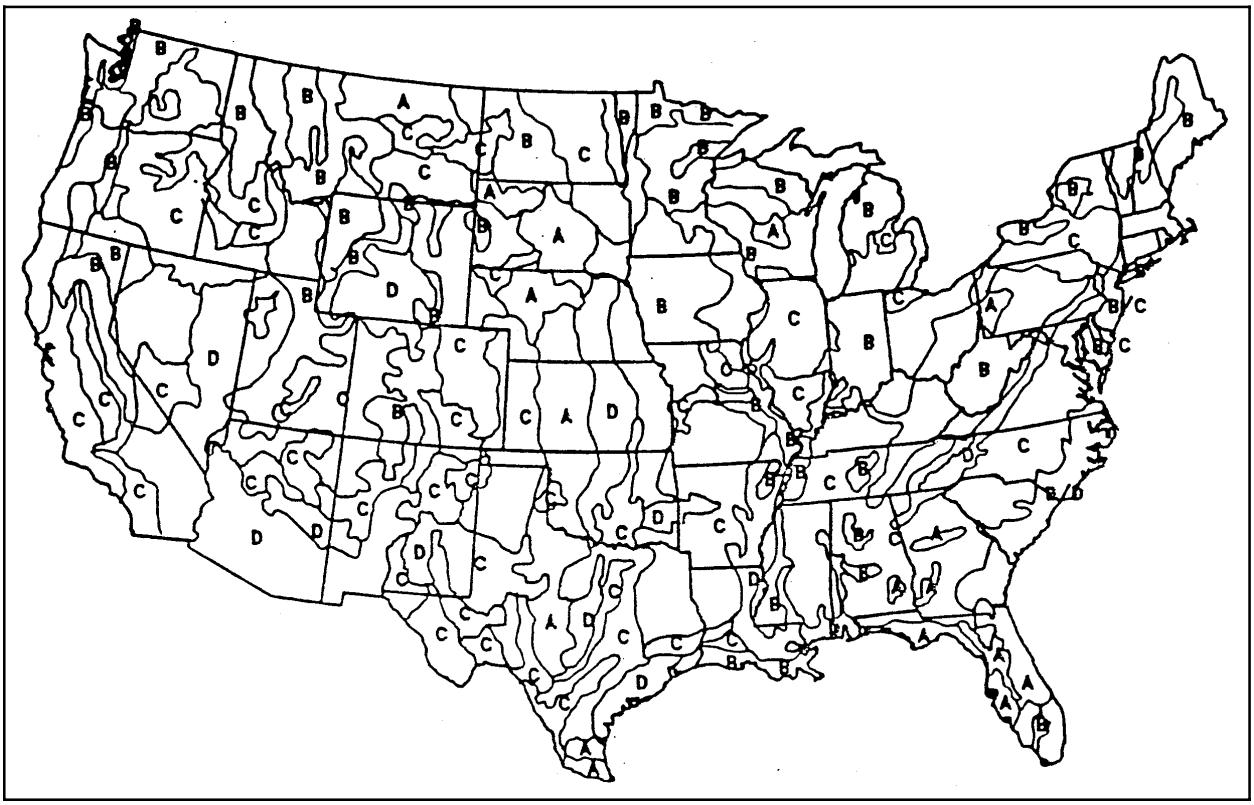


Figure 5.5 Diagram for estimating Soil Conservation Service soil hydrologic groups.

Figure 5.5 from (from EPA Field Guide for Scientific Support Activities Associated with Superfund Emergency Response. U.S. EPA, Corvallis, OR)

Legend:

A: Well drained soils
B: Moderately well drained soils
C: Poorly drained soils
D: Very poorly drained soils

CORED - The total depth of the soil core in centimeters. This value specifies the maximum depth in which PRZM simulates vertical movement. CORED must be greater or equal to the active crop root depth (AMXDR). For simulation using PRZM and VADOFT, the core depth (CORED) is usually equal to the root zone (AMXDR).

COVMAX - This is the maximum areal crop coverage(%). PRZM simulates crop ground cover up to the maximum value, COVMAX, by linear interpolation between the emergence and maturity dates. As a crop grows, its ground cover increases, thereby influencing the mass of pesticide that reaches the ground from an above-surface application event. For most crops, the maximum coverage will be on the order of 80% to 100%.

DAIR - Vapor phase diffusion coefficient. When Henry's law constant (HENRYK) is greater than zero, vapor phase diffusion is used to calculate the equilibrium between vapor and solution phases. Fick's first law defines the diffusion coefficient as the proportionality between the chemical flux and its concentration spacial gradient (Nye 1979). In soil, vapor phase diffusion occurs in the soil air space. Each chemical will have its own characteristic diffusion coefficient depending on its molecular weight, molecular volume, and shape (Streile 1984). Jury et al. (1983b) concluded that the diffusion coefficient will not show significant variations for different pesticides at a given temperature; they recommended using a constant value of 0.43 m^2 day^{-1} for all pesticides. This value is recommended herein unless other chemical-specific data are available. Note that DAIR is entered in PRZM in cm^2 day^{-1}. The user should be sure to convert the above recommended value to the correct units.

DEPI - The depth(s) of pesticide incorporation. This variable is only required when CAM = 4, 5, 6, 7, 8, 9, or 10. Typical depths are 5 to 10 centimeters. Representative values for several soil application methods are given in Table 5.15. If DEPI is set to zero, or to a depth less than that of the surface soil compartment, pesticide is incorporated to the depth of that first compartment.

DGRAT1, DGRAT2 - Vapor phase degradation rate constant(s). DGRAT1 is used for single phase vapor degradation or as the first phase of a bi-phase reaction. DGRAT2 is only used if simulating a second phase of a bi-phase reaction. Pesticides are degraded by different mechanisms, and at different rates, depending upon whether they are in the vapor, liquid or absorbed phase (Streile 1984). A lumped, first-order rate is assumed for DGRATx. In general, a zero value of DGRATx is recommended, unless chemical-specific data are available to justify a non-zero value. For example, if the user is calibrating for a highly volatile and/or photo-sensitive chemical, vapor phase attenuation processes in the upper 1 to 2 mm of the soil surface may be very important. Field studies have shown that photo chemical loss of organic chemicals can be rapid and substantial immediately following application to the land surface, especially in the case of hydrophobic or cationic organics that sorb to soil particles (Miller et al. 1987).

DISP - Dispersion of pesticide(s). The dispersion or "smearing out" of the pesticide as it moves down in the soil profile is attributed to a combination of molecular diffusion and hydrodynamic dispersion. Molecular diffusion, D_m, in soils will be lower than free-water diffusion, and has been estimated by Bresler (1973):

$$D_m = D_w a e^{b\theta}$$

where

D_w	=	molecular diffusion in free water, cm^2 day^{-1}
a	=	soil constants having a range of 0.001 to 0.005
b	=	soil constants (approximately 10)
θ	=	volumetric water content, cm^3 cm^{-3}

Hydrodynamic dispersion is more difficult to estimate because of its site-soil specificity and its apparent strong dependence on water velocity. Most investigators have established an “effective” diffusion or dispersion coefficient that combines molecular and hydrodynamic terms. Most notable among these is

$$D = 0.6 + 2.93\, v^{1.11} \qquad \textbf{(5.2)}$$

where

D	=	“effective” dispersion coefficient, cm^2 day^{-1}
v	=	pore water velocity, cm day^{-1}

by Biggar and Nielsen (1976). Note in equation 5.2 that *D* is a time and depth varying function since v is both time and depth-varying. The problem remains to estimate the assumed constant for DISP, the effective dispersion coefficient. As noted earlier, the backward difference numerical scheme in PRZM produces numerical dispersion. This dispersion is also related to the magnitude of the velocity term. Other variables that influence the truncation error include the time and space steps. A sensitivity test was performed to examine the influence of the spatial step, $\triangle x$. Results are given in **Figure 5.7**. For these runs, the DISP parameter was set to 0.0. The influence of DISP superimposed on the numerical dispersion created by the model at a $\triangle$x value of 5.0 cm is shown in **Figure 5.7**. A number of studies were performed to investigate the impact of model parameters other than DISP on the apparent dispersion. From these, the following guidance is offered:

1) A spatial step or compartment size of 5.0 cm will mimic the observed field effective dispersion quite well and should be used as an initial value.
2) No fewer than 30 compartments should be used in order to minimize mass balance errors created by numerical dispersion.
3) The DISP parameter should be set to 0.0 unless field data are available for calibration.
4) If DISP calibration is attempted, the compartment size should be reduced to 1.0 cm to minimize numerical dispersion.
5) The Biggar and Nielsen (1976) equation previously noted can be used to bound the values should the need arise to increase dispersion beyond that produced by the numerical scheme.

If the user chooses the MOC algorithm to simulate advection transport, then numerical dispersion will be eliminated and a typical value for field-observed data dispersion should be entered. Use of the MOC algorithm will result in increased model execution time.

DKFLG2, DKDAY, DKMNTH, DKNUM - Flag to allow input of bi-phase degradation of chemicals and/or bi-phase transformation of chemicals to daughter products. First-phase rates are initiated by a user-specified month and day (DKMNTH, DKDAY). Second-phase rates are enacted after a set number of days as specified by the user (DKNUM). See also chemical decay parameters DWRAT1, DSRAT1, DGRAT1, DWRAT2, DSRAT2, DGRAT2 and transformation parameters DKW112, DKW113, DKW123, DKS112, DKS113, DKS123, DKW212, DKW213, DKW223, DKS212, DKS213, DKS223.

DKW112, DKW113, DKW123, DKS112, DKS113, DKS123 - Transformation rate from a parent chemical (1 or 2) to a daughter chemical (2 and/or 3) for dissolved (DKW) and sorbed (DKS) phase residues. When multiple chemicals are specified in PRZM3.RUN, either a parent/daughter relationship exists or the chemicals are independent (chosen by the user). For a parent/daughter relationship, DKWxx or DKSxx is the mass fraction degrading from parent *x* to daughter x. By setting DKWxx or DKSxx to 0.0, the user is specifying that the multiple chemicals (xx) are independent parents.

DKW212, DKW213, DKW223, DKS212, DKS213, DKS223 - Same as above except that transformation rates reflect the second phase of the bi-phase reaction (see DKFLG2).

DPN - Thickness of the compartments in the horizon. The DPN parameter allows the user to specify a different layer depth for each soil horizon. The value of each DPN can be divided by each horizon thickness (THKNS) to obtain the total number of compartments in PRZM. In general, a smaller DPN will generate more accurate results and provide greater spatial resolution, but will also consume more CPU time. From a volatilization viewpoint, a smaller DPN in the top horizon is required for better estimation of the volatilization flux from the soil surface. In addition, since pesticide runoff is calculated from the surface layer, a smaller layer depth allows a better representation and simulation of surface-applied chemicals. Values of 0.1 cm are recommended for the initial 10 cm of the soil profile and where volatilization is a major loss mechanism. DPN can be gradually increased with depth (i.e., 1.0 cm to 2.5 cm to 5.0 cm in the deeper horizons). For the deepest subsurface soil horizons, DPN values in the range of 5.0 to 30.0 cm can be used depending on the spatial resolution needed at lower depths.

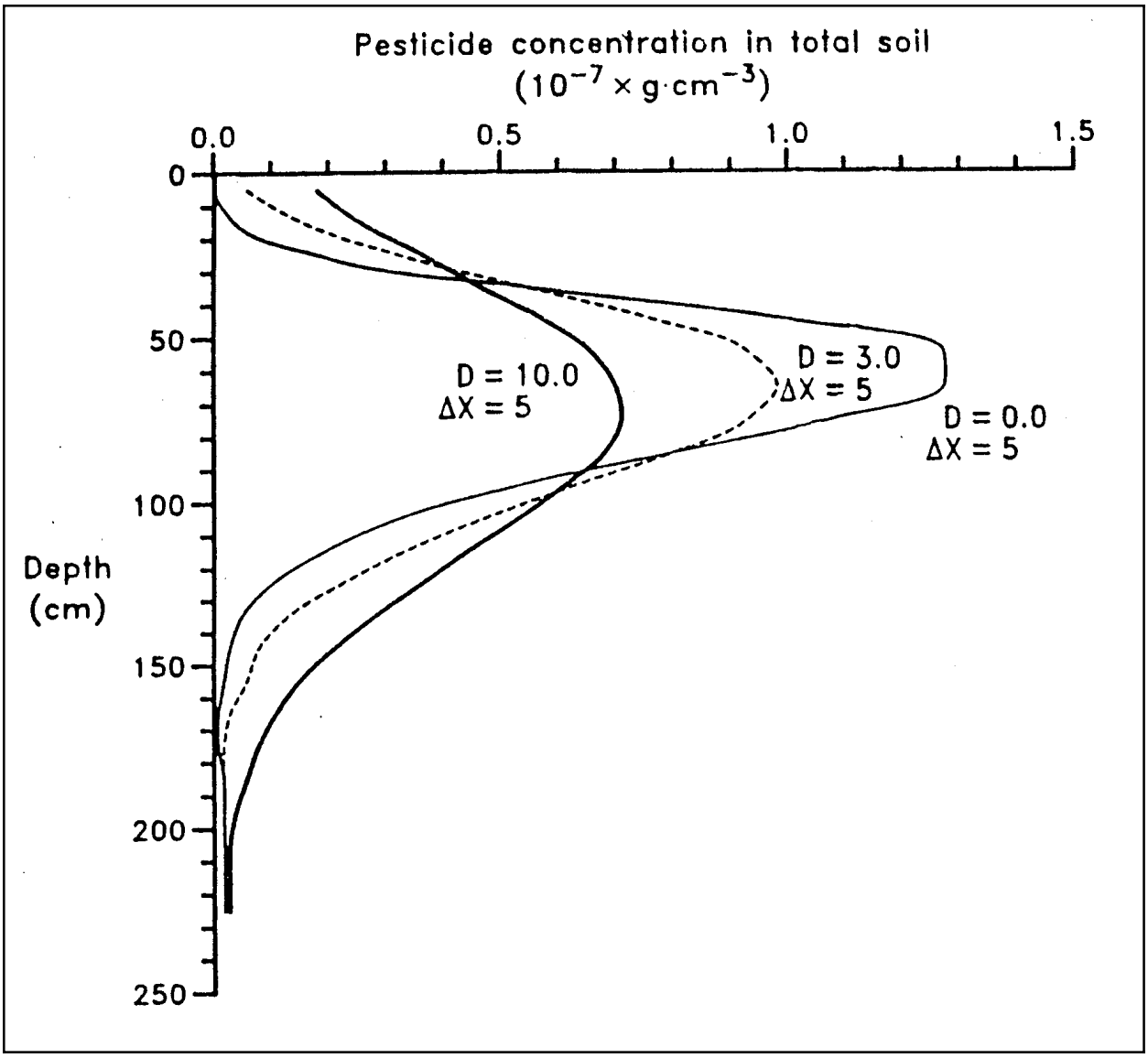


Figure 5.6 Physical dispersion (D) associated with advective transport. (Includes: Numerical dispersion).

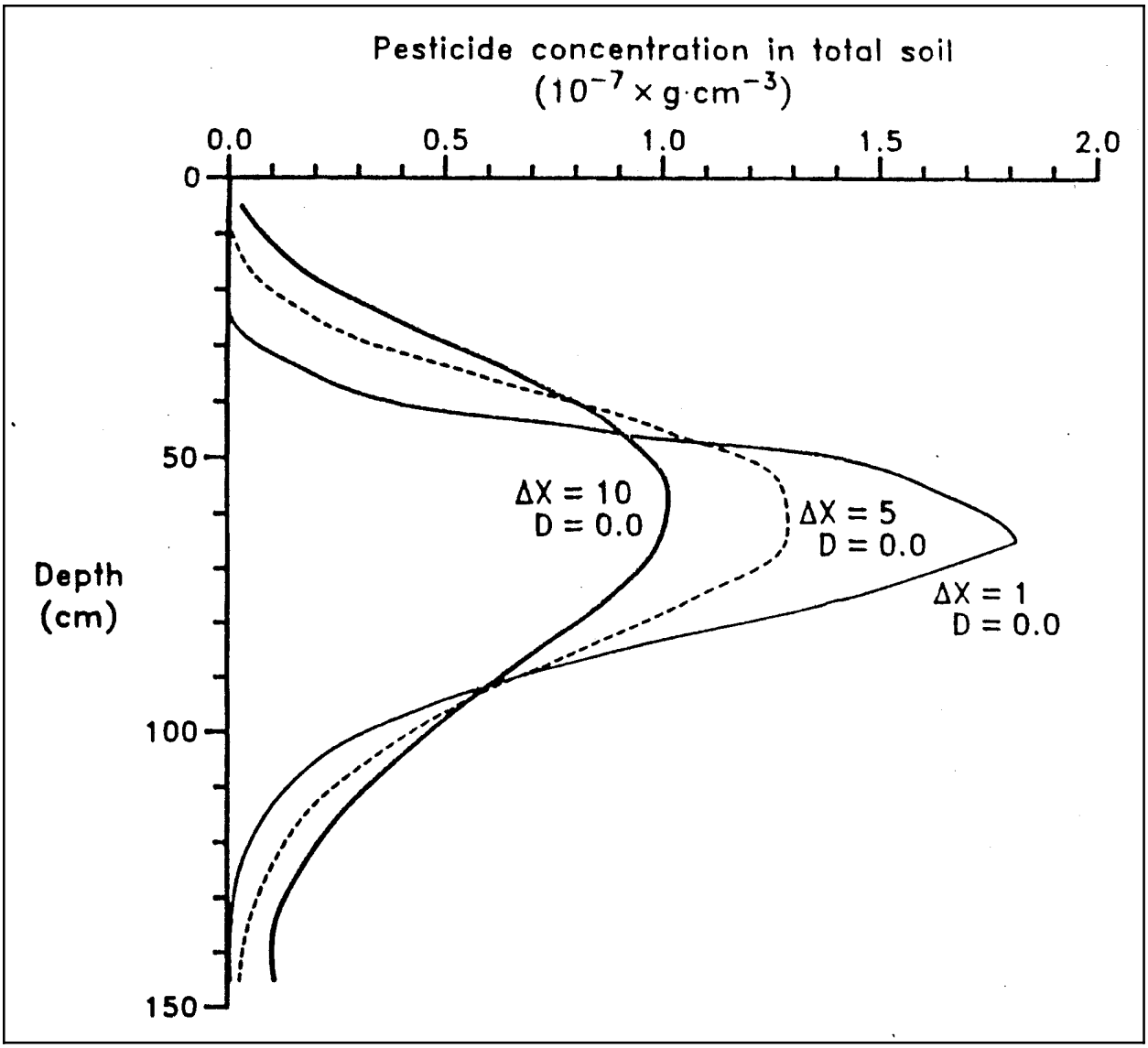


Figure 5.7 Numerical dispersion associated with space step (Δx).

DRFT - Spray drift fraction used to calculate drift loading in the EXAMS transfer file. DRFT is also used for a T-Band application (CAM = 7) to represent the fraction of the chemical application which will be incorporated into the top 2 cm in which drift will be set to 0.0 for the EXAMS transfer file.

DSRAT1, DSRAT2 - Absorbed phase degradation rate constant(s). DSRAT2 is only used with bi-phase reactions (see DKFLG2). See DWRAT1, DWRAT2 for guidance.

DT - Daylight hours for each month in relation to latitude. These values are used to calculate total potential ET if daily pan evaporation data do not exist. Table 5.2 lists monthly daylight hours for the northern hemisphere.

DWRAT1, DWRAT2 - Solution phase degradation rate constant(s). DWRAT1 is used for single phase degradation or as the first phase of a bi-phase reaction. This rate constant contributes to the disappearance of pesticide(s) through

decay. DWRAT2 is only used if simulating a second phase in a bi-phase reaction. For most cases, the same values should be used for solution (DWRATx) and adsorbed (DSRATx) phases for a specific depth. This will allow a lumped first-order degradation rate constant. The dissipation rate of pesticides below the root zone, however, is virtually unknown. Several studies have suggested the rate of dissipation decreases with depth; however, no uniform correction factor was suggested between surface/subsurface rates. First-order dissipation rates for selected pesticides in the root zone were tabulated in Tables 5.19 and 5.20.

EMMISS - Infrared Emissivity. Most natural surfaces have an infrared emissivities lying between 0.9 and 0.99. Values for all natural surfaces are not well known, but it is usually close to unity. Specific values of EMMISS for some natural surfaces are given in Table 5.22.

EN - Manning's roughness coefficient. The well-known measure of the resistance of open channels to flow. Chow (1959) suggests the values of EN range from 0.016 to 0.033 in excavated or dredged earth channels. EN values for the furrows listed in Table 5.34 range from 0.01 to 0.048. Table 5.37 lists the values of EN suggested by the USDA Soil Conservation Service for drainage ditches with various hydraulic radii (defined as the flow area divided by the wetted perimeter).

ENPY - Enthalpy of vaporization. This parameter is used in the temperature correction equation for Henry's Law constant. In a limited literature search, we could find only two pesticides for which ENPY values reported: 18.488 kcal $mole^{-1}$ for lindane and 20.640 kcal $mole^{-1}$ for napropamide (Streile 1984). Chemical-specific values are needed for ENPY, but a value of 20 kcal $mole^{-1}$ is a reasonable approximation.

ERFLAG - Erosion flag used to determine whether erosion losses are to be calculated during a simulation. The total mass of pesticide loss by erosion is determined using the chemicals affinity for soil. The amount of pesticide loss by these means is quite small for highly soluble pesticides. If the apparent distribution coefficient is less than or equal to 5.0, erosion can usually be neglected. For a compound having a greater distribution coefficient, erosion losses should be estimated. To not simulate erosion set ERFLAG =0.

EXMFLG - Flag for reporting output into the EXAMS model file format. This flag allows a user to create an input file for the EXAMS model through PRZM output if so desired. The EXAMS input file created has the name PRZM3EXA.Dxx where xx is the year of PRZM simulation. ERFLAG must be set to 1.

FEXTRC - Foliar washoff extraction coefficient. Washoff from plant surfaces is modeled using a relationship among rainfall, foliar mass of pesticide, and an extraction coefficient. The parameter (FEXTRC) is the required input parameter to estimate the flux of pesticide washoff. Exact values are variable and depend upon the crop, pesticide properties, and application method. Smith and Carsel (1984) suggest that a value of 0.10 is suitable for most pesticides.

FILTRA - The filtration parameter of initial foliage to soil distribution. This parameter relates to the equation for partitioning the applied pesticide between foliage and the ground. Lassey (1982) suggests values in the range of 2.3 to 3.3 m^2 kg^{-1}. Miller (1979) suggested a value of 2.8 m^2 kg^{-1} for pasture grasses. Most of the variation appears to be due to the vegetation and not the aerosol. FILTRA only applies if CAM=3.

FLEACH - The leaching factor as a fraction of irrigation water depth. This factor is used to specify the amount of water added by irrigation to leach salts from saline soil and is defined as a fraction of the amount of water required to meet the soil water deficit. For instance, a value of 0.25 indicates that 25% extra water is added to meet the soil water deficit.

FRMFLG - Flag for testing of ideal soil moisture conditions. This flag specifies whether to check preceding days (WINDAY) after the target application date (APD) for moisture levels being ideal for pesticide application. If a preceding date has adequate moisture levels and the target date does not, then the application date is changed automatically. If the soil moisture after a specified number of days (WINDAY) fails to meet ideal conditions, execution is halted.

HENRYK - Henry's constant is a ratio of a chemical's vapor pressure to its solubility. It represents the equilibrium between the vapor and solution phases (see Equation 6.17). It is quite common to express HENRYK as a dimensionless number. Specific values for HENRYK for selected pesticides can be found in Table 5.18.

HF - Suction parameter. HF represents water movement due to suction in unsaturated soils, and has units of length (meters). As with KS, HF has been correlated with SCS hydrologic soil groups (Brakensiek and Rawls 1983) and are shown in Table 5.39.

HORIZN - Horizon number. The horizon number in relation to the total number of horizons (NHORIZ) must be specified when inputing parameters for each of the PRZM horizons.

HSWZT - Flag to indicate soil water drainage calculation. The HSWZT flag indicates which drainage model is invoked for simulating the movement of recharging water. Drainage model 1 (HSZWT = 0) is for freely draining soils; drainage model 2 (HSZWT = 1) is for more poorly drained soils and requires the user to enter a soil water drainage rate (AD).

HTMAX - Maximum canopy height of the crop at maturation in centimeters. Canopy height increases during crop growth resulting in pesticide flux changes in the plant compartment. Users should have site-specific information on HTMAX since it varies with climate, crop species, and environmental conditions. General ranges for different crops are listed in Table 5.16.

ICNAH - This is the surface condition after crop harvest. Three values are allowed— fallow, cropping, and residue (foliage remains on ground).

ICNCN - The crop number of the different crop. This value is in relation to NDC (number of different crops). This allows separate crop parameters to be specified for each different crop in a simulation.

IDFLAG - Thermal conductivity and volumetric heat capacity flag. This flag allows a user to simulate soil temperature profiles. If IDFLAG = 0, the user must enter thermal conductivity (THCOND) and volumetric heat capacity (VHTCAP). If IDFLAG = 1, the model automatically simulates soil temperature profiles.

ILP - Initial pesticide levels flag. ILP should be set to 1 when evidence of pesticide is present before the simulation start date (STARTDATE). See also CFLAG and PESTR.

INCROP - The crop number associated with the number of different crops (NDC). INCROP should be an increasing integer from the first different crop to the last different crop grown.

INICRP - Initial crop flag. This flag indicates that before the simulation date occurs, a previous crop existed. The

IREG - SCS rainfall distribution region. For time period May 1 to September 15, IREG will be used in time of concentration calculation of peak flow. For rest of year IREG=2. See ? for appropriate region.

?

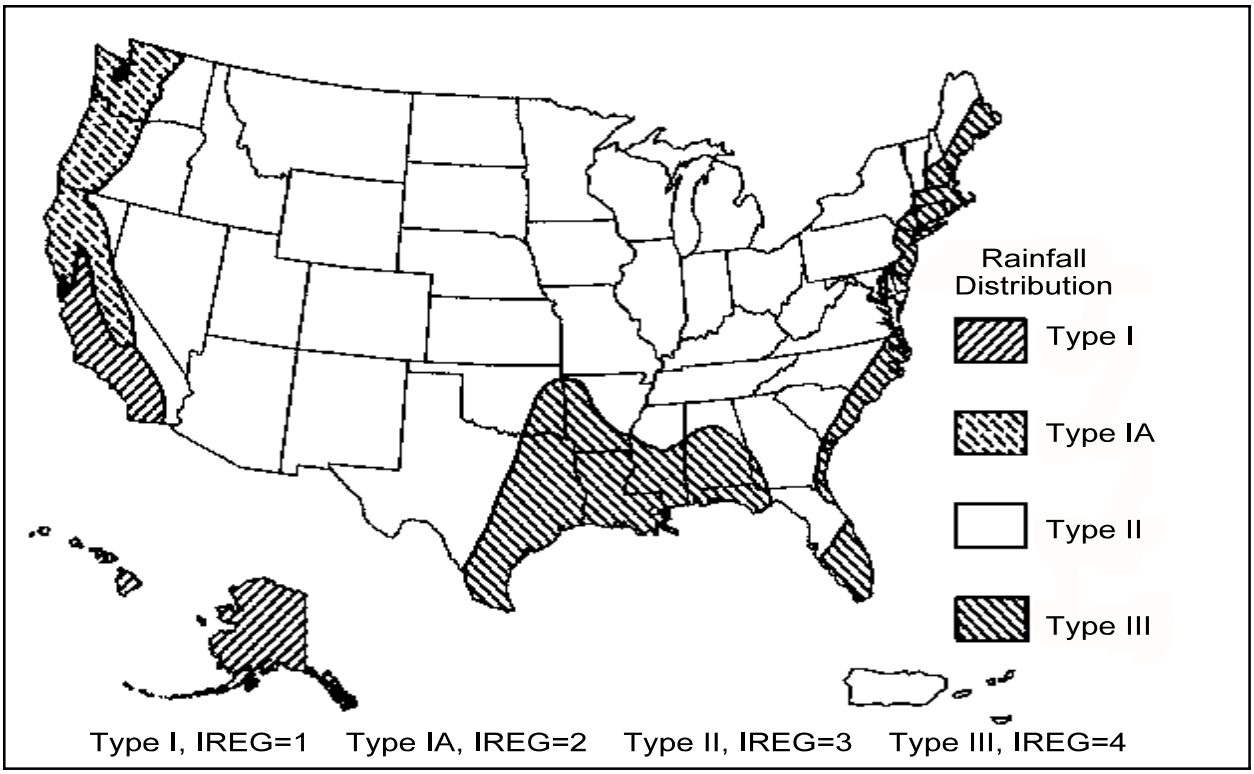


Figure 5.8 Approximate geographic boundaries for SCS rainfall distribution

Figure 5.8 from Soil Conservation Service {, 1986 #220}

IRFLAG - Flag to simulate irrigation. If irrigation is desired, the user has a choice of applying water for the whole year or during a cropping period whenever a specified deficit exists.

IRTYP - Specifies the type of irrigation used. See Table 5.32.

IPEIND - Pan Factor flag. When this flag is set to 0, daily pan evaporation is read from the meteorological file. When this flag is set to 1, pan data are calculated from daylight hours according to latitude. When this flag is set to 2, pan data are calculated through either the met file or daylight hours according to availability.

IPSCND - Flag indicating the disposition of pesticide remaining on foliage after harvest. This flag only applies if CAM = 2 or 3. If IPSCND = 1, pesticide remaining on foliage is converted to surface application to the top soil layer. If IPSCND = 2, remaining pesticide on foliage is completely removed after harvest. If IPSCND = 3, remaining pesticide on foliage is retained as surface residue and continues to undergo decay.

ISCOND - The surface condition for the initial crop if applicable.

ITFLAG - Flag for soil temperature simulation. This flag allows a user to specify soil temperatures (BBT) for shallow core depths. For deep cores (CORED), temperatures will remain relatively constant.

KC - Saturation constant of the co-metabolizing X_c population. See KSM and KCM for further explanation.

KCM - Saturation constant of the metabolizing X_m population with respect to carbon concentration. This value represents an inhibition of growth rate in relation to soil carbon. Lower saturation constants result in decreased carbon content consequently resulting in a lower growth rate.

KE - Average enzyme content of the X_c population. This parameter specifies the amount of the enzyme necessary to allow the population to break a pesticide down.

KD - Pesticide soil-water distribution coefficient. The user can enter KD directly if KDFLAG = 0 (see PCMC and SOL) or allow the model to calculate KD automatically (KDFLAG = 1).

KDFLAG - Flag to indicate soil/pesticide adsorption coefficient. A user may choose to enter KD by setting this flag to 0 else the model automatically calculates the adsorption coefficient.

KIN - Inhibition constant of the X_i population. Evolution of the population requires a finite value controlling growth. KIN accounts for natural variations found in metabolic activities affecting growth rates.

KL1 - Second-order death rate of the X_i population.

KL2 - Dissociation constant of the enzyme substrate complex.

KLDC - Death rate of the co-metabolizing X_c population.

KLDM - Death rate of the metabolizing X_m population.

KLDR - Death rate of the non-sensitive X_r population.

KLDS - Death rate of the sensitive X_s population.

KR - Saturation constant of the non-sensitive X_r population. See KSM and KCM for further explanation.

KS - Saturated hydraulic conductivity. This parameter represents the limiting infiltration rate when the soil column is saturated and suction pressure is no longer important. KS depends upon soil mineralogy, texture, and degree of compaction. Ranges for various unconsolidated materials are given in Table 5.38. KS has also been correlated with SCS hydrologic soil groups (Brakensiek and Rawls 1983) shown in Table 5.39.

KSK - Carbon solubilization constant.

KSM - Saturation constant of the metabolizing X_m population with respect to pesticide concentration. This value represents an inhibition of growth rate. Lower saturation constants result in lower bacteria rates, consequently resulting in lower growth rates. Higher saturation constants increase bacteria growth, resulting in higher growth rates.

MKS - Saturation constant of the sensitive X_s population. See KSM and KCM for further explanation.

MNGS - Mannings roughness coefficient for field. Up to 32 values may be entered per year. Value of 0.17 recommended as default value for typical row crop tillage. See Table 5.45 for values.

MOC - Flag to indicate method of characteristics calculation. The MOC algorithm is a two-pass solution technique used to simulate advection and dispersion. The solution technique reduces truncation error. Because of the 24 hour time step in PRZM, this method can lead to significant losses of mass under high velocity (greater than 120 cm per day) conditions.

MUC - Specific growth rate of the co-metabolizing X_c population.

NAPS - Number of pesticide applications. This is the total number of application dates specified during the simulation. It is possible to apply up to three chemicals on the same application date, but for PRZM this still constitutes one application.

NCHEM - Number of chemicals in the simulation. PRZM and VADOFT allow up to three chemicals to be specified. Using more than one chemical (i.e., NCHEM=3) indicates either a parent-daughter relationship or multiple separate chemicals (determined by transformation mass fractions). NCHEM should be consistent with the number of chemicals specified in the Execution Supervisor file.

NCPDS - Number of cropping periods. This is entered as a sum of all cropping dates from the beginning simulation date to the ending simulation date.

NDC - The number of different crops in the simulation. This value determines how many separate crops will be grown during a simulation. If only one type of crop is grown (ex: corn), then NDC = 1. This includes the crop type of the initial crop also (INICRP).

NHORIZ - Total number of horizons. PRZM allows the user to specify how many horizons are to be simulated within the core depth (CORED). The horizon should serve as a distinct morphologic zone generally described by layers (i.e., surface, subsurface, substratum) according to soil pedon descriptions or soil interpretation records, if available.

NPLOTS - Number of time series plots. PRZM can report several output variables (PLNAME) to a time series file. NPLOTS specifies how many are written in a single simulation.

OC - Percent of soil organic carbon. OC is conventionally related to soil organic matter as %OC = %OM/1.724. Guidance on estimating OM is found in Table 5.31. Information is categorized by hydrologic soil group and by depth. Also shown are coefficients of variation for each soil group and depth. Carsel et al. (1988) determined that the Johnson SB distribution provides the best fit to this data. Rao and Wagenet (Rao and Wagenet 1985) and Nielsen et al. (1973) have reported that these values are often normally distributed. Carsel et al. (1988) noted that organic carbon is weakly correlated with field capacity and wilting point water content with the correlation coefficients ranging from 0.1 to 0.74. Strength of correlation decreases with depth, as shown previously in Table 5.28.

PCDEPL - Fraction of available water capacity where irrigation is triggered. The moisture level where irrigation is required is defined by the user as a fraction of the available water capacity. This fraction will depend upon the soil-moisture holding characteristics, the type of crop planted, and regional agricultural practices. In general, PCDEPL should range between 0.0 and 0.6, where a value of 0.0 indicates that irrigation begins when soil moisture drops to wilting point, and 0.6 indicates the more conservative practice of irrigating at 60 percent of the available water capacity. Schwab et al. (1966) recommend values between 0.45 and 0.55. PRZM will accept values of PCDEPL between 0.0 and 0.90; if the input value is outside this range, PRZM sets PCDEPL to 0.5 and issues a warning message.

PCMC - Flag for estimating distribution coefficients (KD). PRZM allows the user to estimate the KD by multiplying the organic carbon partition coefficient (K_{oc}) derived from the solubility (SOL). PCMC is the flag for using one of four different models for estimating K_{oc}. The four models are:

PCMC1 $\text{Log } K_{oc} = (-0.54 \times \text{Log SOL}) + 0.44$
K_{oc} = organic carbon distribution coefficient
where SOL = water solubility, mole fraction

PCMC2 $\text{Log } K_{oc} = 3.64 - (0.55 \times \text{Log SOL})$
where SOL = water solubility, mg L^{-1}

PCMC3 $\text{Log } K_{oc} = 4.40 - (0.557 \times \text{Log SOL})$
where SOL = water solubility, micromoles L^{-1}

PCMC4 $K_{oc} = \text{SOL}$
where SOL = K_{oc}, dimensionless

PESTR - Initial pesticide(s) levels. PESTR levels are required if evidence of pesticide(s) is present before the simulation start date (ILP = 1). PESTR is entered in units specified by CFLAG for each compartment in each horizon and for all chemicals (NCHEM).

PFAC - The pan factor is a dimensionless number used to convert daily pan evaporation to daily potential evapotranspiration (ET). Pan factor general ranges are between 0.60 to 0.80. See **Figure 5.9** for specific regions of the United States.

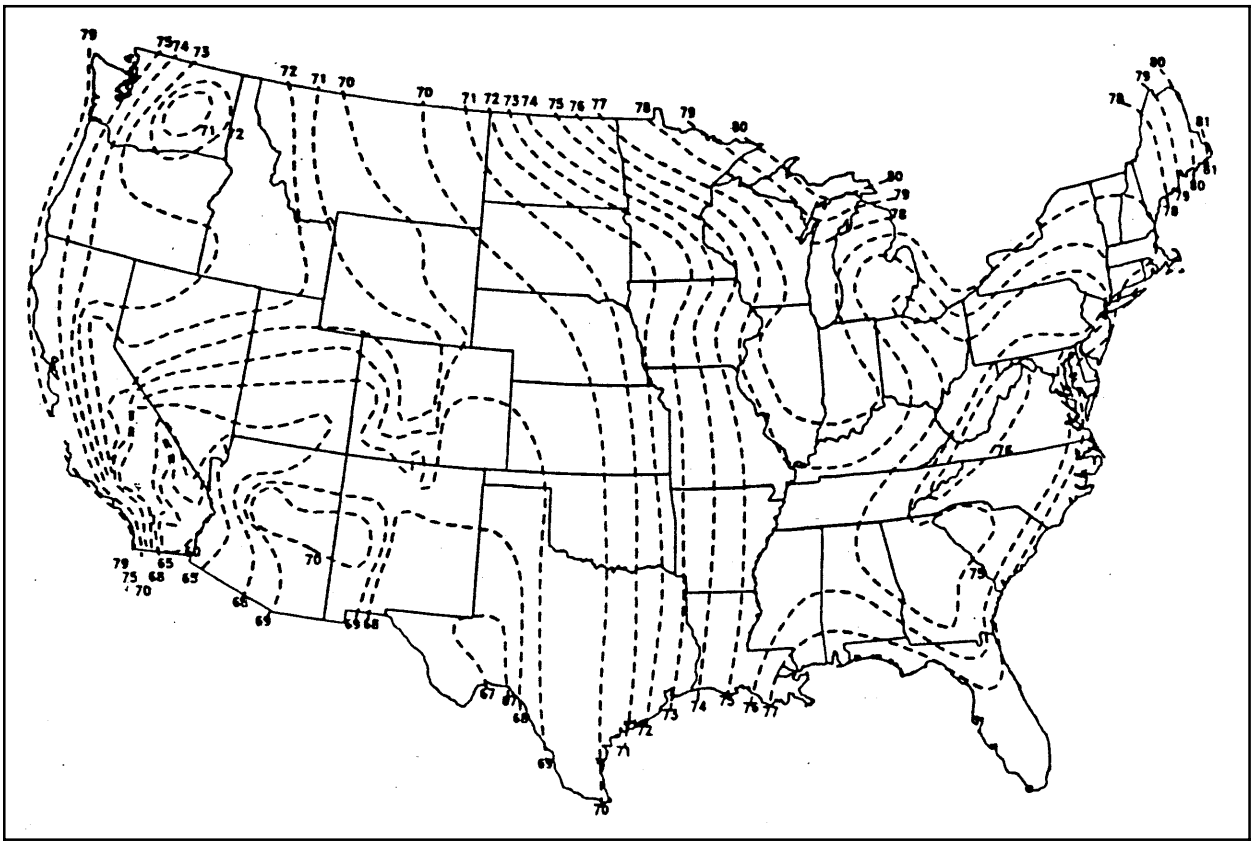


Figure 5.9 Pan evaporation correction factors

Figure 5.9 (from U.S. Weather Bureau)

PLDKRT - Foliage pesticide first-order decay rate. Pesticide degradation rates on plant leaf surfaces is represented as a first-order process controlled by PLDKRT. The user must be consistent in specifying PLDKRT and PLVKRT rates. If PLDKRT includes volatilization processes, then PLVKRT should be zero. If PLVKRT is non-zero then PLDKRT should include all attenuation processes except volatilization. Recent information (Willis and McDowell 1987) is available for estimating degradation rates of pesticides on plant foliage. In the work cited above, observed half-lives (days) were grouped by chemical family. These were:

- Organochlorine 5.0 ± 4.6
- Organophosphorus 3.0 ± 2.7
- Carbamate 2.4 ± 2.0
- Pyrethroid 5.3 ± 3.6

These mean half-lives correspond to degradation rates of 0.14, 0.23, 0.29, and 0.13 day^{-1}, respectively. These are in reasonable agreement with values in Table 5.17.

PLNAME - Name of plotting variable. When creating a time series plot, PLNAME specifies the variable in Table 4.1 for which that output data are written.

PLVKRT - Foliage pesticide first-order volatilization rate. Pesticide volatilization from plant leaf surfaces is represented as a first-order process controlled by PLVKRT. For organophosphate insecticides, Stamper et al. (1979) has shown that the disappearance rate from leaf surfaces can be estimated by a first-order kinetic approach. Similar observations of first-order kinetics were found for volatilization of 2,4-D iso-octyl ester from leaf surfaces by Grover et al. (1985). Volatilization losses of toxaphene and DDT from cotton plants decreased exponentially with time and were linearly related to the pesticide load on these plants (Willis et al. 1983). Table 5.17 shows disappearance rates for selected pesticides on plant foliage. These rates are applicable to estimation of PLVKRT since the overall decay rate (PLDKRT) includes loss associated with volatilization.

PSTNAM - Pesticide(s) name. This is a label used to identify pesticide output. Pesticide names should be placed in order of chemical 1, chemical 2, and chemical 3 if applicable (NCHEM=3)

PTRN12, PTRN13, PTRN23 - lumped foliar transformation rate ($days^{-1}$)

Q - Average carbon content of the X_i population.

Q0 - Flow rate into a single furrow. Q0 is defined as the volume of water entering the furrow per unit time. Flow rates are usually set so that sufficient water reaches the end of the furrow without causing excessive erosion. Table 5.35 lists the maximum non-erosion flow rates for various furrow channel slopes.

QFAC - Factor for rate increase when temperature increases by 10°C. Set to 2 for doubling of microbial degradation rate

RATEAP - Maximum sprinkler application rate. RATEAP is used to limit sprinkler applications to volumes that the sprinkler system is capable of delivering per time step. This value is defined as a maximum depth (cm) of water delivered per hour. Table 5.33 lists sprinkler rates.

SF - Channel slope. SF is determined by regional topography and the design grades of the furrows, and is defined as vertical drop in elevation per horizontal distance of the bed. Furrows are usually used only in relatively level terrain, with slopes no greater than 0.03 (Todd 1970). A few representative slopes are listed in Table 5.34.

SFAC - The snowmelt factor is a used to calculate snowmelt rates in relation to temperature. Snow is considered any precipitation that falls when the air temperature is below 0°C. In areas where climatology prevents snow fall, SFAC should be set to 0.0. Typical ranges for SFAC are provided in Table 5.1.

SLP - Slope of hydraulic flow path.

SOL - Pesticide water solubility. By specifying a water solubility (SOL) for pesticides, the model can calculate the K_{oc} and KD by using one of the models specified for PCMC. SOL must be entered according to the PCMC model selected. Table 5.19 provides pertinent values for selected pesticides for obtaining SOL. Methods are also available to calculate K_{oc} (SOL if PCMC=4). The octanol-water distribution coefficient can be used for calculating K_{oc} with a relationship to organic carbon (OC). Karickhoff et al. (1979) proposed a relationship between K_{ow} and K_{oc} given by

$$\log(K_{oc}) = 1.0 \log(K_{ow}) - 0.21$$

where

K_{ow}	=	octanol-water distribution coefficient ($cm^3\ g^{-1}$)
K_{oc}	=	organic carbon distribution coefficient ($cm^3\ g^{-1}$)

Selected pesticides having properties suitable for use with the octanol-water distribution model by Karickhoff are provided in Table 5.20.

SPACT - Special action variable. During the course of a PRZM simulation, there may be a change in chemical behavior or agricultural management practices. SPACT allows the user to specify a special action variable from Section 4 and change its value at a user-specified time (SADAY,SAMON,SAYR). Also the SPACT variable 'SNAPSHOT' can allow a user to output soil profile pesticide concentrations at a user-specified time during the simulation.

SPT - Initial soil temperature profile. To simulate the soil temperature profile, initial SPT values for each soil horizon must be specified. Since PRZM is often used for long periods of simulation, the initial temperature profile will not have any significant effect on the predicted temperature profile after a few days or weeks of simulation unless the core depth (CORED) is deep. Lower horizons in the core should be assigned values corresponding approximately to the bottom boundary temperature (BBT).

TAPP - Target application rate for pesticide(s). For each pesticide and each application date, the amount of pesticide is entered in kg-active ingredient ha^{-1}. Typical rates are included on the product's registration label. Actual rates used in the model are reduced by an application efficiency (APPEFF).

TBASE - temperature at which microbial degradation was determined

THCOND,VHTCAP - Thermal conductivity and volumetric heat capacity of soil horizon. If the user chooses to have the model simulate the soil temperature profile and sets the IDFLAG flag to zero, then the thermal conductivity (THCOND) and heat capacity (VHTCAP) must be specified. Representative values for some soil types are given in Table 5.24. Note that the value of THCOND is entered in PRZM in units of cal cm^{-1} $°C^{-1}$ day^{-1}; therefore, the values in Table 5.24 should be multiplied by 86,400. If IDFLAG = 1, then THCOND and VHTCAP are calculated by the model from %Sand, %Clay, and %OC, based on the method described in de Vries (1963).

THEFC,THEWP - Field capacity and wilting point. Often these soil-water properties have been characterized and can be found from soil data bases. Where such data are not available, one of three following estimation methods can be used. Method one requires the textural properties (percent sand, silt, and clay), organic matter content (%), and bulk density (g cm^{-3}) of a specific soil. Method two utilizes a soil texture matrix for estimating soil water content if only the sand (%) and clay (%) contents are known. Method three provides mean field capacity and wilting points if only soil texture is known.

Method 1 - (Rawls 1983)

$$\theta_x = a + b \times \%Sand + c \times \%Clay + d \times \%Organic_Matter + e \times Bulk_Density$$

where

θ_x = water retention cm^3 cm^{-3} for a given matric potential (field capacity = -0.33 bar and wilting point = -15.0 bar)

a-e = regression coefficients
Bulk_Density measured in g cm^{-3}

Step 1. From Table 5.23 find the matric potential for field capacity and wilting point.
Step 2. For each matric potential, find the regression coefficient (a-e) that are in the Rawls and Brakensiek equation.
Step 3. For any given soil solve the equation for the -0.33 and -15.0 potential.

Method 2

Use **Figure 5.10** for estimating the field capacity and **Figure 5.11** for estimating the wilting point, given the percent sand and clay.

Method 3

Use Table 5.25 to locate the textural class of the soil of choice. After locating the textural class, read the

mean field capacity and wilting point potentials ($cm^3\ cm^{-3}$), to the right of the textural class.

Guidance for estimating distributional properties for THEFC and THEWP is given in Tables 5.26 and 5.27.

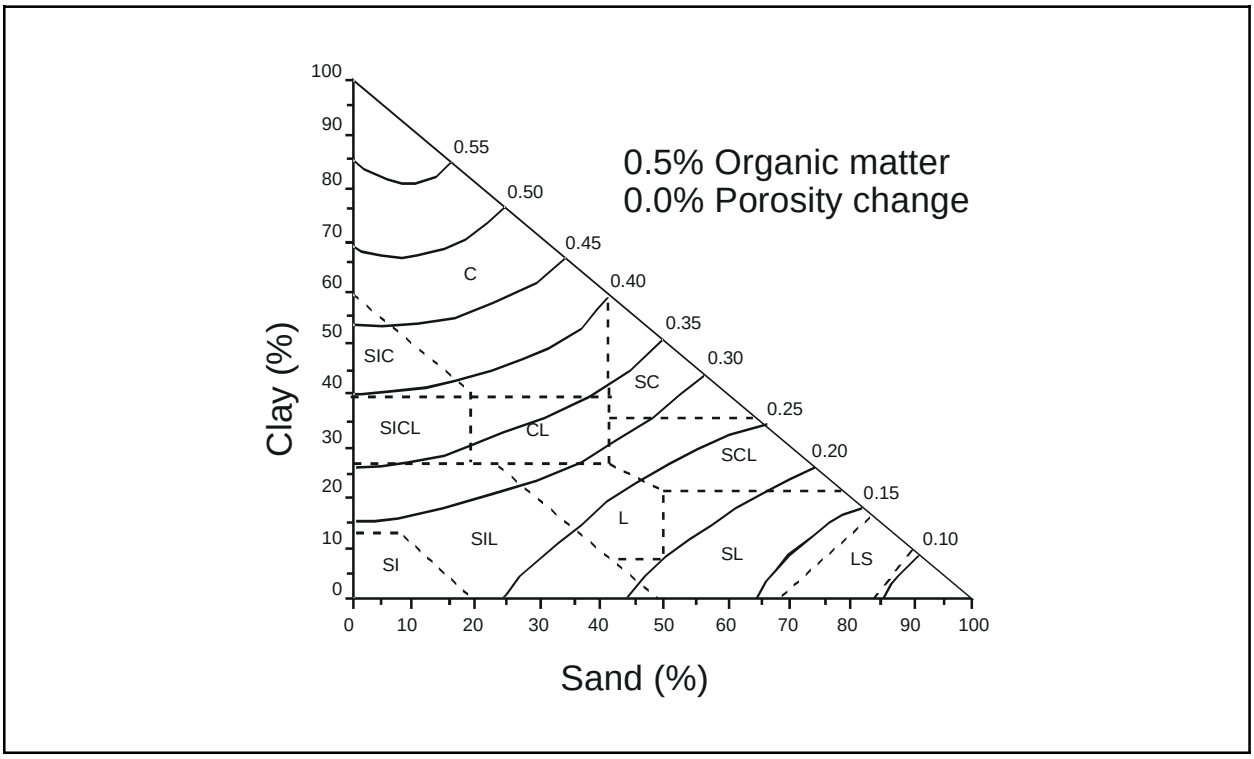


Figure 5.10 1/3-bar soil moisture by volume.

Figure 5.10 (provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland).

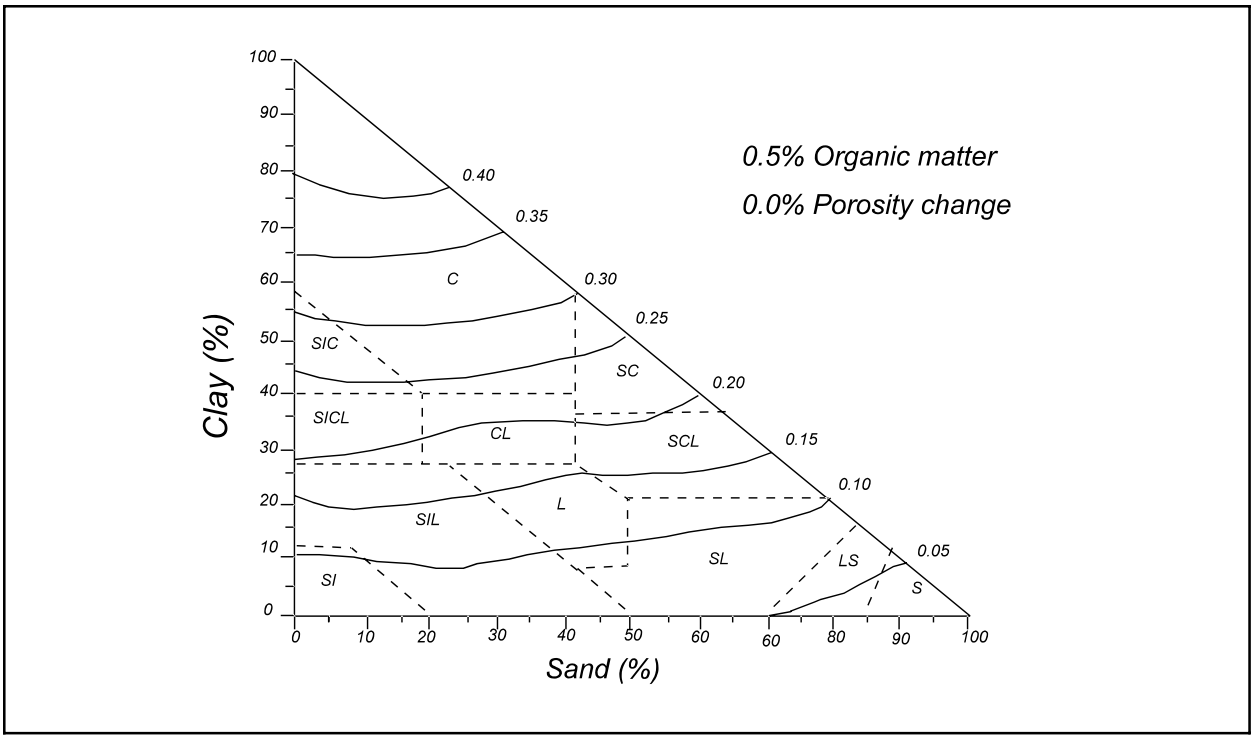


Figure 5.11 15-bar soil moisture by volume.

Figure 5.11 provided by Dr. Walter J. Rawls, U.S. Department of Agriculture, Agricultural Research Service, Beltsville, Maryland.

THETO - Initial water content of the soil. This value provides the model with a starting calculation for moisture. If site-specific data are not available, field capacity value is recommended for THETO.

THEWP - See THEFC for guidance.

THFLAG - Flag to indicate field capacity and wilting point calculation.

THKNS - Thickness of the horizon. This value is the depth (cm) of the horizon specified (HORIZN) in relation to core depth (CORED).

TR - Storm duration peak runoff rate. TR is entered as an average, although in reality this parameter changes seasonally as well as with each storm type. This value represents the time period when storms occur producing peak runoff over a short duration. **Table 5.8** provides estimates for TR for selected locations in the U.S. for both mean summer and annual time periods while **Figure 5.12** provides regionalized values for different areas in the United States.

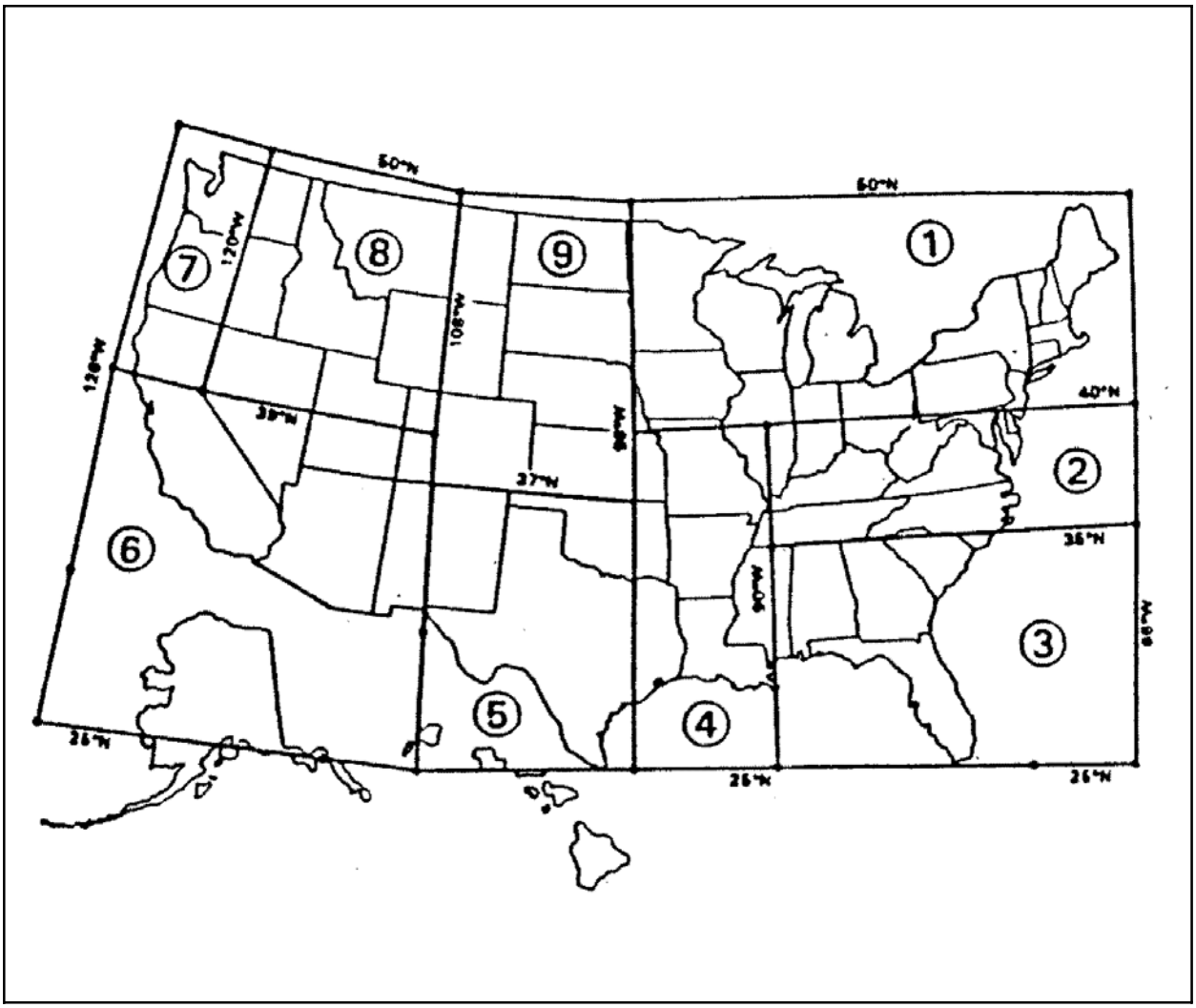


Figure 5.12 Representative regional mean storm duration (hours) values for the U.S.

Mean Storm duration (hours)									
	Zone								
Period	1	2	3	4	5	6	7	8	9
Mean (Annual)	5.8	5.9	6.2	7.3	4.0	3.6	20.0	4.5	4.4
C.V. (Annual)	1.05	1.05	1.22	1.17	1.07	1.02	1.23	0.92	1.20
Mean (Summer)	4.4	4.2	4.9	5.2	3.2	2.6	11.4	2.8	3.1
C.V. (Summer)	1.14	1.09	1.33	1.29	1.08	1.01	1.20	0.80	1.14

Mean – mean storm duration (hours)
C.V. – Coefficient of variation (hours)
Source: (Woodward-Clyde Consultants 1988a, b)

UPTKF - Plant uptake efficiency factor. This value provides for removal of pesticides by plants. It is also a function of the crop root distribution and the interaction of soil, water, and the pesticide. Several approaches to modeling the uptake of nutrients/pesticides have been proposed ranging from process models that treat the root zone system as a distribution sink of known density or strength to empirical approaches that assume a relationship to the transpiration rate. Dejonckheere et al. (1983) reported the mass of uptake into sugarbeets for the pesticides aldicarb and thiofanox for three soils (sandy loam, silt loam, and sandy clay loam). Mass removal expressed as a percentage of applied material for aldicarb on sandy loam, silt loam, and clay loam ranged from 0.46% to 7.14%, 0.68% to 2.32%, and 0.15% to 0.74%, respectively. For thiofanox, 2.78% to 20.22%, 0.81% to 8.70%, and 0.24% to 2.42% removals were reported for the respective soils. Other reviews have suggested ranges from 4% to 20% for removal by plants. Sensitivity tests conducted with PRZM indicate an increase in the uptake by plants as the crop root zone (AMXDR) increases and the partition coefficient (KD) decreases. For highly soluble pesticides and for crop root zones of greater than 120 cm, values of greater than 20% were simulated. Briggs et al. (1982) have developed an empirical relationship between plant uptake of a pesticide, expressed in terms of a transpiration stream concentration factor (TSCF), and the pesticide's octanol/water partition coefficient (K_{ow}). The TSCF is defined as the ratio of the concentration of a pesticide in a plant's transpiration stream to the concentration of the pesticide in external solution; extensive laboratory results suggest that the TSCF is not time dependent (i.e., it is an equilibrium value), and it is independent of external concentrations for dilute solutions. The concentration in the transpiration stream is measured indirectly from the mass of chemical accumulated in the shoots for a known volume of water transpired; the TSCF has a maximum value of 1.0 for passive uptake. The laboratory TSCF values have been fitted to a Gaussian curve, and values for 18 pesticides (O-methyl-carbamamoyloximes and substituted phenylureas) in barley fit the following formula:

$$\text{TSCF} = 0.784 \exp\left[-(\log K_{ow} - 1.78)^2 / 2.44\right]$$

Briggs' laboratory results for TSCFs ranged from 0.11 to 0.94 for the 17 of the 18 pesticides that were tested. For initial estimates, a value of 1.0 for UPTKF is recommended. Using this value results in uptake being estimated as equal to the transpiration times dissolved phase concentration (i.e., passive uptake).

USLEC - The universal soil loss cover management factor © value). Values for USLEC are dimensionless and range from 0.001 (well managed) to 1.0 (fallow or tilled condition). Up to 32 values may be entered for the year dependent on crop growth and tillage operations. Specific values can be calculated via Wischmeier and Smith (1978) or obtained from a local SCS office. Generalized values are provided in Table 5.7.

USLEK - The universal soil loss equation (K) of soil erodibility. This is a soil-specific parameter developed by the USDA. Specific values can be obtained from the local SCS office. Approximate values are listed in Table 5.3.

USLELS - The universal soil loss equation (LS) topographic factor. This is a slope length and steepness parameter developed by the USDA. The value is dimensionless and can be estimated from Table 5.5.

USLEP - The universal soil loss equation (P) practice factor. This value is developed by the USDA to describe conservative agricultural practices. Values are dimensionless and range from 0.10 (extensive practices) to 1.0 (no supporting practices). Specific values can be estimated in Table 5.6.

UCM - Specific growth rate of the metabolizing X_m population with respect to carbon concentration.

UR - Specific growth rate of the non-sensitive X_r population.

US - Specific growth rate of the sensitive X_s population.

USM - Specific growth rate of the metabolizing X_m population with respect to pesticide concentration.

VHTCAP - See THCOND for guidance.

WINDAY - An integer number of days. This specifies the number of days after the target date (APD) that the code

checks for ideal moisture conditions. For this value to be valid, FRMFLG must equal 1. WINDAY should be less than the difference of the target date (APD) to the next chronological target date.

WFMAX - The maximum dry foliar weight. This value is used only if a user desires to have the model estimate the distribution between plants and the soil by an exponential function when a pesticide is applied. WFMAX of the plant above ground (kg m^{-2}) is the exponent used in the exponential foliar pesticide application model. Estimates of WFMAX for several crops are given in Table 5.14.

X2 - Length of the furrow. X2 will depend upon the size of the field and the local topography. Table 5.35 lists maximum furrow lengths for various slope textures, irrigation application depths, and furrow slopes.

XFRAC - Location of the furrow. XFRAC is a fraction of furrow length (X2) that specifies where PRZM infiltration calculations are performed. To use the average depth of furrow infiltration depths, set XFRAC to -1.

Y1 - Metabolizing (X_m) microbial population.

Y2 - Co-metabolizing (X_c) microbial population.

Y3 - Sensitive (X_s) microbial population.

Y4 - Non-sensitive (X_r) microbial population.

YC - True growth yield of the co-metabolizing X_c population.

YCM - True growth yield of the metabolizing X_m population with respect to carbon concentration.

YR - True growth yield of the non-sensitive X_r population.

YS - True growth yield of the sensitive X_s population.

YSM - True growth yield of the metabolizing X_m population with respect to pesticide concentration.

ZRS - Side slope of the furrows. This parameter is defined as the slope of the channel walls, horizontal distance/vertical distance. ZRS will depend upon the cohesiveness of soils and the type of equipment used to dig the furrows. Table 5.36 lists the suitable side slopes for different types of soils, with values ranging from 1.5 to 3.0 for unconsolidated materials.

ZWIND - Height of wind speed measuring instrument. The wind speed anemometer is usually fixed at 10 meters (30 feet) above the ground surface. This height may differ at some weather stations such as at a class A station where the anemometer may be attached to the evaporation pan. The correct value can be obtained from the meteorological data reports for the station whose data are in the simulation.

5.2.1 Nitrogen Calibration Procedures and Parameter Estimation

Application of the nitrogen simulation capabilities in the PRZM-3 code focuses on the model's ability to reproduce target levels of nitrogen storages and fluxes, along with available site-specific data; this approach necessitates *model calibration*. Calibration of soil nitrogen models involves defining model inputs, estimating the nitrogen balance expected for the soil/plant system being modeled, and adjusting model parameters to mimic the expected or observed nitrogen balance, including both soil and plant storages and fluxes. Most of the soil nitrogen modeling work to date, and the majority of the currently available literature on nitrogen balances, is based on studies of agricultural systems, with a significantly smaller portion directed to forested systems. Table 5.45, from Frissel (1978, pp. 203-243) shows examples of nitrogen balances developed from selected field studies for cultivated crops, grasslands, and a few

forested ecosystems. This presentation of a nitrogen balance shows the N inputs or additions, such as fertilizer/manure applications, N fixation, irrigation, and atmospheric deposition (described as 'sediments added' in Table 5.45); the N removals, including crop harvest, denitrification, volatilization, and leaching and erosion/runoff; and recycling process within the soil, such as mineralization, plant uptake, and residue return. It is important to note that the largest components of most agricultural systems are the N additions (e.g. N applications and fixation) and resulting plant uptake and removal. Thus, accurately defining these two components is key to modeling soil nitrogen processes for these systems.

As noted previously, the soil N process algorithms that were integrated into PRZM-3 are the same as those included in the most recent version of the HSPF model. Consequently, the best current source of relevant nitrogen parameter information are prior and recent HSPF applications. Donigian (Donigian 1996) has compiled an (unpublished) bibliography of HSPF-related documents that identifies nitrogen modeling applications in Iowa, Nebraska, Tennessee, Georgia, Pennsylvania, Maryland, Virginia, and the general Chesapeake Bay Region. Bicknell et al. (1996) describe the most recent modifications to the HSPF nitrogen modeling algorithms, which are included in PRZM-3, and their application to forested watersheds in Maryland and Virginia. Donigian et al. (1995) describe the nitrogen plant uptake formulations in HSPF, included in PRZM-3, along with parameter estimation and calibration guidance for agricultural systems. Expected nitrogen balances for a variety of land uses, including cropland, hay, pasture, forest, and urban, are presented by Donigian and Chinnaswamy (Donigian and Chinnaswamy 1996),along with a discussion of their use in watershed modeling. The original report on the PRZM-3 nitrogen algorithms (Imhoff et al. 1995) includes its application for nitrogen leaching from septic systems, along with an expected nitrogen balance and initial parameters for an application site in Colorado; the example PRZM nitrogen input in Section 4.5.1 includes the parameters used for the Colorado septic system application.

Users of the nitrogen capabilities in PRZM-3 should consult the above sources of parameter information, along with the parameter definitions (Section 4.5.2) and the example input (Section 4.5.1), as part of the nitrogen parameter estimation and calibration process, especially when site-specific data is not available for the application site.

5.3 VADOFT Input Parameters

Input data for variably saturated flow simulations include the following:

(1)System Geometry

- Soil column dimensions (L)

(2)Porous Medium Properties

- Saturated hydraulic conductivity, K_s (LT^{-1})
- Specific storage, S_s (L^{-1})
- Effective porosity, ϕ

(3)Constitutive Relationships for Variably Saturated Flow

- Tabulated data of K_{rw} versus S_w, or values of parameters of analytic expressions for K_{rw} versus S_w
- Tabulated data of S_w versus ψ, or values of parameters of analytic expressions for S_w versus ψ.

(4)Initial and Boundary Conditions

- Prescribed values of pressure head, ψ (L)
- Prescribed values of nodal fluid flux (infiltration rate), I (LT^{-1})

Input data for the transport model include the following:

(1)System Geometry

- Soil column dimensions (L)

(2)Porous Medium Properties

- Longitudinal dispersivity α_L, (L)
- Molecular diffusion coefficients, D^* (L^2T^{-1})
- Effective porosity, ϕ

(3)Properties of Solute Species

- Decay coefficient, λ (T^{-1})
- Retardation coefficient, R

(4)Darcy Velocity, V (LT^{-1})

(5)Water Saturation, S_w

(6)Initial and Boundary Conditions

- Prescribed value of concentration, c_o (ML^{-3})
- Prescribed value of solute flux, Vc_o ($ML^{-2}\ T^{-1}$)

Guidance for certain of these parameters is given in the following paragraphs.

Saturated Hydraulic Conductivity - represents the rate at which a porous medium can transmit water under saturated conditions. Table 5.40 gives representative values for various soil types. Also note the values of the coefficient of variation in column three. These CVs are for many soils nationwide that fall into this texture category. CVs for a single soil are likely to be lower. Jury (1985) gives a CV of 120% for this parameter, which may be more representative. The most likely shape for the distribution is lognormal.

Soil-Water Characteristic Data - The user is allowed two options: either to input these data as a set of paired functions (water saturation [S_w] versus relative conductivity [K_{rw}] and pressure head [ψ] versus water saturation [S_w] or to input parameters of the analytic expressions for these functions in the code. The parameterization of the latter functions is discussed here.

To provide a linkage for these parameters to widely known or easily obtained soils data (such as soil texture), Carsel and Parrish (1988) fit these analytic functions to data from soils all over the United States and tabulated corresponding parameter values by texture. These are shown in Table 5.41. The required parameters are α, β, and γ of the van Genuchten model. Mean values of these parameters are shown along with CVs for each by soil texture. Other parameters required to use these relationships are the air entry pressure head (ψ_a) and the residual water phase saturation (S^{wr}). The air entry pressure head is normally taken to be zero. Values of the residual water phase saturation are given in Table 5.42 along with their respective CVs. Table 5.43 from Carsel and Parrish (1988) shows the types of probability density functions used to fit the sample distributions of saturated hydraulic conductivity, residual water phase saturation, and van Genuchten parameters α and β. Note that γ is related to β by the relationship $\gamma = 1 - 1/\beta$.

In addition, Table 5.44 gives the correlations between these parameters by soil textural classification.

Specific Storage - For unsaturated zone flow, set the specific storage to 0.

Effective Porosity - Mean values of saturated water content (θ_s) and residual water content (θ_r) shown in Table 5.42 can be used to estimate effective porosity. The saturation water content (θ_s) is equal to the total porosity of the soil. The effective porosity can be roughly approximated as the difference of θ_s and θ_r in Table 5.43. CVs for soil texture categories are also shown in Table 5.43. According to Jury (1985) the normal distribution is an appropriate probability density function for this parameter.

Longitudinal Dispersivity - (The user should refer to the discussion of the dispersion coefficient having units of $cm^2\ day^{-1}$.) Dispersion coefficients are calculated by the model as the product of the seepage velocity and the dispersivity input by the user. In the absence of site-specific values it is recommended that the dispersivity be chosen

as one-tenth of the distance of the flow path or:

$$\alpha = 0.1\ x_v$$

where

x_v = the thickness of the vadose zone.

Molecular Diffusion - See the discussion in Section 5.2 for the variable DISP.

Pesticide Decay Coefficients - See the discussion in Section 5.2 for pesticide decay in PRZM.

Retardation Factors - In VADOFT, in contrast to PRZM, the user inputs the retardation factor R instead of the distribution coefficient, K_d ($cm^3\ g^{-1}$). The retardation factor is defined for saturated conditions in the input:

$$R = 1 + \frac{K_d \rho}{\theta_s}$$

and is adjusted internally for values of $\theta < \theta_s$. In the above equation, ρ is the soil bulk density ($g\ cm^{-3}$) and θ_s is the saturation water content ($cm^3\ cm^{-3}$). In making this calculation, the user should directly use the value for ρ, if known. If necessary, ρ can be approximated according to:

$$\rho = 2.65\,(1 - \theta_s)$$

The coefficient of variation (CV) of the retardation factor, *R*, can be computed knowing the uncertainties in K_d, ρ and θ_s (Taylor 1982). The fractional uncertainties may be added to determine an upper bound error on *R* (CV_{max}),

$$CV_{\max} = CV(\theta_s) + CV(K_d) + CV(\rho)$$

or are combined as a root mean square for independent random errors,

$$CV_{rms} = 100 \cdot \sqrt{\left(\frac{CV(\theta_s)}{100}\right)^2 + \left(\frac{CV(K_d)}{100}\right)^2 + \left(\frac{CV(\rho)}{100}\right)^2}$$

The uncertainty in the value of K_d will depend upon whether it is measured, calculated as the product of K_{oc} and the percent organic carbon, and whether the K_{oc} is calculated from a surrogate parameter such as octanol water partition coefficient (K_{ow}) or solubility (*s*). Directly measured values would obviously have lower *CV*s. Assuming that K_d is calculated from a measured soluble concentration, then it is possible that the *CV* would be on the order of 60 to 130% (Jury 1985). For K_d derived from K_{ow} or solubility, the *CV* could be on the order of 1000%.

Table 5.1 Typical Values of Snowmelt (SFAC) as Related to Forest Cover

	Snowmelt Factor, (cm °C^{-1} day^{-1})	
FOREST COVER	**MINIMUM**	**MAXIMUM**
Coniferous - quite dense	0.08 - 0.12	0.20 - 0.32
Mixed forest - coniferous,deciduous, open	0.10 - 0.16	0.32 - 0.40
Predominantly deciduous forest	0.14 - 0.20	0.40 - 0.52
Open areas	0.20 - 0.36	0.52 - 0.80

Source: (Anderson 1978)

Table 5.2 Mean Duration (Hours) of Sunlight for Latitudes in the Northern and Southern Hemispheres[a]

		Latitude North*							
Month	**Days In Month**	**00**	**10**	**20**	**30**	**35**	**40**	**45**	**50**
Jan	31	12.1	11.6	11.0	10.5	10.1	9.8	9.3	8.6
Feb	28	12.1	11.7	11.6	11.2	10.9	10.7	10.4	10.0
Mar	31	12.1	12.0	12.0	12.0	12.0	12.0	11.8	11.8
Apr	30	12.1	12.4	12.6	13.0	13.1	13.3	13.6	13.8
May	31	12.1	12.5	13.1	13.7	14.1	14.4	14.9	15.4
Jun	30	12.1	12.7	13.3	14.0	14.5	15.0	15.5	16.3
Jul	31	12.1	12.5	13.2	13.9	14.3	14.7	15.2	15.9
Aug	31	12.1	12.4	12.9	13.2	13.5	13.7	14.1	14.5
Sep	30	12.1	12.2	12.2	12.4	12.4	12.5	12.5	12.7
Oct	31	12.1	11.8	11.6	11.4	11.3	11.1	10.9	10.7
Nov	30	12.1	11.8	11.2	10.7	10.3	10.0	9.5	9.1
Dec	31	12.1	11.5	10.9	10.2	9.9	9.4	8.7	8.1

[a] -(Criddle 1958)

* - Values for the southern hemisphere were assumed equal to the northern hemisphere lagged by six months, e.g., the duration for January in the northern hemisphere is the same as July in the southern hemisphere.

Table 5.3 Indications of the General Magnitude of the Soil erodibility Factor, K[a]

	Organic Matter Content		
Texture Class	**< 0.5%**	**2%**	**4%**
Sand	0.05	0.03	0.02
Fine sand	0.16	0.14	0.10
Very Fine Sand	0.42	0.36	0.28
Loamy Sand	0.12	0.10	0.08
Loamy Fine Sand	0.24	0.20	0.16
Loamy Very Fine Sand	0.44	0.38	0.30
Sandy Loam	0.27	0.24	0.19
Fine Sandy Loam	0.35	0.30	0.24

Table 5.3 Indications of the General Magnitude of the Soil erodibility Factor, K[a]			
	Organic Matter Content		
Texture Class	**< 0.5%**	**2%**	**4%**
Very Fine Sandy Loam	0.47	0.41	0.33
Loam	0.38	0.34	0.29
Silt Loam	0.48	0.42	0.33
Silt	0.60	0.52	0.42
Sandy Clay Loam	0.27	0.25	0.21
Clay Loam	0.28	0.25	0.21
Silty Clay Loam	0.37	0.32	0.26
Sandy Clay	0.14	0.13	0.12
Silty Clay	0.25	0.23	0.19
Clay		0.13 – 0.29	

[a] The values shown are estimated averages of broad ranges of specific-soil values. When a texture is near the borderline of two texture classes, use the average of the two K values. For specific soils, Soil Conservation Service K-value tables will provide much greater accuracy. (Stewart et al. 1975).

Table 5.4 Interception Storage for Major Crops		
Crop	**Density**	**CINTCP (cm)**
Corn	Heavy	0.25 - 0.30
Soybeans	Moderate	0.20 - 0.25
Wheat	Light	0.0 - 0.15
Oats	Light	0.0 - 0.15
Barley	Light	0.0 - 0.15
Potatoes	Light	0.0 - 0.15
Peanuts	Light	0.0 - 0.15
Cotton	Moderate	0.20 - 0.25
Tobacco	Moderate	0.20 - 0.25

Table 5.5 Values of the Erosion Equation's Topographic Factor, LS, for Specified Combinations of Slope Length and Steepness[a]

	Slope Length (feet)										
% Slope	**25**	**50**	**75**	**100**	**150**	**200**	**300**	**400**	**500**	**600**	**800**
0.5	.07	.08	.09	.10	.11	.12	.14	.15	.16	.17	.19
1	.09	.10	.12	.13	.15	.16	.18	.20	.21	.22	.24
2	.13	.16	.19	.20	.23	.25	.28	.30	.33	.34	.38
3	.19	.23	.26	.29	.33	.35	.40	.44	.47	.49	.54
4	.23	.30	.36	.40	.47	.53	.62	.70	.76	.82	.92
5	.27	.38	.46	.54	.66	.76	.93	1.1	1.2	1.3	1.4
6	.34	.48	.58	.67	.82	.95	1.2	1.4	1.5	1.7	1.9
8	.50	.70	.86	.99	1.2	1.4	1.7	2.0	2.2	2.4	2.8
10	.69	.97	1.2	1.4	1.7	1.9	2.4	2.7	3.1	3.4	3.9
12	.90	1.3	1.6	1.8	2.2	2.6	3.1	3.6	4.0	4.4	5.1
14	1.2	1.6	2.0	2.3	2.8	3.3	4.0	4.6	5.1	5.6	6.5
16	1.4	2.0	2.5	2.8	3.5	4.0	4.9	5.7	6.4	7.0	8.0
18	1.7	2.4	3.0	3.4	4.2	4.9	5.7	6.4	7.0	8.0	9.0
20	2.0	2.9	3.5	4.1	5.0	5.8	7.0	8.2	9.1	10.0	12.0
25	3.0	4.2	5.1	5.9	7.2	8.3	10.0	12.0	13.0	14.0	17.0
30	4.0	5.6	6.9	8.0	9.7	11.0	14.0	16.0	18.0	20.0	23.0
40	6.3	9.0	11.0	13.0	16.0	18.0	22.0	25.0	28.0	31.0	—
50	8.9	13.0	15.0	18.0	22.0	25.0	31.0	—	—	—	—
60	12.0	16.0	20.0	23.0	28.0	—	—	—	—	—	–

[a]Values given for slopes longer than 300 feet or steeper than 18% are extrapolations beyond the range of the research data, and therefore, less certain than others. (Stewart et al. 1975).

Table 5.6 Values of Support-practice Factor, P[a]

	Land Slope (percent)				
Practice	**1.1-2.0**	**2.1-7.0**	**7.1-12.0**	**12.1-18.0**	**18.1-24.0**
	(Factor P)				
Contouring (P_c)	0.60	0.50	0.60	0.80	0.90

Table 5.6	Values of Support-practice Factor, P[a]				
	Land Slope (percent)				
Practice	**1.1-2.0**	**2.1-7.0**	**7.1-12.0**	**12.1-18.0**	**18.1-24.0**
	(Factor P)				
Contour Strip cropping (P_{sc})[b]					
R-R-M-M	0.30	0.25	0.30	0.40	0.45
R-W-M-M	0.30	0.25	0.30	0.40	0.45
R-R-W-M	0.45	0.38	0.45	0.60	0.68
R-W	0.52	0.44	0.52	0.70	0.90
R-O	0.60	0.50	0.60	0.80	0.90
Contour listing or ridge					
planting (P_{cl})	0.30	0.25	0.30	0.40	0.45
Contour terracing					
(P_t)[c]	[d] $0.6\sqrt{n}$	$0.5\sqrt{n}$	$0.6\sqrt{n}$	$0.8\sqrt{n}$	$0.9\sqrt{n}$
No support practice	1.0	1.0	1.0	1.0	1.0

[a] (Stewart et al. 1975)

[b] R = rowcrop, W = fall-seeded grain, O = spring-seeded grain, M = meadow. The crops are grown in rotation and so arranged on the field that rowcrop strips are always separated by a meadow or winter-grain strip.

[c]These P_t values estimate the amount of soil eroded to the terrace channels and are used for conservation planning. For prediction of off-field sediment, the P_t values are multiplied by 0.2.

[d]n = number of approximately equal-length intervals into which the field slope is divided by the terraces. Tillage operations must be parallel to the terraces.

Table 5.7	Generalized Values of the Cover and Management Factor, C, in the 37 States East of the Rocky Mountains[a,b]		
Line Crop, Rotation, and Management [c] No.		**Productivity Level [d]**	
		High	**Mod.**
		C Value	
Base value: continuous fallow, tilled up and down		**1.00**	**1.00**
Corn			
1	C, RdR, fall TP, conv (1)	0.54	0.62
2	C, RdR, spring TP, conv (1)	.50	.59

Table 5.7 Generalized Values of the Cover and Management Factor, C, in the 37 States East of the Rocky Mountains[a,b]

Line Crop, Rotation, and Management [c] No.		**Productivity Level [d]**	
		High	**Mod.**
		C Value	
Base value: continuous fallow, tilled up and down		**1.00**	**1.00**
3	C, RdL, fall TP, conv (1)	.42	.52
4	C, RdR, wc seeding, spring TP, conv (1)	.40	.49
5	C, RdL, standing, spring TP, conv (1)	.38	.48
6	C, fall shred stalks, spring TP, conv (1)	.35	.44
7	C(silage)-W(RdL, fall TP) (2)	.31	.35
8	C,RdL, fall chisel, spring disk, 40-30% rc(1)	.24	.30
9	C(silage),W wc seeding, no-till pl in c-k(1)	.20	.24
10	C(RdL)-W(RdL, spring TP) (2)	.20	.28
11	C, fall shred stalks, chisel pl, 40-30% rc(1)	.19	.26
12	C-C-C-W-M, RdL, TP for C, disk for W (6)	.17	.23
13	C, RdL, strip till row zones, 55-40% rc (1)	.16	.24
14	C-C-C-W-M-M, RdL, TP for C, disk for W (6)	.14	.20
15	C-C-W-M, RdL, TP for C, disk for W (4)	.12	.17
16	C, fall shred, no-till pl, 70-50% rc (1)	.11	.18
17	C-C-W-M-M, RdL, TP for C, disk for W (5)	.087	.14
18	C-C-C-W-M, RdL, no-till pl 2nd & 3rd C (5)	.076	.13
19	C-C-W-M, RdL, no-till pl 2nd C (4)	.068	.11
20	C, no-till pl in c-k wheat, 90-70% rc (1)	.062	.14
21	C-C-C-W-M-M, no-till pl 2nd & 3rd C (6)	.061	.11
22	C-W-M, RdL, TP for C, disk for W (3)	.055	.095
23	C-C-W-M-M, RdL, no-till pl 2nd C (5)	.051	.094
24	C-W-M-M, RdL, TP for C, disk for W (4)	.039	.074
25	C-W-M-M-M, RdL, TP for C, disk for W (5)	.032	.061
26	C, no-till pl in c-k sod, 95-80% rc (1)	.017	.053
Cotton[e]			
27	Cot, conv (Western Plains) (1)	0.42	0.49

Table 5.7 Generalized Values of the Cover and Management Factor, C, in the 37 States East of the Rocky Mountains[a,b]

Line Crop, Rotation, and Management [c] No.		Productivity Level [d] C Value High	Productivity Level [d] C Value Mod.
Base value: continuous fallow, tilled up and down		**1.00**	**1.00**
28	Cot, conv (South) (1)	.34	.40
Meadow			
29	Grass & Legume mix	.004	0.01
30	Alfalfa, lespedeza or Sericia	.020	
31	Sweet clover	.025	
Sorghum, grain (Western Plains)[e]			
32	RdL, spring TP, conv (1)	0.43	0.53
33	No-till pl in shredded 70-50% rc	.11	.18
Soybeans[e]			
34	B, RdL, spring TP, conv (1)	0.48	0.54
35	C-B, TP annually, conv (2)	.43	.51
36	B, no-till pl	.22	.28
37	C-B, no-till pl, fall shred C stalks (2)	.18	.22
Wheat			
38	W-F, fall TP after W (2)	0.38	
39	W-F, stubble mulch, 500 lbs rc (2)	.32	
40	W-F, stubble mulch, 1000 lbs rc (2)	.21	
41	Spring W, RdL, Sept TP, conv (N&S Dak) (1)	.23	
42	Winter W, RdL, Aug TP, conv (Kansas) (1)	.19	
43	Spring W, stubble mulch, 750 lbs rc (1)	.15	
44	Spring W, stubble mulch, 1250 lbs rc (1)	.12	
45	Winter W, stubble mulch, 750 lbs rc (1)	.11	
46	Winter W, stubble mulch, 1250 lbs rc (1)	.10	
47	W-M, conv (2)	.054	
48	W-M-M, conv (3)	.026	

Table 5.7 Generalized Values of the Cover and Management Factor, C, in the 37 States East of the Rocky Mountains[a,b]

Line Crop, Rotation, and Management [c] No.		Productivity Level [d] High C Value	Productivity Level [d] Mod. C Value
Base value: continuous fallow, tilled up and down		**1.00**	**1.00**
49	W-M-M-M, conv (4)	.021	

[a] This table is for illustrative purposes only and is not a complete list of cropping systems or potential practices. Values of C differ with rainfall pattern and planting dates. These generalized values show approximately the relative erosion-reducing effectiveness of various crop systems, but locationally derived C values should be used for conservation planning at the field level. Tables of local values are available from the Soil Conservation Service.
[b] (Stewart et al. 1975)
[c] Numbers in parentheses indicate number of years in the rotation cycle. No. (1) designates a continuous one-crop system.
[d] High level is exemplified by long-term yield averages greater than 75 bu. corn or 3 tons grass-and-legume hay; or cotton management that regularly provides good stands and growth.
[e] Grain sorghum, soybeans, or cotton may be substituted for corn in lines 12, 14, 17-19, 21-25 to estimate C values for sod-based rotations.

Abbreviations defined:
B - soybeans
F - fallow
C - Corn
M - grass & legume hay
c-k - chemically killed
pl - plantconv - conventional
W - wheat
cot - cotton
we - cover
lbs rc - pounds of crop residue per acre remaining on surface after new crop seeding
% rc - percentage
7-50% rc - 70% cover for C values in first column; 50% for second column
RdR - residues (corn stover, straw, etc.) removed or burned
RdL - all residues left on field (on surface or incorporated)
TP - turn plowed (upper 5 or more inches of soil inverted, covering residues

Table 5.8 Mean Storm Duration* (TR) Values for Selected Cities

	Storm Duration (hrs)			Storm Duration (hrs)	
Location	**Mean Annual**	**Summer (June-Sept)**	**Location**	**Mean Annual**	**Summer (June-Sept)**
Great Lakes			Southeast		
Champaign-Urbana,IL	6.1	4.6	Greensboro, NC	5.0	3.6
Chicago, IL	5.7	4.5	Columbia, SC	4.5	3.5

Table 5.8 Mean Storm Duration* (TR) Values for Selected Cities

	Storm Duration (hrs)			Storm Duration (hrs)	
Location	**Mean Annual**	**Summer (June-Sept)**	**Location**	**Mean Annual**	**Summer (June-Sept)**
Davenport, IA	6.6	5.3	Atlanta, GA	8.0	6.2
Detroit, MI	4.4	3.1	Birmingham, AL	7.2	5.0
Louisville, KY	6.7	4.5	Gainesville, FL	7.6	6.6
Minneapolis, MN	6.0	4.5	Tampa, FL	3.6	3.1
Stubenville, OH	7.0	5.9			
Toledo, OH	5.0	3.7	Rocky Mountains		
Zanesville, OH	6.1	4.3	Denver, CO (8 Yr)	4.3	3.2
Lansing, MI (30 Yr)	5.6	4.2	Denver, CO (25 Yr)	4.8	3.2
Lansing, MI (21 Yr)	6.2	5.1	Denver, CO (24 Yr)	9.1	4.4
			Rapid City, SD	8.0	6.1
Lower Mississippi Valley			Salt Lake City, UT	4.5	2.8
Memphis, TN	6.9	4.7	Salt Lake City, UT	7.8	6.8
New Orleans, LA	6.9	5.0			
Shreveport, LA (17)	7.8	5.3	California		
Lake Charles, LA	7.7	5.9	Oakland, CA	4.3	2.9
			San Francisco, CA	5.9	11.2
Texas and Southwest					
Abilene, TX	4.2	3.3	Northeast		
Austin, TX	4.0	3.3	Caribou, ME	5.8	4.4
Brownsville, TX	3.5	2.8	Boston, MA	6.1	4.2
Dallas, TX	4.2	3.2	Lake George, NY	5.4	4.5
El Paso, TX	3.3	2.6	Kingston, NY	7.0	5.0
Waco, TX	4.2	3.3	Poughkeepsie, NY	6.9	4.9
Phoenix, AZ	3.2	2.4	New York City, NY	6.7	4.8
			Mineola, LI, NY (2)	5.6	4.0
Northwest			Upton LI, NY	6.3	4.6

Table 5.8 Mean Storm Duration* (TR) Values for Selected Cities

	Storm Duration (hrs)			Storm Duration (hrs)	
Location	**Mean Annual**	**Summer (June-Sept)**	**Location**	**Mean Annual**	**Summer (June-Sept)**
Portland, OR (25yr)	5.4	4.5	Wantagh, LI, NY (2)	5.6	4.0
Portland, OR (10yr)	15.5	9.4	Long Island, NY	4.2	3.4
Eugene, OR	29.2	15.0	Washington, DC	5.9	4.1
Seattle, WA	21.5	12.7	Baltimore, MD	6.0	4.2

Source: (U.S. Environmental Protection Agency 1986)

* These values may be misleading in arid regions or regions with pronounced seasonal rainfall patterns.

Table 5.9 Agronomic Data for Major Agricultural Crops in the United States

Crop	Representative States of Major States Production[a]	Planting Window, Month, Day (Days from (Julian Day)[b] Planting)	Crop Emergency (Days from Planting)	Crop Maturity Month, Day (Julian Day)[b]	Harvest Window,Yield/ Acre 1977-1979[c]	Average Rooting Depth (cm)	Range of Active Plant
Corn	IA, IL, IN, NE, OH	April 25 (115) to June 15 (166)	5-15 5-15	110-130 110-130	Sept. 25 (268 to Dec. 10 (344)	110 bu	60-120
Soybeans	IA, IL, IN,MS,OH	May 1 (121) to June 25 (176)	5-15	110-130	Sept. 15 (258) to Dec. 10 (344)	35 bu	30-60
Cotton	TX, MS, CA, AZ, AR	March 1 (60) to May 25 (145)[TX to June 20 (171)]	5-15	110-130	Sept. 1 (244) to Jan. 15 (015) [TX Aug. 1 (213) to Dec. 20 (354)]	670 lbs	30-90
Wheat	KS, OK, CA, ND, MT, WA, MN, ID	Aug. 15 (227) to Oct. 25 (298) [WA to Nov. 20 (324),CA to Feb. 15 (046)]	5-15	200-225	June 15 (166) to Sept. 20 (263)	40 bu	15-30
Potatoes	Long Island NY, ME, ID, WA, CA, OR	April 1 (091) to May 1 (121)	5-15	150-170	Sept. 1 (244) to Oct. 1 (274)	335 cwt	15-45
Peanuts	GA, TX, AL, NC, VA	April 5 (095) to June 5 (156) [TX Mar. 31 (090) to July 20 (201)]	5-15	150-175	Aug. 10 (222) to Dec. 15 (349)	2550 lbs	30-60
Tobacco	NC, SC, TN, KY, VA	April 5 (095) to June 20 (171)	Planted in Field as Seedling	120-150	July 1 (182) to Oct. 1 (274)	2000 lbs	30-60

Table 5.9 Agronomic Data for Major Agricultural Crops in the United States

Crop	Representative States of Major States Production[a]	Planting Window, Month, Day (Days from (Julian Day)[b] Planting)	Crop Emergency (Days from Planting)	Crop Maturity Month, Day (Julian Day)[b]	Harvest Window,Yield/ Acre 1977-1979[c]	Average Rooting Depth (cm)	Range of Active Plant
Grain Sorghum	TX, KS, NE	TX Mar. 1 (060) to July 1 (182) KS, NE May 5 (125) to July 1 (182)	5-15	120-150 to Nov. 20 (324)	TX July 1 (182) KS, NE Sept. 20 (263) to Dec. 1 (335)	62 bu	15-30

[a](Bay and Bellinghausen 1979)

[b](Burkhead et al. 1972)

(Kirkbride 1980)

Table 5.10 Runoff Curve Numbers for Hydrologic Soil-cover Complexes[a] (Antecedent Moisture Condition II, and $I_a = 0.2\ S$)

	Cover		Hydraulic Soil Group			
Land Use	**Treatment or Practice**	**Hydrologic Condition**	**A**	**B**	**C**	**D**
Fallow Row crops	Straight Row	—	77	86	91	94
	Straight Row	Poor	72	81	88	91
	Straight row	Good	67	78	85	89
	Contoured	Poor	70	79	84	88
	Contoured	Good	65	75	82	86
	Contoured and terraced	Poor	66	74	80	82
	Contoured and terraced	Good	62	71	78	81
Small grain	Straight row	Poor	65	76	84	88
	Straight row	Good	63	75	83	87
	Contoured	Poor	63	74	83	87
	Contoured	Good	61	73	81	84
	Contoured and terraced	Poor	61	72	79	82
	Contoured and terraced	Good	59	70	78	81
Close-seeded legumes[b] or rotation meadow	Straight row	Poor	66	77	85	89
	Straight row	Good	58	72	81	85
	Contoured	Poor	64	75	83	85
	Contoured	Good	55	69	78	83
	Contoured and terraced	Poor	63	73	80	83
	Contoured and terraced	Good	51	67	76	80
Pasture or range		Poor	68	79	86	89
		Fair	49	69	79	84
		Good	39	61	74	80
	Contoured	Poor	47	67	81	88
	Contoured	Fair	25	59	75	83
	Contoured	Good	6	35	70	79

Table 5.10 Runoff Curve Numbers for Hydrologic Soil-cover Complexes[a] (Antecedent Moisture Condition II, and $I_a = 0.2\ S$)

	Cover		Hydraulic Soil Group			
Land Use	**Treatment or Practice**	**Hydrologic Condition**	**A**	**B**	**C**	**D**
Meadow		Good	30	58	71	78
Woods		Poor	45	66	77	83
		Fair	36	60	73	79
		Good	25	55	70	77
Farmsteads		—	59	74	82	86
Roads (dirt)[c]		—	72	82	87	89
(hard surface)[c]		—	74	84	90	92

[a] (Mockus 1972)
[b] Close-drilled or broadcast.
[c] Including right-of-way.

Table 5.11 Method for Converting Crop Yields to Residue[a]

Crop[b]	**Straw/Grain Ratio**	**Bushel Weight (lbs)**
Barley	1.5	48
Corn	1.0	56
Oats	2.0	32
Rice	1.5	45
Rye	1.5	56
Sorghum	1.0	56
Soybeans	1.5	60
Winter wheat	1.7	60
Spring Wheat	1.3	60

Table 5.11 Method for Converting Crop Yields to Residue[a]		
Crop[b]	**Straw/Grain Ratio**	**Bushel Weight (lbs)**

[a] Crop residue = (straw/grain ratio) *x* (bushel weight in lb/bu) *x* (crop yield in bu/acre).

[b] (Knisel 1980)

Table 5.12 Residue Remaining from Tillage Operations[a]	
Tillage[b] Operation	**Residue Remaining(%)**
Chisel Plow	65
Rod weeder	90
Light disk	70
Heavy disk	30
Moldboard plow	10
Till plant	80
Fluted coulter	90
V Sweep	90

[a] Crop residue remaining = (crop residue from Table 5.11) ×(tillage factor(s).

[b] (Knisel 1980)

Table 5.13 Reduction in Runoff Curve Numbers Caused by Conservation Tillage and Residue Management[a]			
Large Residue Crop[b] (lb/acre)	**Medium Residue Crop[b] (lb/acre)**	**Surface Covered by Residue (%)**	**Reductive in Curve Number[d] (%)**
0	0	0	0
400	150	10	0
700	300	19	2
1,100	450	28	4
1,500	700	37	6
2,000	950	46	8
2,500	1,200	55	10
6,200	3,500	90	10

[a] (Knisel 1980)

[b] Large-residue crop (corn).

[c] Medium residue crop (wheat, oats, barley, rye, sorghum, soybeans).

[d] Percent reduction in curve numbers can be interpolated linearly. Only apply 0 to ½ of these percent reductions to CNs for contouring and terracing practices when they are used in conjunction with conservation tillage.

Table 5.14 Values for Estimating Wfmax in Exponential Foliar Model

Crop	Yield[a] (Bu/Ac)	Bushel[a] dry wt.(lbs/Bu)	Straw/Grain Ratio	Units Conversion Factor	WFMAX
Corn	110	56	1.0	1.1214×10^{-4}	1.38
Sorghum	62	56	1.0	1.1214×10^{-4}	0.78
Soybeans	35	60	1.5	1.1214×10^{-4}	0.59
Winter wheat	40	60	1.7	1.1214×10^{-4}	0.72

[a] 10-year average

Table 5.15 Pesticide Soil Application Methods and Distribution

Method of Application	Common Procedure	Distribution	CAM
Broadcast	Spread as dry granules or spray over the whole surface	Remains on the soil surface	4
Disked-in	Disking after broadcast application	Assume uniform distribution to tillage depth	1 or 6
Chisel-plowed	Chisel plowing after broadcast	Assume linear distribution to tillage depth	4
Surface banded	Spread as dry granules or a spray over a fraction of the row	Remains on soil surface	4
Banded - incorporated	Spread as dry granules or a spray over a fraction of the row and incorporated in planting operation	Assume uniform distribution to depth of incorporation	7

Table 5.16 Maximum Canopy Height at Crop Maturation

Crop	Height (cm)	Reference
Barley	20 - 50	A

Grain Sorghum	90 - 110	B
Alfalfa	10 - 50	A
Corn	80 - 300	A
Potatoes	30 - 60	A
Soybeans	90 - 110	B
Sugarcane	100 - 400	A

References:
A. (Szeicz et al. 1969)
B. (Smith et al. 1978)

Table 5.17 Degradation Rate Constants of Selected Pesticides on FOLIAGE[a]

Class	**Group**	**Decay Rate (days^{-1})**
Organochlorine	Fast (aldrin, dieldrin, ethylan, heptachlor, lindane, methoxychlor).	0.231 - 0.1386
	Slow (chlordane, DDT, endrin, toxaphene).	0.1195 - 0.0510
Organophosphate	Fast (acephate, chlorphyrifos-methyl, cyanophenphos, diazinon, depterex, ethion, fenitrothion, leptophos, malathion, methidathion, methyl parathion, phorate, phosdrin, phosphamidon, quinalphos, alithion, tokuthion, triazophos, trithion).	0.2772 - 0.3013
	Slow (azinphosmethyl, demeton, dimethoate, EPN, phosalone).	0.1925 - 0.0541
Carbamate	Fast (carbofuran)	0.630
	Slow (carbaryl)	0.1260 - 0.0855
Pyrethroid	(permethrin)	0.0196
Pyridine	(pichloram)	0.0866
Benzoic acid	(dicamba)	0.0745

[a] (Knisel 1980)

Table 5.18 Estimated Values of Henry's Constant for Selected Pesticides

Compound	Henry's Constant (dimensionless)	References
Alachlor	1.3E-06	A
Aldrin	6.3E-04	D
Anthracene	4.4E-05	D
Atrazine	2.5E-07	A
Bentazon	2.0E-10	A
Bromacil	3.7E-08	C
Butylate	3.3E-03	A
Carbaryl	1.1E-05	A
Carbofuran	1.4E-07	A
Chlorpyrifos	1.2E-03	A
Chrysene	4.7E-05	D
Cyanazine	1.2E-10	A
DDT	2.0E-03	C
Diazinon	5.0E-05	C
Dicamba	3.3E-08	A
Dieldrin	6.7E-04	C
Diuron	5.4E-08	C
Endrin	1.8E-05	D
EPTC	5.9E-04	C
Ethoprophos	6.0E-06	C
Fenitrothion	6.0E-06	B
Fonofos	2.1E-04	A
Heptachlor	1.7E-02	D
Lindane	1.3E-04	B
Linuron	2.7E-06	A
Malathion	2.4E-06	B
Methomyl	4.3E-08	A
Methyl Parathion	4.4E-06	A

Table 5.18 Estimated Values of Henry's Constant for Selected Pesticides

Compound	Henry's Constant (dimensionless)	References
Metolachlor	3.8E-07	A
Metribuzin	9.8E-08	A
Monuron	7.6E-09	C
Napropamide	7.9E-07	C
Parathion	6.1E-06	C
Permethrin	6.2E-05	A
Picloram	1.9E-08	B
Prometryne	5.6E-07	C
Simazine	1.3E-08	A
Terbufos	1.1E-03	A
Toxaphene	2.3E+00	A
Triallate	7.9E-04	C
Trichlorfon	1.5E-09	B
Trifluralin	6.7E-03	A
2,4-D (acid)	5.6E-09	A
2,4,5-T (acid)	7.2E-09	B

References:
A. (Donigian et al. 1986)
B. (Spencer et al. 1984)
C. (Jury et al. 1984)
D. (Schnoor et al. 1987)

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Actellic	pirimiphosmethyl	5	a	X					274	b	3.28×10^{-7}	5	18		
Alachlor	alachlor	220	b	X					269.9	b	1.47×10^{-5}	220	815	.0384	f
Antor	diethatyl ethyl	105	a		X				311.5	c	6.07×10^{-6}	105	337	.0099-.0173	g
Aresin	monol inuron	735	a		X				214.6	b	6.17×10^{-6}	735	3430		
Balan	benefin	70	b		X				335.3	b	3.76×10^{-6}	70	209	0.3349	f
Basalin	fluchloralin	0.7	b		X				355.7	b	3.55×10^{-8}	0.7	2	0.0169	f
Baygon	propoxur	2000	a	X					209	b	1.72×10^{-4}	2000	9600		
Baygon Meb	plifenate	50	a	X					336.2	d	2.68×10^{-6}	50	149		
Bayleton	triadimefon	70	a			X			267.45	d	4.72×10^{-6}	70	262		
Baythion	phoxim	7	b	X					298	b	4.23×10^{-7}	7	24		
Baythion C	chlorphoxim	1.7	a	X					301.45	d	1.02×10^{-7}	1.7	5.6		
Betasan	bensulide	25	c		X				397.5	b	1.13×10^{-6}	25	63		
Bromophos	bromophos	40	a	X					366	b	1.97×10^{-6}	40	109	.0198	f

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Butachlor	butachlor	23	a		X				312	e	1.33×10^{-6}	23	74		
Bux	bufencarb	1	b	X					221.3	b	8.14×10^{-8}	1.0	5		
Carbamult	promecarb	92	a	X					207	d	8.01×10^{-6}	92	444		
Carbyne	barban	11	c		X				258.1	b	7.70×10^{-7}	11	43	.0347	g
Chlordimeform	chlordimeform	250	a	X				X	196.7	b	2.30×10^{-5}	250	1270		
Chlorfenvinphos	chlorfenvinphos	110	a	X					359.5	b	5.51×10^{-6}	110	306	.0055	f
Chloro IPC	chlorpropham	108	b		X				213.7	b	9.11×10^{-6}	108	505	.0058-.00267	g
Chlorpyrifos	chlorpyrifos	2	b	X					350.5	b	1.03×10^{-7}	2.0	6		
Co-Ral	coumaphos	1.5	b	X					362.8	b	7.45×10^{-8}	1.5	4		
Counter	terbufos	15	a	X			X		288	d	9.38×10^{-7}	15	52		
DNOC	DNOC	130	a	X	X	X			198.1	b	1.18×10^{-5}	130	656		
Dichlorprop	dichlorprop	350	a		X				235	b	2.68×10^{-5}	350	1490	.0578-.0866	f
Dimetan	dimetan	30000	b	X					197.3	b	2.74×10^{-3}	30000	152000		

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Dimethoate	dimethoate	X=25000	a	X					229.1	b	1.97×10^{-3}	25000	109000	.0057	
Dinitramine	dinitroamine	1	a		X				322.2	c	5.60×10^{-8}	1	3	.0193-.0856	f
Dinoseb	dinoseb	52	c		X				240.2	b	3.90×10^{-6}	52	217	.0462-.0231	g
Dazomet	dazomet	1200	b		X	X	X		162.3	b	1.33×10^{-4}	1200	7390		
Devrinol	napropamide	73	a		X				271.36		4.85×10^{-6}	73	269		
Elocron	dioxacarb	6000	a	X					223	b	4.85×10^{-4}	6000	26900	.3465-.0248	f
Evik	ametryn	185	a		X				227	b	1.47×10^{-5}	185	815	.0231-.0077	g
Far-Go	triallate	4	b			X			304.6	b	2.37×10^{-7}	4	13	.0231-.0713	g
Fongarid	furalaxyl	230	a			X			301	d	1.38×10^{-5}	230	764		
Fornothion	fornothion	2600	a	X				X	257	b	1.82×10^{-4}	2600	10100		
Fuji-one	isoprothiolane	48	a	X		X			290	d	2.98×10^{-6}	48	166		
Gardona	tetrachlorvinphos	11	b	X					366	b	5.42×10^{-7}	11	30	.1732-1386	
Gesaran	methoprotryne	320	a		X				271	b	2.13×10^{-5}	320	1180		

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Goal	oxyfluorfen	0.1	c		X				361.7	c	4.98×10^{-9}	0.1	0.3	.0231-.0173	c
Guthion	azinphos-methyl	29	a	X					317.3	b	1.65×10^{-5}	29	91	.0533-.0014	f
Hoelon	diclofop methyl	30	a		X				340.9	d	1.59×10^{-6}	30	88		
Imidan	phosmet	25	b	X					317.3	b	1.42×10^{-6}	25	79		
IPC	propham	250	b		X				179.2	b	2.51×10^{-5}	250	1400	.0347-.0116	g
Linuron	linuron	75	a		X				249.1	b	5.42×10^{-6}	75	300	.0280-.0039	f
Malathion	malathion	145	a	X					330.4	b	7.91×10^{-6}	145	439	2.91-.4152	f
Mecoprop	mecoprop	620	a		X				214.6	b	5.21×10^{-5}	620	2890		
MEMC	MEMC	50000	a			X			295	d	3.05×10^{-3}	50000	169000		
Merpelan AZ	isocarbamid	13000	a		X				185	d	1.27×10^{-3}	13000	70300		
Mesoranil	aziprotryn	75	b		X				225	b	6.01×10^{-6}	75	333		
Mesurol	mercaptodimethur	2.7×10^{7}	a	X					225.3	b	2.16	2.7×10^{7}	1.2×10^{8}		
Methomyl	methomyl	58000	a	X					162.2	b	6.44×10^{-3}	58000	358000		

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Methoxychlor	methoxychlor	0.1	b	X					345.7	b	5.21×10	0.1	0.3	.0046-.0033	f
Meth-Parathion	methyl Parathion	$\bar{X}$ = 57.5	a	X					263.2	b	3.94×10^{-6}	57.5	219	.2207	f
Nemacur	fenamiphos	400	a			X			300	b	2.38×10^{-5}	400	1320		
Nortron	ethofumesate	110	a		X				286	d	6.93×10^{-6}	110	385		
Orthene	acephate	6.5×10^{5}	b	X					183.2	b	0.06 6.5×10^{5}	650000	3550000		
Oxamyl	oxamyl	2.8×10^{5}	a	X			X	X	219	b	0.023 2.8×10^{5}	280000	1280000	.0354-.0646	f
Parathion	parathion	24	b	X					291.3	b	1.48×10^{-6}	24	82	.2962-.0046	f
Patoran	metabromuron	330	a		X				258.9	d	2.30×10^{-5}	330	1280	.0234	f
Phorate	phorate	50	b	X					260.4	b	3.46×10^{-6}	50	192	.0363-.0040	f
Propachlor	propachlor	580	c		X				211.7	b	4.94×10^{-5}	580	2740	.0231-.0139	g
Propanil	propanil	500	c		X				218	b	4.13×10^{-5}	500	2290	.693-.231	g
Prowl	pendimethalin	0.5	c		X				281.3	c	3.20×10^{-8}	0.5	1.8		

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Prynachlor	prynachlor	500	a		X				221.7	b	4.06×10^{-5}	500	2260		
Quinalphos	quinalphos	22	a	X				X	298	d	1.33×10^{-6}	22	74		
Ronstar	oxadiazon	0.7	b		X				345.23	b	3.65×10^{-8}	0.7	2.0		
Sancap	dipropetryn	16	a		X				255.4	b	1.13×10^{-6}	16	63		
Semeron	desmetryn	580	a		X				213	b	4.91×10^{-5}	580	2720		
Supracide	methidathion	240	a	X				X	302	b	1.43×10^{-5}	240	795	.0495-.0108	f
Tachigareu	hymexazol	85000	a			X			99.05	b	0.02	85000	858000		
Temik	aldicarb	6000	a	X			X	X	190.3	b	5.68×10^{-4}	6000	31500	.0322-.0116	f
Tolban	profluralin	0.1	a		X				347.3	c	5.19×10^{-9}	0.1	0.3	.0049	f
Trifluralin	trifluralin	24	b		X				335.3	b	1.29×10^{-6}	24	71	.0956-.0026	f
Tsumacide	MTMC	2600	a	X					165	d	2.84×10^{-4}	2600	15800		
Tordon	picloram	430	c		X				241.5	b	3.21×10^{-5}	430	1780	.0354-.0019	f
Toxaphene	toxaphene	3	b	X					413	b	1.31×10^{-7}	3	7	.0046	f

Table 5.19 Physical Characteristics of Selected Pesticides for Use in Development of Partition Coefficients (Using Water Solubility) and Reported Degradation Rate Constants in Soil Root Zone

				Mode of Action							Partitioning Model				
Chemical	Common Name	Solubility in water (20 - 25°C) (mg/l)	Reference	Insecticide	Herbicide	Fungicide	Nematocide	Acaricide	Molecular weight (g)	Reference	PCMC1 (mole fraction)	PMCM2 (mg/l)	PCMC3 (µm/l)	Degradation Rate Constant in Soil Root Zone ($days^{-1}$)	Reference
Trichlorfon	trichlorfon	120000	a	X					257.35	d	8.40×10^{-3}	120000	466000		

Calculations for the Karickhoff and Chiou partitioning equations are:

PCMC1:

- millimole solubility (MMS) = (ppm solubility) / [molecular weight (g)]
- molar solubility (MS) = MMS / 10^3
- mole fraction = MS / [55.5 (molar conc. water)]

Chiou:

- millimole solubility (MMS) = (ppm solubility) / [molecular weight (g)]
- µm/l = MMS × 10^6 / 10^3

References:

[a] Farm Chemicals Handbook (Meister Publishing Company 1981)
[b] Pesticide Manual (Martin 1968)
[c] Herbicide Handbook (Mullison 1979)
[d] Calculations based on information from Farm Chemicals Handbook (Meister Publishing Company 1981).
[e] (Beroza et al. 1981)
[f] (Nash 1980)
[g] (Stewart et al. 1975)

Table 5.20 Octanol Water Distribution Coefficients (Log K_{ow}) and Soil Degradation Rate Constants for Selected Chemicals

Chemical Name	Log K_{ow}[b]	Degradation Rate Constant (days^{-1})	Reference
Alachlor	2.78	0.0384	A
Aldicarb	0.70	0.0322 - 0.0116	A
Altosid	2.25		
Atrazine	2.45	0.0149 - 0.0063	A
Benomyl	2.42	0.1486 - 0.0023	A
Bifenox	2.24	0.1420	A
Bromacil	2.02		
Captan	2.35		
Carbaryl	2.56	0.1196 - 0.0768	A
Carbofuran	2.44	0.0768 - 0.0079	A
Chloramben	1.11		
Chlordane	4.47	0.0020 - 0.0007	
Chloroacetic Acid	-0.39		
Chloropropham	3.06	0.0058 - 0.00267	D
Chloropyrifos	4.97		
Cyanazine	2.24	0.0495	C
Dalapon	0.76	0.0462 - 0.0231	D
Dialifor	4.69		
Diazinon	3.02	0.0330 - 0.0067	A
Dicamba	0.48	0.2140 - 0.0197	A
Dichlobenil	2.90	0.0116 - 0.0039	
Dichlorofenthion	5.14		
2,4,-Dichlorophenoxy-acetic Acid	2.81	0.0693 - 0.0231	D
Dichloropropene	1.73		
Dicofol	3.54		
Dinoseb	2.30	0.0462 - 0.0231	D
Diuron	2.81	0.0035 - 0.0014	D

Table 5.20 Octanol Water Distribution Coefficients (Log K_{ow}) and Soil Degradation Rate Constants for Selected Chemicals

Chemical Name	Log K_{ow} [b]	Degradation Rate Constant (days^{-1})	Reference
Endrin	3.21		
Fenitrothion	3.36	0.1155 - 0.0578	A
Fluometuron	1.34	0.0231	C
Linuron	2.19	0.0280 - 0.0039	A
Malathion	2.89	02.91 - 0.4152	A
Methomyl	0.69		
Methoxychlor	5.08	0.0046 - 0.0033	A
Methyl Parathion	3.32	0.2207	A
Monolinuron	1.60		
Monuron	2.12	0.0046 - 0.0020	D
MSMA	-3.10		
Nitrofen	3.10		
Parathion	3.81	0.2961 - 0.0046	A
Permethrin	2.88	0.0396	E
Phorate	2.92	0.0363 - 0.0040	A
Phosalone	4.30		
Phosmet	2.83		
Picloram	0.30	0.0354 - 0.0019	A
Propachlor	1.61	0.0231 - 0.0139	D
Propanil	2.03	0.693 - 0.231	D
Propazine	2.94	0.0035 - 0.0017	D
Propoxur	1.45		
Ronnel	4.88		
Simazine	1.94	0.0539 - 0074	A
Terbacil	1.89		
Terbufos	2.22		
Toxaphene	3.27	0.0046	E

Table 5.20 Octanol Water Distribution Coefficients (Log K_{ow}) and Soil Degradation Rate Constants for Selected Chemicals

Chemical Name	Log K_{ow} [b]	Degradation Rate Constant ($days^{-1}$)	Reference
Trifluralin	4.75	0.0956 - 0.0026	A
Zineb	1.78	0.0512	A

[A] (Nash 1980)
[B] (Smith 1981)
[C] (Mullison 1979)
[D] (Stewart et al. 1975)
[E] (Smith and Carsel 1984)

Table 5.21 Albedo Factors of Natural Surfaces for Solar Radiation*

Surface	Reflectivity
Fresh Dry Snow	0.80-0.90
Clean, Stable Snow Cover	0.60-0.75
Old and Dirty Snow Cover	0.30-0.65
Dry Salt Cover	0.50
Lime	0.45
White Sand, Lime	0.30-0.40
Quartz Sand	0.35
Granite	0.15
Dark Clay, Wet	0.02-0.08
Dark Clay, Dry	0.16
Sand, Wet	0.09
Sand, Dry	0.18
Sand, Yellow	0.35
Bare Fields	0.12-0.25
Wet Plowed Field	0.05-0.14
Newly Plowed Field	0.17
Grass, Green	0.16-0.27
Grass, Dried	0.16-0.19
Grass, High Dense	0.18-0.20

Table 5.21 Albedo Factors of Natural Surfaces for Solar Radiation*	
Surface	**Reflectivity**
Prairie, Wet	0.22
Prairie, Dry	0.32
Stubble Fields	0.15-0.17
Grain Crops	0.10-0.25
Alfalfa, Lettuce, Beets, Potatoes	0.18-0.32
Coniferous Forest	0.10-0.15
Deciduous Forest	0.15-0.25
Forest with Melting Snow	0.20-0.30
Yellow Leaves (fall)	0.33-0.36
Desert, Dry Soils	0.20-0.35
Desert, Midday	0.15
Desert, Low Solar Altitude	0.35
Water (0°C to 30°C)[a]	0.02
Water (60°C)[a]	0.06
Water (85°C)[a]	0.58

References:
(Brutsaert 1982)
(van Wijk 1963)

[a] angle of solar incidence.

Table 5.22 Emissivity Values for Natural Surfaces at Normal Temperatures*	
Surface	**Emissivity**
Sand (dry-wet)	0.95-0.98
Mineral Soil (dry-wet)	0.95-0.97
Peat (dry-wet)	0.97-0.98
Firs	0.97
Tree Vegetation	0.96-0.97
Grassy Vegetation	0.96-0.98
Leaves	0.94-0.98

Table 5.22 Emissivity Values for Natural Surfaces at Normal Temperatures*	
Surface	**Emissivity**
Water	0.95
Snow (old)	0.97
Snow (fresh)	0.99

References:
(van Wijk 1963)
(Brutsaert 1982)

Table 5.23 Coefficients for Linear Regression Equations for Prediction of Soil Water Contents at Specific Matric Potentials[a]

Matric Coefficient	**Intercept a**	**Sand (%) b**	**Clay (%) c**	**Organic Matter (%) d**	**Bulk Density (g cm^{-3}) e**	**R^2**
-0.20	0.4180	-0.0021	0.0035	0.0232	-0.0859	0.75
-0.33	0.3486	-0.0018	0.0039	0.0228	-0.0738	0.78
-0.60	0.2819	-0.0014	0.0042	0.0216	-0.0612	0.78
-1.0	0.2352	-0.0012	0.0043	0.0202	-0.0517	0.76
-2.0	0.1837	-0.0009	0.0044	0.0181	-0.0407	0.74
-4.0	0.1426	-0.0007	0.0045	0.0160	-0.0315	0.71
-7.0	0.1155	-0.0005	0.0045	0.0143	-0.0253	0.69
-10.0	0.1005	-0.0004	0.0044	0.0133	-0.0218	0.67
-15.0	0.0854	-0.0004	0.0044	0.0122	-0.0182	0.66

[a] Rawls, W. J., U.S. Department of Agriculture, Agricultural Research Service, Beltsville, MD. Personal Communication.

Table 5.24 Thermal Properties of Some Soil and Reference Materials*

Material	**Water Content (%)**	**Heat Capacity (cal cm^{-3} °C^{-1})**	**Thermal Cond. (cal cm^{-1} °C^{-1} sec^{-1})**
Clay		1.44	0.00288
Light Soil w/Roots		0.09	0.00027
Wet Sandy Soil		0.64	0.0064
Dead Air		0.000312	0.00005

Table 5.24 Thermal Properties of Some Soil and Reference Materials*

Material	Water Content (%)	Heat Capacity (cal cm^{-3} °C^{-1})	Thermal Cond. (cal cm^{-1} °C^{-1} sec^{-1})
Hudson River Sand	4.5	0.2	0.0091
	18.1	0.336	0.03
Podunk Fine Sandy Loam	6.6	0.221	0.0012
	20.2	0.371	0.0026
Leonardtown Silt Loam	9.0	0.316	0.0018
	18.4	0.338	0.0021
Muck Soil	23.0	0.251	0.00076
	59.0	0.321	0.00108
Yolo Clay	0.0	0.236	0.0014
	29.0	0.72	0.0083
Granite Sandy Loam	0.0	0.291	0.0017
	22.7	0.706	0.0071
Fine Calcareous Loam	0.0	0.175	0.00079
	24.4	0.430	0.0048
Granitic Sand	0.0	0.269	0.00137
	13.1	0.636	0.0108
Barns Loam	5.1	0.29	0.00041
	26.0	0.35	0.00086
Chester Loam	2.0	0.32	0.00045
	13.4	0.37	0.00087
Herman Sandy Loam	1.3	0.30	0.00049
	13.4	0.37	0.00087
Kalkaska Loamy Sand	0.8	0.32	0.0006
	5.7	0.37	0.00124
Northway Silt Loam	6.6	0.38	0.0013
	22.5	0.636	0.0025
Fairbanks Silty Clay Loam	12.3	0.436	0.002
	25.4	0.625	0.0028

Table 5.24 Thermal Properties of Some Soil and Reference Materials*

Material	Water Content (%)	Heat Capacity (cal cm^{-3} °C^{-1})	Thermal Cond. (cal cm^{-1} °C^{-1} sec^{-1})
Dakota Sandy Loam	1.9	0.269	0.00059
	4.9	0.483	0.0054
Black Cotton Soil		0.336	0.00037

References:
(Rosenberg 1974)
(Kilmer 1982)

Table 5.25 Hydrologic Properties by Soil Texture[a]

	Range of Textural Properties (Percent)				
Texture Class	**Sand**	**Silt**	**Clay**	**Water Retained at -0.33 Bar Tension cm^3 cm^{-3}**	**Water Retained at -15.0 Bar Tension cm^3 cm^{-3}**
Sand	85-100	0-15	0-10	0.091[b] (0.018 - 0.164)[c]	0.033[b] (0.007 - 0.059)[c]
Loamy Sand	70-90	0-30	0-15	0.125 (0.060 - 0.190)	0.055 (0.019 - 0.091)
Sandy Loam	45-85	0-50	0-20	0.207 (0.126 - 0.288)	0.095 (0.031 - 0.159)
Loam	25-50	28-50	8-28	0.270 (0.195 - 0.345)	0.117 (0.069 - 0.165)
Silt Loam	0-50	50-100	8-28	0.330 (0.258 - 0.402)	0.133 (0.078 - 0.188)
Sandy Clay Loam	45-80	0-28	20-35	0.257 (0.186 - 0.324)	0.148 (0.085 - 0.211)
Clay Loam	20-45	15-55	28-50	0.318 (0.250 - 0.386)	0.197 (0.115 - 0.279)
Silty Clay Loam	0-20	40-73	28-40	0.366 (0.304 - 0.428)	0.208 (0.138 - 0.278)
Sandy Clay	45-65	0-20	35-55	0.339 (0.245 - 0.433)	0.239 (0.162 - 0.316)
Silty Clay	0-20	40-60	40-60	0.387 (0.332 - 0.442)	0.250 (0.193 - 0.307)
Clay	0-45	0-40	40-100	0.396 (0.326 - 0.466)	0.272 (0.208 - 0.336)

[a] (Rawls et al. 1982)
[b] Mean value.
[c] One standard deviation about the mean.

Table 5.26 Descriptive Statistics and Distribution Model for Field Capacity (Percent by Volume)

Original Data

Stratum(m)	Sample Size	Mean	Median	s.d.	CV(%)	Distribution Model		s.d.
						Transform	Mean	
Class A								
0.0-0.3	52	11.8	9.4	9.2	78	ln	2.25	0.65
0.3-0.6	50	9.6	8.1	7.9	82	ln	1.99	0.73
0.6-0.9	42	7.3	5.9	5.8	79	ln	1.73	0.73
0.9-1.2	39	7.1	5.8	5.0	70	ln	1.73	0.71
Class B								
0.0-0.3	456	19.5	19.1	8.3	42	s_U	0.316	0.13
0.3-0.6	454	18.8	18.8	7.4	39	s_U	0.311	0.12
0.6-0.9	435	18.7	18.7	7.1	39	s_U	0.298	0.11
0.9-1.2	373	17.5	17.5	7.6	43	s_U	0.288	0.12
Class C								
0.0-0.3	371	22.4	22.5	7.8	35	s_U	0.363	0.12
0.3-0.6	362	22.8	23.2	7.8	34	s_U	0.369	0.12
0.6-0.9	336	22.7	22.9	8.6	38	s_U	0.368	0.13
0.9-1.2	290	22.2	21.3	8.9	40	s_U	0.359	0.13
Class D								
0.0-0.3	230	24.1	24.2	9.1	38	s_U	0.387	0.14
0.3-0.6	208	26.1	26.3	9.3	36	s_U	0.419	0.14
0.6-0.9	178	25.0	25.6	8.2	33	s_U	0.403	0.13
0.9-1.2	146	24.1	24.4	8.1	33	s_U	0.390	0.12

CV = coefficient of variation
s.d. = standard deviation

Source: (Carsel et al. 1988)

Table 5.27 Descriptive Statistics and Distribution Model for Wilting Point (Percent by Volume)

Original Data								
						Distribution Model		
Stratum(m)	**Sample Size**	**Mean**	**Median**	**s.d.**	**CV(%)**	**Transform**	**Mean**	**s.d.**
Class A								
0.0-0.3	118	4.1	3.1	3.4	82	ln	1.83	0.64
0.3-0.6	119	3.2	2.3	2.4	75	ln	0.915	0.71
0.6-0.9	113	2.9	2.1	2.3	81	s_B	3.32	0.88
0.9-1.2	105	2.6	1.9	2.3	87	s_B	3.43	0.92
Class B								
0.0-0.3	880	9.0	8.7	4.0	45	s_U	0.150	0.066
0.3-0.6	883	9.4	9.3	4.3	46	s_U	0.156	0.071
0.6-0.9	866	9.1	8.9	4.4	48	s_U	0.151	0.072
0.6-1.2	866	8.6	8.4	4.6	53	s_U	0.143	0.076
Class C								
0.3-0.3	678	10.8	10.4	5.1	48	s_U	1.63	0.62
0.3-0.6	677	12.2	12.1	5.6	46	s_U	0.202	0.091
0.6-0.9	652	12.2	11.9	6.0	49	s_U	0.201	0.096
0.9-1.2	582	11.8	11.5	5.7	48	s_U	0.194	0.092
Class D								
0.0-0.3	495	14.6	13.8	7.6	52	s_U	1.26	0.76
0.3-0.6	485	16.9	17.0	7.3	43	s_U	0.277	0.12
0.6-0.9	437	16.6	16.3	7.4	45	s_U	0.271	0.12
0.9-1.2	401	15.7	15.1	7.6	48	s_U	0.257	0.12

CV = coefficient of variation
s.d. = standard deviation
Source: (Carsel et al. 1988)

Table 5.28 Correlations among Transformed Variables of Organic Matter, Field Capacity, and Wilting Point

Stratum (m)	OM + WP		FC + OM		FC + WP	
	N	Corr.	N	Corr.	N	Corr.
Class A						
0.0-0.3	118	0.738	52	0.624	51	0.757
0.3-0.6	119	0.630	49	0.404	49	0.759
0.6-0.9	111	0.487	42	0.427	42	0.811
0.9-1.2	98	0.456	38	0.170	39	0.761
Class B						
0.0-0.3	877	0.545	459	0.609	455	0.675
0.3-0.6	870	0.372	446	0.384	450	0.639
0.6-0.9	844	0.375	419	0.336	429	0.714
0.9-1.2	780	0.392	347	0.412	370	0.762
Class C						
0.0-0.3	673	0.495	369	0.577	370	0.745
0.3-0.6	664	0.473	355	0.409	361	0.775
0.6-0.9	627	0.457	321	0.434	334	0.784
0.9-1.2	543	0.434	264	0.456	289	0.751
Class D						
0.0-0.3	488	0.538	228	0.496	226	0.847
0.3-0.6	472	0.434	201	0.454	204	0.845
0.6-0.9	420	0.456	171	0.369	174	0.782
0.9-1.2	384	0.415	137	0.106	145	0.687

OM = organic matter; WP = wilting point; FC = field capacity; N = sample size; Corr. = correlation.
Source: (Carsel et al. 1988)

Table 5.29 Mean Bulk Density (g cm^{-3}) for Five Soil Textural Classifications [a]		
Soil Texture	**Mean Value**	**Range Reported**
Silt Loams	1.32	0.86 - 1.67
Clay and Clay Loams	1.30	0.94 - 1.54
Sandy Loams	1.49	1.25 - 1.76
Gravelly Silt Loams	1.22	1.02 - 1.58
Loams	1.42	1.16 - 1.58
All Soils	1.35	0.86 - 1.76

[a] (Baes and Sharp 1983)

Table 5.30 Descriptive Statistics for Bulk Density (g cm^{-3})					
Stratum(m)	**Sample Size**	**Mean**	**Medium**	**s.d.**	**CV(%)**
Class A					
0.0-0.3	40	1.45	1.53	0.24	16.2
0.3-0.6	44	1.50	1.56	0.23	15.6
0.6-0.9	38	1.57	1.55	0.16	10.5
0.9-1.2	34	1.58	1.59	0.13	8.4
Class B					
0.0-0.3	459	1.44	1.45	0.19	13.5
0.3-0.6	457	1.51	1.53	0.19	12.2
0.6-0.9	438	1.56	1.57	0.19	12.3
0.9-1.2	384	1.60	1.60	0.21	12.9
Class C					
0.0-0.3	398	1.46	1.48	0.22	15.0
0.3-0.6	395	1.58	1.59	0.23	14.5
0.6-0.9	371	1.64	1.65	0.23	14.2
0.9-1.2	326	1.67	1.68	0.23	14.0
Class D					
0.0-0.3	259	1.52	1.53	0.24	15.9
0.3-0.6	244	1.63	1.66	0.26	16.0

Table 5.30 Descriptive Statistics for Bulk Density (g cm^{-3})

Stratum(m)	Sample Size	Mean	Medium	s.d.	CV(%)
0.6-0.9	214	1.67	1.72	0.27	16.3
0.9-1.2	180	1.65	1.72	0.28	17.0

CV = coefficient of variation
s.d. = standard deviation
Source: (Carsel et al. 1988)

Table 5.31 Descriptive Statistics and Distribution Model for Organic Matter (Percent by Volume)

	Original Data						
						Distribution Model	
Stratum(m)	Sample Size	Mean	Median	s.d.	CV(%)	Mean	s.d.
Class A							
0.0-0.3	162	0.86	0.62	0.79	92	-4.53	0.96
0.3-0.6	162	0.29	0.19	0.34	114	-5.72	0.91
0.6-0.9	151	0.15	0.10	0.14	94	-6.33	0.83
0.9-1.2	134	0.11	0.07	0.11	104	-6.72	0.87
Class B							
0.0-0.3	1135	1.3	1.1	0.87	68	-4.02	0.76
0.3-0.6	1120	0.50	0.40	0.40	83	-5.04	0.77
0.6-0.9	1090	0.27	0.22	0.23	84	-5.65	0.75
0.9-1.2	1001	0.18	0.14	0.16	87	-6.10	0.78
Class C							
0.0-0.3	838	1.45	1.15	1.12	77	-3.95	0.79
0.3-0.6	822	0.53	0.39	0.61	114	-5.08	0.84
0.3-0.9	780	0.28	0.22	0.27	96	-5.67	0.83
0.9-1.2	672	0.20	0.15	0.21	104	-6.03	0.88
Class D							
0.0-0.3	638	1.34	1.15	0.87	66	-4.01	0.73
0.3-0.6	617	0.65	0.53	0.52	80	-4.79	0.78
0.6-0.9	558	0.41	0.32	0.34	84	-5.29	0.82

Table 5.31	Descriptive Statistics and Distribution Model for Organic Matter (Percent by Volume)						
			Original Data				
						Distribution Model	
Stratum(m)	**Sample Size**	**Mean**	**Median**	**s.d.**	**CV(%)**	**Mean**	**s.d.**
0.9-1.2	493	0.29	0.22	0.31	105	-5.65	0.86

CV = coefficient of variation
s.d. = standard deviation
Source: (Carsel et al. 1988)
[a] Johnson s_B transformation is used for all cases in this table.

Table 5.32	Adaptations and Limitations of Common Irrigation Methods	
Irrigation Method	**Adaptations**	**Limitations**
Furrow	Light, medium and fine.	Slopes up to 3 percent in textured soils; row crops.direction of irrigation; row crops; 10 percent cross slope.
Sprinklers	All slopes; soils; crops.	High initial equipment cost; lowered efficiency in wind and hot climate.
Flood	Light, medium, and heavy soils.	Deep soils; high cost of land preparation; slopes less than 2 percent.

Source: (Todd 1970)

Table 5.33	Water Requirements for Various Irrigation and Soil Types				
	Typical Application Rate (Inches/Hour) by Sprinklers				
	Slope (%)	**Coarse Sandy Loam**	**Light Sandy Loam**	**Medium Silt Loam**	**Clay Loam Soils**
Sprinkling	0-2	2.0	0.75	0.5	0.20
	2-5	2.0	0.75	0.5	0.20
	5-8	1.5	0.50	0.4	0.15
	8-12	1.0	0.40	0.3	

Source: (Todd 1970)

Table 5.34 Representative Furrow Parameters Described in the Literature

Reference	Location	Soil	Crop	Channel Slope	Flow Rate(m^3/s)	Furrow Length(m)	Bottom Width(cm)	Manning's Roughness Coefficient
(Elliott et al. 1982)	Colorado	Clay loam	Corn	.0044	.001-.003	625	–	.02-.03
		Clay loam	Corn	.0092-.0095	.00085-.00096	425-450	—	.02-.03
		Loamy sand	Corn	.0023-.0025	.003-.005	350	—	.02-.03
(Hall 1956)	—	Medium	Corn	.005		200	—	.035
(Fangmeier and Ramsey 1978)	Arizona	Fine sandy loam	None (test furrows)	.01	.0004-.0018	9	—	.02-.04
(Karmeli et al. 1978)	Colorado	Clay loam	None	.0045	.0011	625	10-20	.01-.048

Table 5.35 Furrow Irrigation Relationships for Various Soils, Slopes, and Depths of Application

Soil Texture		**Coarse**				**Medium**				**Fine**			
Max allowable nonerosive Slope furrow stream		**Depth of irrigation application (inches)**											
		2	**4**	**6**	**8**	**2**	**4**	**6**	**8**	**2**	**4**	**6**	**8**
(percent)	**(gpm)**	**Maximum allowable length of run (feet)**											
0.25	40	500	720	875	1,000	820	1,150	1,450	1,650	1,050	1,500	1,750	2,140
0.50	20	345	480	600	680	560	800	975	1,120	730	1,020	1,250	1,460
0.75	13	270	380	480	550	450	630	775	900	580	820	1,000	1,150
1.00	10	235	330	400	470	380	540	650	760	500	750	850	990
1.50	7	190	265	330	375	310	430	530	620	400	570	700	800
2.00	5	160	225	275	320	260	370	450	530	345	480	600	675
3.00	3	125	180	220	250	210	295	360	420	270	385	470	550
5.00	2	95	135	165	190	160	225	270	320	210	290	350	410

Table 5.36 Suitable Side Slopes for Channels Built in Various Kinds of Materials	
Material	**Side slope**
Rock	Nearly vertical
Muck and peat soils	¼:1
Stiff clay or earth with concrete lining	½:1 to 1:1
Earth with stone lining, or earth for large channels	1:1
Firm clay or earth for small ditches	1½:1
Loose sandy earth	2:1
Sandy loam or porous clay	3:1
Source: Adapted from (Chow 1959).	

Table 5.37 Value of "N" for Drainage Ditch Design	
Hydraulic radius (ft)	**EN**
less than 2.5	0.040 – 0.045
2.5 to 4.0	0.035 – 0 .040
4.0 to 5.0	0.030 – 0 .035
more than 5.0	0.025 – 0 .030
Source: Adapted from U.S. Dept. of Agric. Soil Conservation Service.	

Table 5.38 Representative Permeability Ranges for Sedimentary Materials			
Material	**Hydraulic Conductivity (m/s)**	**Material**	**Hydraulic Conductivity (m/s)**
Clay	10^{-12} - 10^{-9}	Very fine sand	10^{-7} - 10^{-4}
Silty clay	10^{-12} - 10^{-9}	Find sand	10^{-6} - 10^{-3}
Sandy clay	10^{-11} - 10^{-8}	Medium sand	10^{-5} - 10^{-3}
Silty clay loam	10^{-10} - 10^{-7}	Coarse sand	10^{-5} - 10^{-2}
Sandy loam sand	10^{-9} - 10^{-6}	Gravel and sand	10^{-5} - 10^{-2}
Silt	10^{-9} - 10^{-6}	Gravel	10^{-5} - 10^{-2}
Silt loam	10^{-9} - 10^{-6}	Sandstone	10^{-6} - 10^{-3}
Loam	10^{-9} - 10^{-6}	Limestone*	10^{-7} - 10^{-4}

Table 5.38 Representative Permeability Ranges for Sedimentary Materials			
Material	**Hydraulic Conductivity (m/s)**	**Material**	**Hydraulic Conductivity (m/s)**
Sandy loam	10^{-8} - 10^{-7}	Shale	10^{-7} - 10^{-4}

* Excluding cavernous limestone.
Source: Adapted from (Todd 1970).
[a] See also Table 5.40.

Table 5.39 Values of Green-ampt Parameters for SCS Hydrologic Soil Groups		
SCS Hydrologic Soil Group	**Saturated Hydraulic[a] Conductivity KS (cm hr^{-1})**	**Suction Parameter HF(cm)**
A	1.0 - 10.0	10
B	0.60 - 1.0	10 - 20
C	0.20 - 0.60	15 - 10
D	0.005 - 0.20	20 - 150

Source: Adapted from (Brakensiek and Rawls 1983)
[a] Also see Table 5.30.

Table 5.40 Descriptive Statistics for Saturated Hydraulic Conductivity (cm hr^{-1})				
	Hydraulic Conductivity (K)*			
Soil Type	**$\bar{x}$**	**s**	**CV**	**n**
Clay**	0.20	0.42	210.3	114
Clay Loam	0.26	0.70	267.2	345
Loam	1.04	1.82	174.6	735
Loamy Sand	14.59	11.36	77.9	315
Silt	0.25	0.33	129.9	88
Silt Loam	0.45	1.23	275.1	1093
Silty Clay	0.02	0.11	453.3	126
Silty Clay Loam	0.07	0.19	288.7	592
Sand	29.70	15.60	52.4	246
Sandy Clay	0.12	0.28	234.1	46
Sandy Clay Loam	1.31	2.74	208.6	214

Table 5.40	Descriptive Statistics for Saturated Hydraulic Conductivity (cm hr^{-1})			
	Hydraulic Conductivity (K)*			
Soil Type	**x̄**	**s**	**CV**	**n**
Sandy Loam	4.42	5.63	127.0	1183

* n = Sample size, x̄ = Mean, s = Standard deviation, CV = Coefficient of variation (percent)
** Agricultural soil, less than 60 percent clay
Source: (Carsel and Parrish 1988)

Table 5.41 Descriptive Statistics for Van Genuchten Water Retention Model Parameters, α, β, γ ((Carsel and Parrish 1988))

	Parameter α, cm^{-1}				**Parameter β**				**Parameter γ**			
Soil Type	**X**	**SD**	**CV**	**N**	**X**	**SD**	**CV**	**N**	**X**	**SD**	**CV**	**N**
Clay[a]	0.008	0.012	160.3	400	1.09	0.09	7.9	400	0.08	0.07	82.7	400
Clay Loam	0.019	0.015	77.9	363	1.31	0.09	7.2	364	0.24	0.06	23.5	364
Loam	0.036	0.021	57.1	735	1.56	0.11	7.3	735	0.36	0.05	13.5	735
Loamy Sand	0.124	0.043	35.2	315	2.28	0.27	12.0	315	0.56	0.04	7.7	315
Silt	0.016	0.007	45.0	88	1.37	0.05	3.3	88	0.27	0.02	8.6	88
Silt Loam	0.020	0.012	64.7	1093	1.41	0.12	8.5	1093	0.29	0.06	19.9	1093
Silty Clay	0.005	0.005	113.6	126	1.09	0.06	5.0	374	0.09	0.05	51.7	374
Silty Clay Loam	0.010	0.006	61.5	641	1.23	0.06	5.0	641	0.19	0.04	21.5	641
Sand	0.145	0.029	20.3	246	2.68	0.29	20.3	246	0.62	0.04	6.3	246
Sandy Clay	0.027	0.017	61.7	46	1.23	0.10	7.9	46	0.18	0.06	34.7	46
Sandy Clay Loam	0.059	0.038	64.6	214	1.48	0.13	8.7	214	0.32	0.06	53.0	214
Sandy Loam	0.075	0.037	49.4	1183	1.89	0.17	9.2	1183	0.47	0.05	10.1	1183

x̄ = Mean, SD = Standard Deviation, CV = Coefficient of Variation, N = Sample size
[a]Agricultural Soil, Clay 60%

Table 5.42 Descriptive Statistics for Saturation Water Content (Θ_s) and Residual Water Content (Θ_r)

	Saturation Water Content (θ_s)				Residual Water Content (θ_r) Statistic*			
Soil Type	**x̄**	**s**	**CV**	**n**	**x̄**	**s**	**CV**	**n**
Clay**	0.38	0.09	24.1	400	0.068	0.034	49.9	353

Table 5.42 Descriptive Statistics for Saturation Water Content (Θ_s) and Residual Water Content (Θ_r)

	Saturation Water Content (θ_s)				Residual Water Content (θ_r)			
Soil Type	**$\bar{x}$**	**s**	**CV**	**n**	**$\bar{x}$**	**s**	**CV**	**n**
Clay Loam	0.41	0.09	22.4	364	0.095	0.010	10.1	363
Loam	0.43	0.10	22.1	735	0.078	0.013	16.5	735
Loamy Sand	0.41	0.09	21.6	315	0.057	0.015	25.7	315
Silt	0.46	0.11	17.4	82	0.034	0.010	29.8	82
Silt Loam	0.45	0.08	18.7	1093	0.067	0.015	21.6	1093
Silty Clay	0.36	0.07	19.6	374	0.070	0.023	33.5	371
Silty Clay Loam	0.43	0.07	17.2	641	0.089	0.009	10.6	641
Sand	0.43	0.06	15.1	246	0.045	0.010	22.3	246
Sandy Clay	0.38	0.05	13.7	46	0.100	0.013	12.9	46
Sandy Clay Loam	0.39	0.07	17.5	214	0.100	0.006	6.0	21
Sandy Loam	0.41	0.09	21.0	1183	0.065	0.017	26.6	1183

* n = Sample size, $\bar{x}$ = Mean, s = standard deviation, CV = coefficient of variation (percent)
** Agricultural soil, less than 60 percent clay.

Table 5.43 Statistical Parameters Used for Distribution Approximation

Soil Texture**	**Hydraulic Variable**	Transformation	**Limits of Variation**		**Mean**	**Estimated* Standard Deviation**	**Truncation Limits on Transformed D*** Variable**
			A	**B**			
S	K_s	SB	0.0	70.0	-0.39387	1.15472	0.045
S	θ_r	LN	0.0	0.1	-3.11765	0.22369	0.053
S	α	SB	0.0	0.25	0.37768	0.43895	0.050
S	β	LN	1.5	4.0	0.97813	0.10046	0.063
SL	K_s	SB	0.0	30.0	-2.49047	1.52854	0.029
SL	θ_r	SB	0.00	0.11	0.38411	0.70011	0.034
SL	α	SB	0.00	0.25	-0.93655	0.76383	0.044
SL	β	LN	1.35	3.00	0.63390	0.08162	0.039

Table 5.43 Statistical Parameters Used for Distribution Approximation

Soil Texture**	Hydraulic Variable	Transformation	Limits of Variation A	Limits of Variation B	Mean	Estimated* Standard Deviation	Truncation Limits on Transformed Variable D***		
LS	K_s	SB	0.0	51.0	-1.26908	1.40000	0.036		
LS	θ_r	SB	0.0	0.11	0.07473	0.56677	0.043		
LS	α	NO	0.0	0.25	0.12354	0.04345	0.027		
LS	β	SB	1.35	5.00	-1.11095	0.30718	0.070		
SIL	K_s	LN	0.0	15.0	-2.18691	1.49414	0.046		
SIL	θ_r	SB	0.0	0.11	0.47752	0.58156	0.073		
SIL	α	LN	0.0	0.15	-4.09937	0.55542	0.083		
SIL	β	SB	1.0	2.0	-0.37036	0.52557	0.104		
SI	K_s	LN***	0.0	2.0	-2.20	0.7000	0.168	-2.564	-0.337
SI	θ_r	ND***	0.0	0.09	0.042	0.0145	0.089	0.013	0.049
SI	α	NO	0.0	0.1	0.01688	0.00611	0.252		
SI	β	NO	1.2	1.6	1.37815	0.03729	0.184		
C	K_s	SB	0.0	5.0	-5.75949	2.32884	0.122		
C	θ_r	SU**	0.0	0.15	0.44537	0.28178	0.058	0.0065	0.834
C	α	SB**	0.0	0.15	-4.14805	1.29310	0.189	-5.01	0.912
C	β	LN**	0.9	1.4	0.00021	0.11800	0.131	0.00	0.315
SIC	K_s	LN	0.0	1.0	-5.68562	1.31421	0.205		
SIC	θ_r	NO	0.0	0.14	0.06971	0.02337	0.058		
SIC	α	LN	0.0	0.15	-5.65849	0.58445	0.164		
SIC	β	SB	1.0	1.4	-1.28378	0.82074	0.069		
SC	K_s	LN	0.0	1.5	-4.04036	2.01721	0.130		
SC	θ_r	SB	0.0	0.12	1.72496	0.70000	0.078		
SC	α	LN	0.0	0.15	-3.76810	0.56322	0.127		
SC	β	LN	1.0	1.5	0.20209	0.07788	0.100		
SICL	K_s	SB	0.0	3.5	-5.31256	1.61775	0.049		
SICL	θ_r	NO	0.0	0.115	0.08871	0.00937	0.056		

Table 5.43 Statistical Parameters Used for Distribution Approximation

Soil Texture**	Hydraulic Variable	Transformation	Limits of Variation A	Limits of Variation B	Mean	Estimated* Standard Deviation	Truncation Limits on Transformed D*** Variable
SICL	α	SB	0.0	0.15	-2.75043	0.60529	0.082
SICL	β	NO	1.0	1.5	1.23640	0.06130	0.082
CL	K_s	SB***	0.0	7.5	-5.87171	2.92220	0.058 -8.92 2.98
CL	θ_r	SU	0.0	0.13	0.67937	0.06005	0.061
CL	α	LN	0.0	0.15	-4.21897	0.71389	0.052
CL	β	SB	1.0	1.6	0.13248	0.72498	0.035
SCL	K_s	SB	0.0	20.0	-4.03718	1.84976	0.047
SCL	θ_r	SB***	0.0	0.12	1.65387	0.43934	0.077 0.928 2.94
SCL	α	SB	0.0	0.25	-1.37920	0.82327	0.048
SCL	β	LN	1.0	2.0	0.38772	0.08645	0.043
L	K_s	SB	0.0	15.0	-3.71390	1.77920	0.019
L	θ_r	SB	0.0	0.12	0.63872	0.48709	0.064
L	α	SB	0.0	0.15	-1.27456	0.78608	0.039
L	β	SU	1.0	2.0	0.53169	0.09948	0.036

* For distribution of transformed variables.
** S = sand, SL = sandy loam, LS = loamy sand, SIL = silty loam, SI = silt, C = clay, SIC = silty clay, SC = sandy clay, SICL = silty clay loam, CL = clay loam, SCL = sandy clay loam, L = loam.
*** Truncated form of the distribution.
**** Kolmogorov-Smirnov test statistic.
Source: (Carsel and Parrish 1988)

Table 5.44 Correlations among Transformed Variables Presented with the Factored Covariance Matrix*

	K_s	θ_r	α	β
Silt **(n = 61)				
K_s	0.5349258	-0.0015813	0.0030541	0.0128700
θ_r	-0.204	0.0075771	0.0000021	-0.0145118
α	0.984	-0.200	0.0005522	0.0144376
β	0.466	-0.610	0.551	0.0133233

Table 5.44 Correlations among Transformed Variables Presented with the Factored Covariance Matrix*

	K_s	θ_r	α	β
Clay (n = 95)				
K_s	1.9614077	0.0701669	0.5645309	0.0475514
θ_r	0.972	0.0170159	-0.0798488	-0.0142394
α	0.948	0.890	0.1716520	0.0021973
β	0.908	0.819	0.910	0.0164640
Silty Clay (n = 123)				
K_s	1.2512845	0.0082067	0.3143268	0.3674505
θ_r	0.949	0.0027392	0.0404171	-0.0858769
α	0.974	0.964	0.0608834	0.0660396
β	0.908	0.794	0.889	0.1305065
Sandy Clay (n = 46)				
K_s	2.0172105	0.8827527	0.5391195	0.0756103
θ_r	0.939	0.3241979	0.0634106	0.0035688
α	0.957	0.937	0.1501651	-0.0010668
β	0.972	0.928	0.932	0.0178225
Sand (n = 237)				
K_s	1.0370702	-0.1092256	0.3276629	0.0805436
θ_r	-0.515	0.1816914	0.2583835	-0.0471785
α	0.743	0.119	0.1429585	-0.0013674
β	0.843	-0.858	0.298	0.0167064
Sandy Loam (n = 1145)				
K_s	1.6026856	-0.1529235	0.0372713	0.2108253
θ_r	-0.273	0.5378436	0.0174500	-0.1943369
α	0.856	0.151	0.0142626	0.0193794
β	0.686	-0.796	0.354	0.1084945
Loamy Sand (n = 313)				
K_s	1.4754063	-0.2005639	0.0372713	0.2108253
θ_r	-0.359	0.5215473	0.0174500	-0.1943369

Table 5.44 Correlations among Transformed Variables Presented with the Factored Covariance Matrix*

	K_s	θ_r	α	β
α	0.986	-0.301	0.0142626	0.0193794
β	0.730	-0.590	0.354	0.1084945
Silt Loam (n = 1072)				
K_s	1.4754063	-0.02005639	0.5245489	0.3525548
θ_r	-0.359	0.5215473	0.0300399	-0.1696100
α	0.986	-0.301	0.0820163	0.2341768
β	0.730	-0.590	0.775	0.1583593
Silty Clay Loam (n = 591)				
K_s	1.6177521	0.0056509	0.5116521	0.0486478
θ_r	0.724	0.0053780	0.0475299	-0.0089569
α	0.986	0.777	0.0731704	0.0080399
β	0.918	0.549	0.911	0.0171716
Clay Loam (n = 328)				
K_s	1.9200165	0.0395603	0.5886263	0.5417671
θ_r	0.790	0.0307122	-0.0619715	-0.1536351
α	0.979	0.836	0.1060875	0.0653030
β	0.936	0.577	0.909	0.1159401
Sandy Clay Loam (n = 212)				
K_s	1.8497610	0.1020156	0.7838769	0.0766289
θ_r	0.261	0.3775754	0.1223451	-0.0305588
α	0.952	0.392	0.2198684	-0.0078559
β	0.909	-0.113	0.787	0.0155766
Loam (n = 664)				
K_s	1.4083953	-0.0995016	0.6110671	0.0545016
θ_r	0.204	0.4775039	0.0727710	-.0545793
α	0.982	-0.086	0.0926351	0.0256843
β	0.632	-0.748	0.591	0.0288861

Table 5.44 Correlations among Transformed Variables Presented with the Factored Covariance Matrix*				
	$\mathbf{K_s}$	$\boldsymbol{\theta_r}$	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$

* Entries in the lower triangular portion of the matrix are sample Pearson product-moment correlations given to three decimal places. The diagonal and upper triangular entries form the triangular Cholesky decomposition of the sample covariance matrix.
** n = Sample size.
Source: (Carsel and Parrish 1988)

Table 5.45 Examples of Nitrogen Gains, Losses, and Transformations (In Kg/ha/yr) for Eight Different Cropping Systems[a]

Description of Change	Grazed Bluegrass (No. Car.)	Corn Grains (Ind.)	Soybean Seeds (Ark.)	Wheat (Kansas)	Irish Potatoes (Maine)	Cotton (Calif.)	Loblolly Pine (Miss.)	Douglas Fir (Wash.)
Additions								
Added Fertilizer	168	112	0	34	168	179	—	—
Irrigation,floodwater	—	10	—	—	—	50	—	—
Sediments added	10	10	10	6	6	3	11	10
N_2-fixation	—	—	123	—	—	—	8	—
Removals								
Harvested product	38	85	90	36	80	79	12	10
Denitrification	5	15	15	5	15	20	1	1
Volatilization of ammonia	98[b]	—	—	—	—	—	—	—
Leaching loss	—	15	10	4	64	83	1	1
Erosion and runoff	14	16	16	5	15	50	3	2
Recycling process								
Uptake from soil	151	126	120	56	145	127	20	35
Manure from grazing	60	—	—	—	—	—	—	—
Plant residues left	113	41	30	20	65	48	9	25
Mineralization from humus	48	50	15	28	65	48	6	—

[a] A dash means that no measurement was made or the item does not apply to the system.
[b] Losses from voided animal urine and feces as ammonia gas.
Source: Data from (Frissel 1978, pp. 203-243)

Table 5.46 Recommended Manning's Roughness Coefficients for Overland Flow

Cover of Treatment	Residue Rate (ton/acre)	Value recommended	Range
Concrete or asphalt		0.011	0.01 - 0.013
Bare sand		0.01	0.010 - 0.016
Graveled surface		0.02	0.012 - 0.03
Bare clay-loam (eroded)		0.02	0.012 - 0.033
Fallow—no residue		0.05	0.006 - 0.16
Chisel plow	1/4	0.07	0.006 - 0.17
	1/4 - 1	0.18	0.07 - 0.34
	1-	0.30	0.19 - 0.47
	3	0.40	0.34 - 0.46
Disk/harrow	1/4	0.08	0.008 - 0.41
	1/4 - 1	0.16	0.10 - 0.41
	1-3	0.25	0.14 - 0.53
	3	0.30	-
No-till	1/4	0.04	0.03 - 0.07
	1/4 - 1	0.07	0.01 - 0.13
	1-3	0.30	0.16 - 0.47
Moldboard Plow (Fall)		0.06	0.02 - 0.10
Coulter		0.10	0.05 - 0.13
Range (natural)		0.13	0.01 - 0.32
Range (clipped)		0.10	0.02 - 0.24
Grass (bluegrass sod)		0.45	0.39 - 0.63
Short grass prairie		0.15	0.10 - 0.20
Dense grass		0.24	0.17 - 0.30
Bermuda grass		0.41	0.30 - 0.48
Woods-Light underbrush		0.40	
Woods-Dense underbrush		0.80	

SECTION 6
Pesticide Root Zone Model (PRZM) Code and Theory

6.1 Introduction and Background (PRZM)

This section describes the theoretical background for the mathematical simulation model (PRZM) that has been developed and tested to evaluate pesticide leaching from the crop root zone under field crop conditions. While the model's focus has traditionally been on pesticides, it has been used over the years to simulate the behavior of other organic chemicals; the most recent version of the model has been expanded to include capabilities for modeling nitrogen species as well. The majority of this section is devoted to the discussion of the model's code and theory related to pesticide simulation. A summary of the features of the new nitrogen code is included in Section 6.2.1; a new section (6.3.8) describes the nitrogen code and theoretical considerations in greater detail.

Following an introduction, Section 6.2 describes the features and limitations of the model. A description of the theory, including a detailed description of the equations solved, is provided in Section 6.3. An outline of the numerical implementation techniques used by the model to apply the theory to the simulation of physical problems follows. Section **6** concludes with a discussion of testing results for new algorithms that have been added in this release.

6.1.1 Introduction

Pesticide leaching from agricultural fields as nonpoint source loads can lead to groundwater contamination. Nonpoint source contamination is characterized by highly variable loadings, with rainfall and irrigation events dominating the timing and magnitude of the loading of pesticides leaching below the root zone. The potentially widespread, areal nature of resulting contamination makes remedial actions difficult because there is no single plume emanating from a "point source" (the more common groundwater problem) that can be isolated and controlled. In any case, a more prudent approach to prevention or reduction of groundwater contamination by pesticides must be based on understanding the relationships among chemical properties, soil system properties, and the climatic and agronomic variables that combine to induce leaching. Knowledge of these relationships can allow a priori investigation of conditions that lead to problems, and appropriate actions can be taken to prevent widespread contamination.

Many investigators have studied the factors contributing to pesticide leaching. These investigations have shown that chemical solubility in water, sorptive properties, volatility, formulation, and soil persistence determine the tendency of pesticides to leach through soil. Similarly, the important environmental and agronomic factors include soil properties, climatic conditions, crop type, and cropping practices. In short, the hydrologic cycle interacts with the chemical characteristics to transform and transport pesticides within and out of the root zone. Vertical movement out of the root zone can result in groundwater contamination and is the problem that the model is designed to investigate.

Numerical models to simulate the movement of solutes in porous media under steady-state, transient, homogenous, and/or multi-layered conditions have been previously developed. Included in such models have been descriptions of linear and nonlinear sorption, ion exchange, and chemical-specific reactions. These prior models and related investigations have proven valuable in interpreting laboratory data, investigating basic transport processes, and identifying the controlling factors in solute transport and transformation. As noted in a recent review of models for simulating the movement of contaminants through groundwater flow systems, the successful use of such models requires a great deal of detailed field data. This unfortunate conclusion arises from the scaling problems associated with using laboratory experiments results for field-scale assessments, and the traditional solution of the appropriate partial differential equations at points or nodes in a finite-difference or finite-element grid network. Each spatial segment modeled must be properly characterized – a most expensive, if not impossible, task for many modeling problems.

Such difficulties in modeling pesticide leaching with existing procedures are even more daunting when one considers the need to evaluate the potential for future problems arising from pesticides not yet widely distributed or

used. Models used to perform such prognostic evaluations should conform to the maximum possible extent to known theory, but must be structured to enable efficient analysis of field situations with minimal requirements for specialized field data. In short, the goal is to integrate the essential chemical-specific processes occurring during leaching with reasonable estimates of water movement through soil systems. Data input must be reasonable for both spatial and temporal requirements, and generally available from existing data bases. PRZM attempts to meet these objectives.

In addition to pesticide simulation, the need has arisen to simulate nitrogen species (in particular, nitrate) in order to assist in delineating rural wellhead protection areas. A model to perform these simulations would need to be able to represent (1) nitrogen introduced as a result of on-site wastewater treatment systems, (2) soil nitrogen transport and transformation processes within the unsaturated zone, and (3) certain potential influxes of nitrogen due to land surface activities related to agriculture and atmospheric deposition. In 1995 the existing PRZM-2 modeling framework was enhanced to develop a tool capable of simulating nitrogen soil fate processes, thereby providing a means to project those loadings to groundwater. PRZM-3 is capable of modeling soil nitrogen transformation and transport processes, thereby providing a valuable tool for defining wellhead protection strategies relative to nitrate contamination.

6.1.2 Background

The Pesticide Root Zone Model (PRZM) (Carsel et al. 1984, Carsel et al. 1985) was designed and developed as a code for Agency in simulating the transport and transformation of agriculturally applied pesticides in the crop root zone. As such, PRZM attained a degree of acceptability in both the regulatory community and in the agricultural chemical industry. Therefore, its utility in accomplishing the objective of this model development effort is obvious.

6.2 Features and Limitations

6.2.1 Features

PRZM Release III is a one-dimensional, dynamic, compartmental model for use in simulating chemical movement in unsaturated soil systems within and immediately below the plant root zone (see **Figure 6.1**). PRZM allows the user to perform simulations of potentially toxic chemicals, particularly pesticides, that are applied to the soil or to plant foliage. Dynamic simulation allows the consideration of pulse loads, the prediction of peak events, and the estimation of time-varying mass emission or concentration profiles, thus overcoming limitations of the more commonly used steady-state models. Time-varying transport by both advection and dispersion in the dissolved phase or diffusion in the gas phase are represented in the program.

PRZM has two major components – hydrology and chemical transformation and transport. The hydrologic component for calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the Universal Soil Loss Equation. Evapotranspiration is estimated from pan evaporation data, or by an empirical formula if input pan data are unavailable. Evapotranspiration is divided among evaporation from crop interception, evaporation from soil, and transpiration by the crop. Water movement is simulated by the use of generalized soil parameters, including field capacity, wilting point, and saturation water content. Irrigation inputs can also be modeled.

Dissolved, adsorbed, and vapor-phase contaminant concentrations in the soil are estimated by simultaneously considering the processes of chemical uptake by plants, surface runoff, erosion, decay, volatilization, foliar washoff, advection, dispersion, and retardation. The user can elect to solve the transport equations using one of two finite-difference numerical techniques, the original backwards-difference implicit scheme featured in the first release, or a Method of Characteristics algorithm that greatly reduces numerical dispersion, but increases model execution time.

The hydrologic components of the chemical transport equations (i.e., soil moisture content and soil-water velocities) are decoupled, solved separately, and used to numerically integrate the equation in succeeding time steps. Predictions are made on a daily basis. Output can be summarized on a daily, monthly, or annual frequency. Daily time series of values for various fluxes or storages can be written to sequential files during program execution.

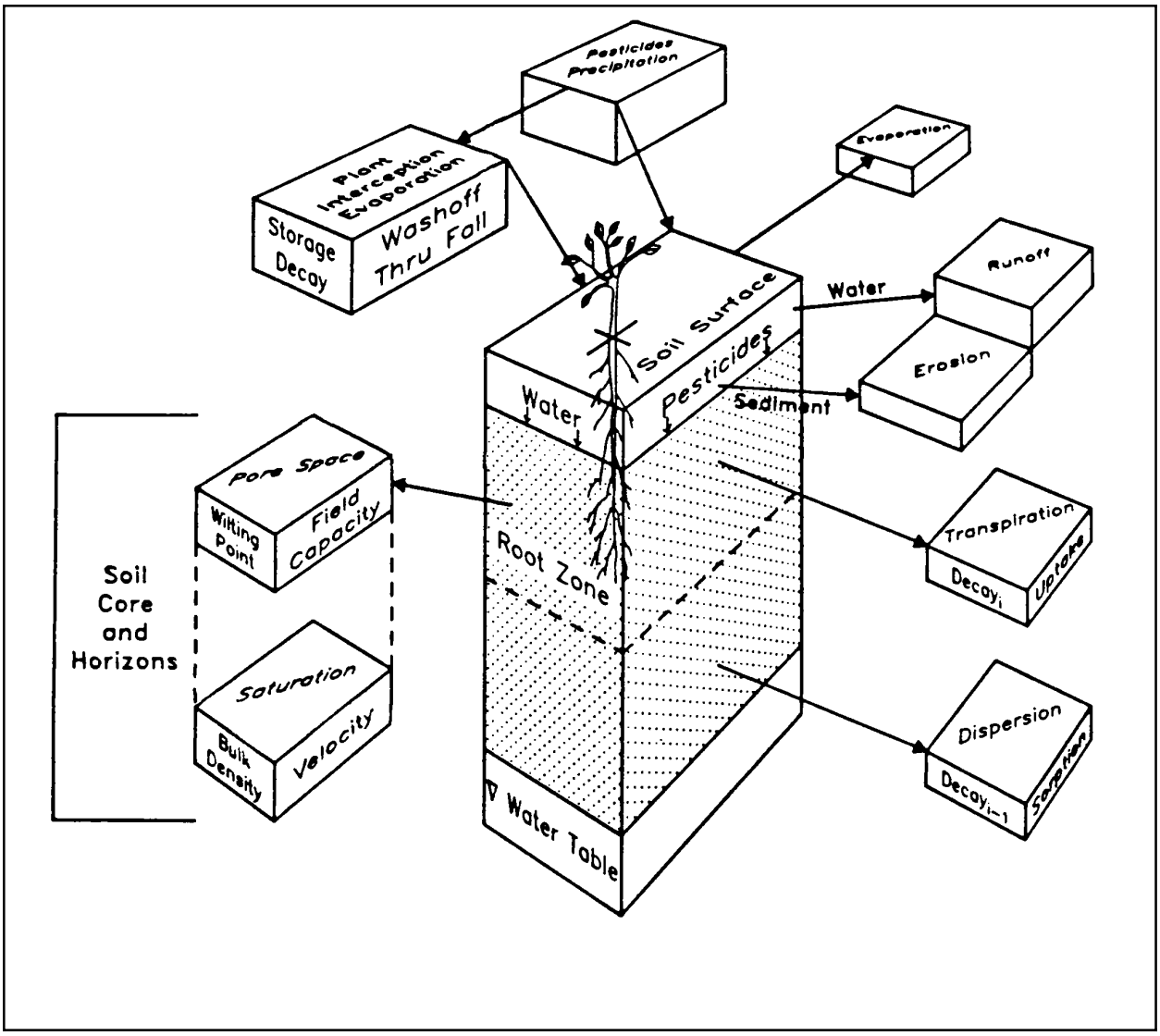


Figure 6.1 Pesticide Root Zone Model.

Enhancements to PRZM in the most recent version of PRZM-3 have added the ability to simulate nitrogen constituents in a manner similar to pesticides. The soil nitrogen storages and transformations included in PRZM-3 are based on the soil nitrogen modeling procedures included in HSPF AGCHEM Version No. 11 (Bicknell et al. 1995), with a few modifications to accommodate the PRZM soil profile representation, include a threshold for denitrification based on soil moisture, and mesh with the daily time step in PRZM. The nitrogen species of nitrate, ammonia, and four forms of organic nitrogen (i.e. particulate organic nitrogen (labile and refractory) and dissolved organic nitrogen (labile and refractory)) are represented. Allowable inputs of nitrogen include atmospheric deposition, septic system effluent, and surface applications. The soil nitrogen fate processes include plant uptake of nitrate and ammonium, return of plant nitrogen to organic nitrogen, denitrification or reduction of nitrate-nitrite, immobilization of nitrate-nitrite and ammonium, mineralization of organic nitrogen, fixation of atmospheric nitrogen, volatilization of ammonium, and the adsorption/desorption of ammonium and the organic forms. All reactions and fluxes are computed on a daily basis and the storages then updated.

All water related transport processes are performed by existing PRZM routines. Water from septic system effluent is introduced into the soil hydraulics routines in the same equations used to calculate lateral outflow. Since the nitrogen reactions are performed in the newly incorporated soil nitrogen module, the water movement generated within

PRZM can used to transport the nitrogen species. This was done by creating a modified version of the existing pesticide transport/reaction routine (SLPST0), that calls the same tri-diagonal matrix solver (TRDIAG) to calculate only transport values. This new routine (NITMOV) uses the water movement calculations within PRZM to account for all water-related nitrogen movement fluxes, including runoff, and erosion, leaching, and lateral outflow.

Agricultural nitrogen applications are modeled using the same rules for incorporation depth (soil application only) as for a pesticide in PRZM-2. The PRZM-3 mass balance model houses the same code for the water balance as is found in PRZM-2's mass balance.

Some processes are simulated in both the PRZM code and the nitrogen module, and it should be clarified which modules are used for which simulation. Ammonia volatilization is performed using the new nitrogen simulation code, not the pesticide volatilization routines in PRZM. Plant growth is simulated in both PRZM and the nitrogen module. The plant growth algorithm used in the nitrogen module is only used in that module. All other plant growth simulation is performed in existing PRZM modules.

Some assumptions from the HSPF nitrogen simulation had to be transferred to the nitrogen simulation in PRZM-3. For example, atmospheric deposition and litter return are only incorporated into the surface and upper zones of HSPF. In PRZM-3, it is assumed that atmospheric deposition and litter return are incorporated into the first horizon only and are divided equally among the compartments in the first horizon.

6.2.2 Limitations

There were some severe limitations of the PRZM Release I Code, that were obvious to the developers, and some that were pointed out subsequently by model users. These limitations can be broken into four categories:

- Hydrology
- Soil hydraulics
- Method of solution of the transport equation
- Deterministic nature of the model

In Release II, many of these limitations to an extent, were overcome, to an extent.

Hydraulic computations are performed in PRZM on a daily time step; however, some of the processes involved (evaporation, runoff, erosion) are clearly among those that might be simulated on a finer time step to ensure greater accuracy and realism. For instance, simulation of erosion by runoff depends on the peak water runoff rate, that is, in turn, dependent on the time base of the water runoff hydrograph. All of this depends, to some extent, on the duration of the precipitation event. PRZM retains its daily time step in this release primarily due to the relative availability of daily versus shorter time step meteorological data. A portion of this limitation has been mitigated, we hope, by enhanced parameter guidance.

The method of computing potential evapotranspiration using Hamon's formula, in the absence of actual evaporation data, has also been retained. However, we noted that evapotranspiration from irrigated citrus in Florida was found to be substantially under-predicted when using this method to estimate potential evapotranspiration (Dean and Atwood 1985a). Users should check the model's hydrologic simulation carefully when using this option.

The capability to simulate soil temperature was added to PRZM-2 and carried-over to PRZM-3 in order to correct Henry's constant for the temperature occurring in various depths in the soil when performing vapor-phase calculations. Removal of water by evaporation versus transpiration from the profile may have a pronounced effect on soil temperature. This is due to the fact that more heat is removed during the process of evaporation because the energy necessary to vaporize water leaves the system, producing a cooling effect. No differentiation is made between evaporation and transpiration in PRZM at this time.

In PRZM Release I, the soil hydraulics were simple – all drainage to the field capacity water content was assumed to occur within 1 day. (An option to make drainage time dependent value was also included, but there is not much

evidence to suggest that this option was utilized by model users to any great extent). This assumption had the effect, especially in deeper soil columns , of inducing a greater-than-anticipated and unrealistic movement of chemical through the soil profile. While this representation of soil hydraulics has been retained in PRZM-3, the user has the option, with the linked modeling system, of coupling PRZM to VADOFT. PRZM-3 is then used to model just the root zone, while VADOFT, with a more rigorous representation of unsaturated flow, is used to simulate the rest of the vadose zone. The difficulties in parameterizing the Richards equation for unsaturated flow in VADOFT is overcome by using the technique of van Genuchten to generate soil water characteristic curves using soil textural information. For thin soil columns, PRZM can be used to represent the entire vadose zone.

The addition of algorithms to simulate volatilization has brought into focus another limitation of the soil hydraulics representation. PRZM-3 simulates only advective, downward movement of water and does not account for diffusive movement due to soil water gradients.. This means that PRZM-3 is unable to simulate the upward movement of water in response to when for simulating the effects of volatilization. This latter process has bee identified by jury at al. (1984) to be important when simulating the effects of volatilization However, this process would seem less likely to affect the movement of chemicals with high vapor pressures. For these later chemicals, vapor diffusion would more likely be the major process for renewing the chemical concentration in the surface soil horizon(s).

Another limitation of the Release I model was the inadequacy of the solution to the chemical transport equation in advection-dominated systems. The backward difference formulation of the advection term tends to produce a high degree of numerical dispersion in such systems. This results in over-prediction of downward chemical movement due to smearing of the dissolved concentration peak and subsequent overestimation of chemical loadings to groundwater. In PRZM-3, a new formulation is available for advection-dominated systems. The advective terms are decoupled from the rest of the transport equation and solved separately using a Method of Characteristics (MOC) formulation. The remainder of the transport equation is then solved as before, using the fully implicit scheme. This approach effectively eliminates numerical dispersion, but with some additional overhead expense in computation time. In low-advection systems, the MOC approach reduces to the original PRZM solution scheme, which is exact for water velocities approaching zero.

The final limitation is the use of field-averaged water and chemical transport parameters to represent spatially heterogeneous soils. Several researchers have shown that this approach produces slower breakthrough times than are observed using stochastic approaches. This concern has been addressed by adding the capability in PRZM-3 to run PRZM in a Monte Carlo framework. Thus, distributional, rather than field-averaged, values can be utilized as inputs thereby producing distributional outputs of the relevant variables (e.g., flux to the water table).

6.3 Description of the Algorithms

The description of the processes simulated by PRZM is broken-down in the following discussion into eight categories:

- Chemical Transport in Soil
- Water Movement
- Chemical Application and Foliar Washoff
- Chemical dissolved in Runoff
- Soil Erosion
- Volatilization
- Irrigation
- Nitrogen Processes

The first two categories plus soil erosion were simulation options originally available in PRZM Release I. Since the capability to simulate ponding is new, the mathematical basis of the ponding algorithms is described in detail. Volatilization and irrigation simulation were added in the PRZM-2 release, and the sections on chemical application, dissolved chemical runoff and nitrogen processes describe enhancements developed for the PRZM-3 release.

6.3.1 Chemical Transport in Soil

The PRZM-3 model was derived from the conceptual, compartmentalized representation of the soil profile as shown in **Figure 6.2**. From consideration of **Figure 6.2**, it is possible to writechemical mass balance equations for both the surface and subsurface zones. Addition of the vapor phase and ponded water compartments in PRZM-3 require the consideration of additional terms compared to previous PRZM releases. The surface zone mass balance expressions for each of the dissolved, adsorbed, and vapor phases are:

$$A\Delta z\frac{\partial(C_w\theta)}{\partial t} = J_D - J_V - J_{DW} - J_U - J_{QR} + J_{APP} + J_{FOF} \pm J_{TRN} \quad \textbf{(6.1)}$$

$$A\Delta z\frac{\partial(C_s\rho_s)}{\partial t} = -J_{DS} - J_{ER} \quad \textbf{(6.2)}$$

$$A\Delta z\frac{\partial(C_g a)}{\partial t} = J_{GD} - J_{DG} \quad \textbf{(6.3)}$$

where

A	= cross-sectional area of soil column (cm^2)
Δz	= depth dimension of compartment (cm)
C_w	= dissolved concentration of pesticide (g cm^{-3})
C_s	= sorbed concentration of pesticide (g g^{-1})
C_g	= gaseous concentration of pesticide (g cm^{-3})
θ	= volumetric water content of soil (cm^3 cm^{-3})
a	= volumetric air content of the soil (cm^3 cm^{-3})
ρ_s	= soil bulk density (g cm^{-3})
t	= time (days)
J_D	= represents the effect of dispersion and diffusion of dissolved phase (g day^{-1})
J_V	= represents the effect of advection of dissolved phase (g day^{-1})
J_{GD}	= represents the effect of dispersion and diffusion in vapor phase (g day^{-1})
J_{DW}	= mass loss due to degradation in the dissolved phase (g day^{-1})
J_{DG}	= mass loss due to degradation in the vapor phase (g day^{-1})
J_U	= mass loss by plant uptake of dissolved phase (g day^{-1})
J_{QR}	= mass loss by removal in runoff (g day^{-1})
J_{APP}	= mass gain due to pesticide deposition on the soil surface (g day^{-1})
J_{FOF}	= mass gain due to washoff from plants to soil (g day^{-1})
J_{DS}	= mass loss due to degradation of sorbed phase chemical (g day^{-1})
J_{ER}	= mass loss by dissolved removal on eroded sediments (g day^{-1})
J_{TRN}	= mass gain or loss due to parent/daughter transformations (g day^{-1})

Equations for the subsurface zones are identical to Equations 6.1, 6.2, and 6.3 except that J_{QR}, J_{FOF}, and J_{ER} are not included. J_{APP} applies to subsurface zones only when the pesticides are incorporated into the soil. For subsurface layers below the root zone, the term J_U is also not utilized.

Note that terms representing phase transfers (e.g., volatilization) are neglected in Equations 6.1 through 6.3 because they cancel when the equations are added (see Equation 6.19).

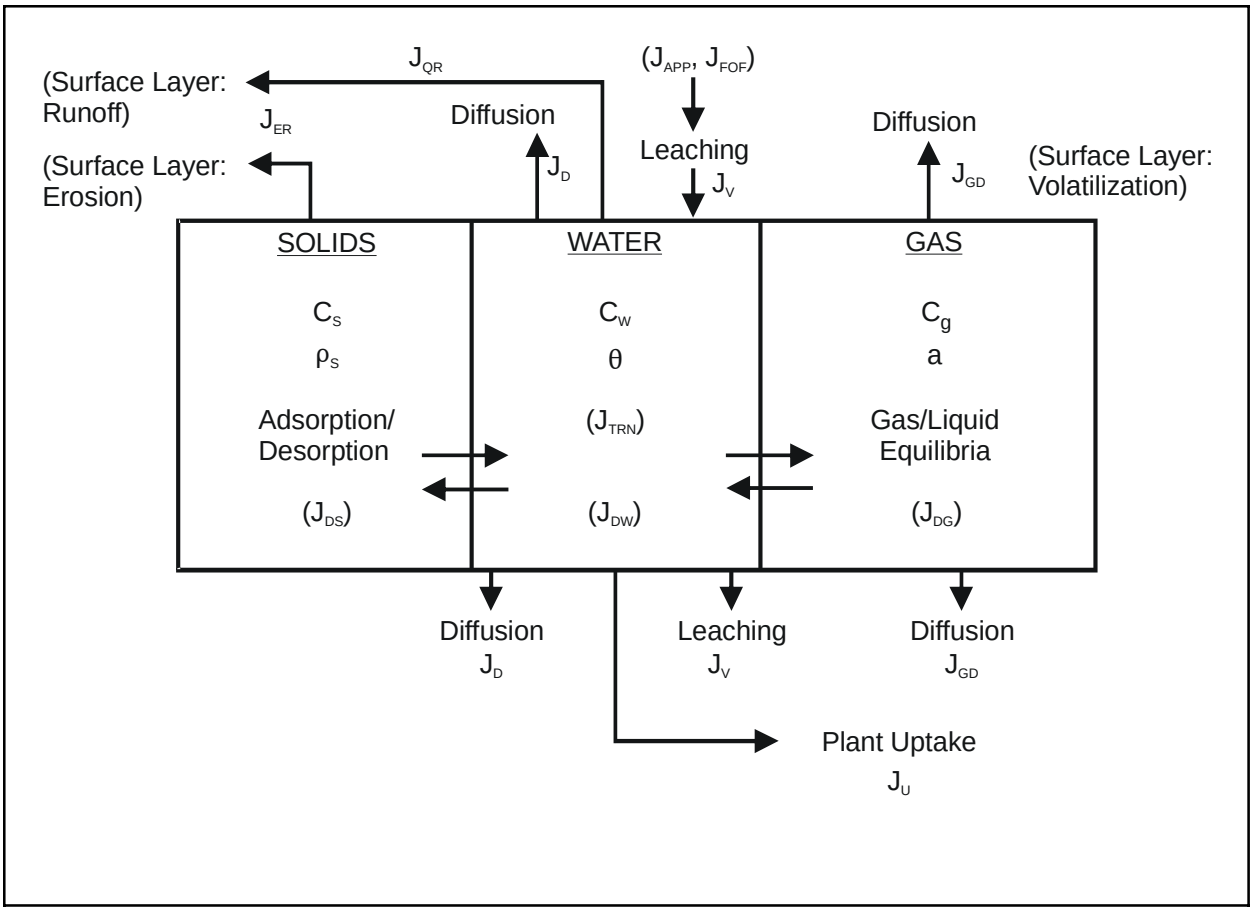


Figure 6.2 Schematic representation of a single chemical in a soil layer.

Each term in Equations 6.1 through 6.3 is now further defined. Dispersion and diffusion in the dissolved phase are combined and are described using Fick's law:

$$J_D = -A\Delta z\, D_w \frac{\partial^2 (C_w \theta)}{\partial z^2} \qquad \textbf{(6.4)}$$

where

D_w = diffusion-dispersion coefficient for the dissolved phase, assumed constant ($cm^2\ day^{-1}$)
C_w = dissolved concentration of pesticide ($g\ cm^{-3}$)
θ = volumetric soil water content ($cm^3\ cm^{-3}$)
z = soil depth dimension (cm)

In a similar manner, dispersion and diffusion in the vapor phase are described by Fick's law:

$$J_{GD} = -A\ \Delta z\ D_g \frac{\partial^2 (C_g a)}{\partial z^2} \qquad \textbf{(6.5)}$$

where

D_g = molecular diffusivity of the pesticide in the air-filled pore space ($cm^2\ day^{-1}$)
C_g = vapor-phase concentration of pesticide ($g\ cm^{-3}$)
a = volumetric soil air content ($cm^3\ cm^{-3}$)

The dependence of the molecular diffusivity of the pesticide in air-filled pore space of the volumetric soil air content

is described by the Millington-Quirk expression (Jury et al. 1983a)

$$D_g = \frac{a^{10/3}}{n^2} D_a \tag{6.6}$$

where

a = the air-filled porosity ($cm^3\ cm^{-3}$)
ϕ = total porosity ($cm^3\ cm^{-3}$)
D_a = molecular diffusivity of the chemical in air, assumed constant ($cm^2\ day^{-1}$)

The mathematical theory underlying the diffusive and dispersive flux of pesticide in the vapor phase within the soil and into the overlying air can be found in the section describing volatilization.

The advective term for the dissolved phase, J_V, describes the movement of pesticide in the bulk flow field:

$$J_V = A\ \Delta z\ V \frac{\partial(C_w \theta)}{\partial z} \tag{6.7}$$

where

V = velocity of water movement ($cm\ day^{-1}$)

Vapor-phase advection has not been included as a flux in the transport equation. A number of researchers have indicated a consensus that vapor-phase advection is not likely to be significant for agricultural situations (Jury et al. 1987). Early studies of water vapor movement suggested that the fluctuation of barometric pressure at the soil surface could act as a pumping mechanism for vapor-phase advective transport (Fukuda 1955, Farrell et al. 1966, Scotter and Raats 1970). However, using models for vapor emissions from landfills, Thibodeaux et al. (1982)found that atmospheric pressure fluctuations increased the total emission rate for benzene by only 15%, compared to constant pressure conditions. Therefore, it appears to be a reasonable assumption at this time to neglect vapor-phase advection in modeling chemical migration for agricultural situations.

Degradation of a pesticide in or on soil can be due to such processes as hydrolysis, photolysis, and microbial decay. If these processes follow pseudo first-order kinetics, the rate coefficients can be combined into a single, overall or lumped decay coefficient. Assuming the same rate constants for the solid and dissolved phases, the rate of change of chemical out of each phase due to decomposition is given by:

$$J_{DW} = K_s\ C_w\ \theta\ A\ \Delta z \tag{6.8}$$

$$J_{DS} = K_s\ C_s\ \rho_s\ A\ \Delta z \tag{6.9}$$

$$J_{DG} = K_g\ C_g\ a\ A\ \Delta z \tag{6.10}$$

where

K_s = lumped, first-order decay constant for solid and dissolved phases (day^{-1})
K_g = lumped, first-order decay constant for vapor phase (day^{-1})
C_s = solid-phase concentration of pesticide ($g\ g^{-1}$)

Plant uptake of pesticides is modeled by assuming that uptake is directly related to transpiration rate. The uptake is given by:

$$J_U = f\ C_w\ \theta\ \varepsilon\ A\ \Delta z \tag{6.11}$$

where

J_u = uptake of pesticide ($g\ day^{-1}$)
f = the fraction of total water in the zone used for transpiration (day^{-1})
ε = an uptake efficiency factor or reflectance coefficient (dimensionless)

Erosion and runoff losses as well as inputs to the surface zone from foliar washoff are considered in the surface layer. The loss of pesticide due to runoff is

$$J_{QR} = \frac{Q}{A_W} C_w A \tag{6.12}$$

where

J_{QR} = pesticide loss due to runoff (g day^{-1})
Q = the daily runoff volume (cm^3 day^{-1})
A_w = watershed area (cm^2)

and the loss of sorbed pesticide due to erosion is

$$J_{ER} = \frac{P X_e r_{om} C_s A}{A_w} \tag{6.13}$$

where

J_{ER} = the pesticide loss due to erosion (g day^{-1})
X_e = the erosion sediment loss (metric tons day^{-1})
r_{om} = the enrichment ratio for organic matter (g g^{-1})
p = a units conversion factor (g tons^{-1})

Soil erosion is discussed in more detail in Section 6.3.5.

Pesticides can be applied to either bare soil if pre-plant conditions prevail or to a full or developing crop canopy if post-plant treatments are desired. The pesticide application is an input mass rate that is calculated by one of the application/deposition models discussed in Section 6.3.3. It is partitioned between the plant canopy and the soil surface, and the rate at which it reaches the soil surface is designated J_{APP}.

Pesticides applied to the plant canopy can be transported to the soil surface as a result of rainfall washoff. This term, J_{FOF}, is defined as:

$$J_{FOF} = E P_r M A \tag{6.14}$$

where

E = foliar extraction coefficient (cm^{-1})
P_r = daily rainfall amount (cm day^{-1})
M = mass of the pesticide on the plant surface projected area basis (g cm^{-2})

The foliar pesticide mass, M, is subject to degradation, transformation to metabolites and losses through volatilization. Its rate of change is given by

$$A \frac{dM}{dt} = - K_f MA - K_t MA - J_{FOF} + A_F bA \tag{6.15}$$

where

K_f = lumped first-order foliar degradation constant (day^{-1})
K_t = lumped first-order foliar transformation constant (day^{-1})
A_F = application rate to the plant (g ha^{-1} day^{-1})
b = a units conversion factor (ha)

Adsorption and desorption in Equations 6.1 through 6.3 are treated as instantaneous, linear, and reversible processes. Using this assumption, we can relate the sorbed phase concentration to the dissolved-phase concentration by:

$$C_s = K_d C_w \tag{6.16}$$

where

K_d = partition coefficient between the dissolved and solid phases ($cm^3\ g^{-1}$)

A similar expression can be developed to express the vapor phase concentration in terms of the dissolved-phase concentration:

$$C_g = K_H C_w \tag{6.17}$$

where

K_H = dimensionless Henry's constant, i.e., distribution-coefficient between the vapor phase and the liquid phase. K_H = (Henry's constant [atm/mol]) / ® T), where T is the temperature [kelvin], and R is the gas constant, 8.20574×10^{-2} [liter atm mol^{-1} K^{-1}].

The transformation of parent to daughter is assumed to be first order and is described by

$$J_{TRN} = - K_{TRN}\ C_w\ A\ \Delta z\ \theta \tag{6.18}$$

where

K_{TRN} = the transformation rate constant (day^{-1})

When simulating an end-of-chain daughter, J_{TRN} can also be a source term equal to the sum of the first-order transfers from any and all parents.

$$J_{TRN} = \sum_k K_{TRN}^k\ C_w^k\ A\ \Delta z\ \theta \tag{6.19}$$

in which the superscript k denotes a parent compound. For intermediate products, the solute transport equation can also contain terms such as those shown in both Equations 6.18 and 6.19. The transformation of parent to daughter compounds is discussed in detail in Section 6.5.4. That section includes a description of the equations used to simulate this scenario.

Summing Equations 6.1, 6.2, and 6.3 and utilizing equations 6.16 and 6.17, produces the following expressions for the mass balance of pesticide in the uppermost soil layer:

$$\begin{aligned}\frac{\partial}{\partial t}[C_w(\theta + K_d\rho_s + aK_H)] &= -D_w\frac{\partial^2}{\partial z^2}(C_w\theta) - D_g\frac{\partial^2}{\partial z^2}(aC_wKH) - V\frac{\partial}{\partial z}(C_w\theta) \\ &- C_w\left[K_s(\theta + K_d\rho_s) + K_g aK_H + f\theta\varepsilon + \frac{Q}{A_w\Delta z} + \frac{PX_e r_{om}K_d}{A_w\Delta z}\right] \\ &+ \frac{J_{APP}}{A\ \Delta z} + \frac{EP_r M}{\Delta z} - K_{TRN}\ C_w\theta + \sum_k K_{TRN_k}\ C_w^k\ \theta\end{aligned} \tag{6.20}$$

Equation 6.20 is solved in PRZM-3 for the surface layer with $f\ \theta = 0$, and an upper boundary condition that allows vapor phase flux upward from the soil surface to the overlying air. This upper boundary condition is described more fully in the section on volatilization. The lower boundary condition is one that allows advection, but no diffusion, out of the bottom of the soil profile.

6.3.2 Water Movement

Because V and θ are not generally known and not generally measured as part of routine monitoring programs, it is necessary to develop additional equations for these variables. In the general case, Darcy's law can be combined with the continuity equation to yield the Richards equation (Richards 1931):

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[K\ (\theta)\ \frac{\partial h}{\partial t}\right] \tag{6.21}$$

where

$K(\theta)$ = hydraulic conductivity at various heads (cm sec^{-1})
θ = soil water content (cm^3 cm^{-3})

and

$$V = -K(\theta)\frac{\partial h}{\partial t} \tag{6.22}$$

or, in simpler terms

$$\frac{\partial \theta}{\partial t} = -\frac{\partial V}{\partial z} \tag{6.23}$$

where

V = soil water velocity (cm day^{-1})

Writing Equation 6.23 in an integrated backwards finite difference form yields

$$\Delta z(\theta^{t+1} - \theta^t) = (V_i - V_{i-1})\,\Delta t \tag{6.24}$$

or

$$\theta^{t+1}\Delta z = (V_i - V_{i-1})\Delta t + \theta^t \Delta z \tag{6.25}$$

In these equations, t and $t+1$ denote the beginning and end of time step values, respectively, and "I" is the soil layer index. These equations can be further simplified by substituting the nomenclature SW for $\theta\Delta z$ so that

$$SW^{t+1} = SW^t + (V_i - V_{i-1})\,\Delta t \tag{6.26}$$

where

SW = soil water content (cm)

The velocities in Equation 6.26 are a function of inputs to the soil (irrigation, precipitation, infiltration) and outflows from the soil (evapotranspiration, runoff).

Water balance equations are separately developed for (a) the surface zone, (b) horizons comprising the active root zones, and © the remaining lower horizons within the unsaturated zone. The equations are:

Surface Zone

$$(SW)_1^{t+1} = (SW)_1^t + INF - I_1 - E_1 - U_1 \tag{6.27}$$

Root Zone

$$(SW)_1^{t+1} = (SW)_1^t + I_{i-1} - U_i - I_i \tag{6.28}$$

Below Root Zone

$$(SW)_1^{t+1} = (SW)_1^t + I_{i-1} - I_i \tag{6.29}$$

where

$(SW)_i^t$ = soil water in layer "I" on day "t" (cm)
E_i = evaporation (cm day^{-1})
U_i = transpiration (cm day^{-1})
I_i = percolation out of zone I (cm day^{-1})
INF = infiltration into layer 1 (cm day^{-1})

Daily updating of soil moisture in the soil profile using the above equations requires the additional calculations for infiltration, evaporation, transpiration, and percolation.

Infiltration is calculated as

$$INF = P + SM - Q - E \tag{6.30}$$

where, assuming a unit area of 1 cm^2,

P	=	precipitation as rainfall, minus crop interception (cm day^{-1})
SM	=	snowmelt (cm day^{-1})
Q	=	runoff (cm day^{-1})
E	=	evaporation (cm day^{-1})

The calculations of precipitation, snowmelt, and runoff on a daily time step are described in the following. The disaggregation of these values and the calculation of the change in the depth of ponding on a finer time step is included in Sections 6.3.7.4 and 6.4.4 that describe the simulation of furrow irrigation and ponded surface water.

Input precipitation is read in and pan evaporation and/or air temperature are additional inputs from which potential evapotranspiration (PET) is estimated. Incoming precipitation is first partitioned between snow or rain, depending on temperature. Air temperatures below 0°C produce snow that can result in the accumulation of a snowpack. Precipitation first encounters the plant canopy, and once the interception storage capacity is depleted, the remaining depth is available for runoff or infiltration.

The runoff calculation partitions the precipitation between infiltrating water and surface runoff. Infiltrating water can pond on the soil surface for a period of time before it infiltrates, but this ephemeral process is described in a following section. Runoff is calculated by a modification of the USDA Soil Conservation Service curve number approach (Haith and Loehr 1979). Snowmelt is estimated on days in which a snowpack exists and above freezing temperatures occur as

$$SM = C_M T \tag{6.31}$$

where

C_M	=	degree-day snowmelt factor (cm $°C^{-1}$ day^{-1})
T	=	average daily temperature (°C)

The precipitation and/or snowmelt are inputs to the SCS runoff equation written as

$$Q = \frac{(P + SM - 0.2S)^2}{P + SM + 0.8S} \tag{6.32}$$

where S, the watershed retention parameter, is estimated by

$$S = \frac{1000}{CN} - 10 \tag{6.33}$$

where

CN	=	SCS runoff curve number

Curve numbers (CN) are a function of soil type, soil drainage properties, crop type, and management practice. Typically, specific curve numbers for a given rainfall event are determined by using the sum of the rainfall totals for the previous 5 days, known as the 5-day antecedent moisture condition. In this release of PRZM, as in the original version, the curve numbers are continuously adjusted each day as a function of the soil water status in the upper soil layers. These algorithms were developed and reported by Haith and Loehr (1979 pp. 325 – 327). The approach used in PRZM does not incorporate all of their modifications, however. The algorithm used by PRZM-3 considers the contribution of snowmelt as a component in the runoff curve equation (via the snowmelt (SM) addition to precipitation), but does not adjust the watershed retention parameter, S, to account for the effects of frozen ground. In addition, field experience suggested an improvement to the mapping of antecedent soil moisture conditions to daily curve numbers (R.F. Carousel 2004, Personal Communication). The initial approach stepped from AMC (Antecedent Moisture Condition) I (driest, CN1) to II (average, CN2) to AMC III (wettest, CN3) based on absolute (1 cm) moisture departures from field capacity. In PRZM-3.12.2, field capacity is mapped to the midpoint between

CN2 and CN3, and the wilting point is mapped to the mid-point between CN1 and CN2. The curve number for each day is a linear interpolation between these set points. Because PRZM-3.12.2 restricts apparent soil moisture to this computational range, the effective CN is similarly restricted to the range from (CN1 + CN2)/2 to (CN2+CN3)/2. CN1 and CN3 are calculated as in Chow et al. (1988):

$$\mathrm{CN1} = \frac{4.2\,\mathrm{CN2}}{10 - 0.058\,\mathrm{CN2}} \tag{6.34}$$

$$\mathrm{CN3} = \frac{23\,\mathrm{CN2}}{10 + 0.13\,\mathrm{CN2}} \tag{6.35}$$

The daily evapotranspiration demand is divided among evaporation from canopy, ponded surface water, soil evaporation, and crop transpiration. Total demand is first estimated and then extracted sequentially from crop canopy storage, ponded surface water, and then from each layer until wilting point is reached in each layer or until total demand is met. Evaporation occurs down to a user-specified depth. The remaining demand, crop transpiration, is met from the active root zone. The root zone growth function is activated at crop emergence and increases stepwise until maximum rooting depth is achieved at crop maturity.

Actual evapotranspiration from a soil layer is estimated as:

$$ET_i = \mathrm{Minimum}\left[(SW_i - WP_i)\, f_{di},\ \ ET_p - \sum_{j=1}^{i-1} ET_j\right] \tag{6.36}$$

where

ET_i	=	the actual evapotranspiration from layer "*I*" (cm)
f_{di}	=	depth factor for layer "*I*"
WP_i	=	wilting point water content in layer "*I*" (cm)
ET_p	=	potential evapotranspiration (cm)

This equation states that the transpiration from any layer "*I*" is the minimum of the available water in layer "*I*" or the demand remaining after extracting available water from layers above "*I*" in the profile.

The depth factor, f_{di}, is internally set in the code. It linearly weights the extraction of *ET* from the root zone with depth. A triangular root distribution is assumed from the surface zone to the maximum depth of rooting, with the maximum root density assumed to be near the surface. This algorithm essentially views the plant as a pump and assumes that it will expend the minimum energy possible in pumping. As long as the soil water is equally available, water closest to the surface meets this criterion.

Evapotranspiration can also be limited by soil moisture availability. The potential rate cannot be met if sufficient soil water is not available to meet the demand. In that case, PRZM-3 modifies the potential rate by

$$ET_p = \begin{cases} ET_p & SW - WP \geq 0.6(FC - WP) \\ SMFAC \times ET_p & WP < SW - WP < 0.6(FC - WP) \\ 0 & SW \leq WP \end{cases} \tag{6.37}$$

where

FC	=	soil moisture content at field capacity (cm)
WP	=	soil moisture content at wilting point (cm)
SMFAC	=	soil moisture factor (dimensionless)
FC-WP	=	maximum soil moisture available to plants (cm)
SW-WP	=	plant-extractable soil moisture (cm)

The *SMFAC* concept has been used in other similar water balance models (Stewart et al. 1976, Haith and Loehr 1979) and is internally set in the code to linearly reduce ET_p when soil water becomes limited. Finally, if pan evaporation input data are available, ET_p is related to this later input value:

$$ET_p = C_p \, PE \tag{6.38}$$

where

PE	=	measured pan evaporation (cm day^{-1})
C_p	=	pan factor (dimensionless)

The pan factor is constant for a given location and is a function of the average daily relative humidity, average daily wind speed, and location of the pan with respect to an actively transpiring crop.

In the absence of pan evaporation data, ET_p can also be estimated by

$$ET_p = 14000 \, L_d^2 \, SVD \tag{6.39}$$

where

L_d	=	possible hours of sunshine per day, in 12-hour units
SVD	=	saturated vapor density at the mean air temperature (g cm^{-1})
SVD	=	$0.622 \, SVP / (R_g \, T_{abs})$
SVP	=	saturated vapor pressure at the mean absolute air temperature (mb)
R_g	=	dry-air gas constant
T_{abs}	=	absolute mean air temperature (K)

The final term in the various soil profile layer water balance equations that must be defined is the percolation value, *I*. Because the Richards equation is not solved in PRZM-3 utilizing soil water characteristic curves to predict water movement, PRZM-3 resorts to "drainage rules" keyed to soil moisture storages and the time available for drainage. Two options are included. Although bothe options are admittedly simplistic representations of soil moisture redistribution, they are consistent with the objectives of PRZM-3 and its intended uses.

6.3.2.1 Option 1

Percolation, *I*, in this option is defined in the context of two bulk soil moisture holding characteristics commonly reported for agricultural soils: field capacity and wilting point. Field capacity is a somewhat imprecise measure of soil water holding properties and is usually reported as the moisture content that field soils attain after all excess water is drained from the system under influence of gravity, usually at tensions of about 0.3 bar. The difficulty with this concept is the fact that some soils will continue to drain for long periods of time, and thus field capacity is not a constant. Admitting the lack of theoretical and physical rigor, we believe that the concept remains a useful measure of soil moisture capacity that has been successfully used in a number of water balance models (Stewart et al. 1976, Haith and Loehr 1979). Wilting point is a function of both the soil and the plants growing in the soil. It is defined as the soil moisture content below which plants are unable to extract water, usually at tensions of about 15 bar.

Field capacity and wilting point are used operationally to define two reference states in each soil layer for predicting percolation. If the soil water, *SW*, in any layer is calculated to be in excess of field capacity, then percolation is allowed to remove the excess water to a lower zone/layer. The entire soil profile excess is assumed to drain within 1 day. The lower limit of soil water permitted is the wilting point. One outcome of these assumed "drainage rules" is that the soil layers below the root zone tend to quickly reach field capacity and remain at that value. When this condition is reached, all water percolated below the root zone is assumed to displace the water in the next lower soil layer simulated, and so on to ground water. There is no allowance for lateral water movement. Water balance accounting in this manner should be most accurate for sandy soils in which water movement is relatively unimpeded, and least accurate for clay soils (Stewart et al. 1976).

6.3.2.2 Option 2

The second option is provided to accommodate soils having low permeability layers that restrict the "free drainage" assumed in Option 1. In the context of the field capacity reference condition, two things can occur. First, conditions may prevail that raise the soil moisture levels above field capacity for periods of time because the water is "backed

up" above a relatively impermeable layer. Second, the excess water may not drain during the 1-day period assumed in Option 1. To accommodate these two conditions, two additional parameters are needed. Maximum soil moisture storage, θ_s, is added to represent moisture contents under saturated conditions. The drainage rate also must be modified to allow drainage to field capacity over periods in excess of 1 day (one time step). The drainage rate is assumed to be a first-order function of the water content above field capacity and is modeled by

$$\frac{d}{dt}(\theta - \theta_{fc}) = -\alpha(\theta - \theta_{fc}) \tag{6.40}$$

which has the solution

$$\theta_i^{t+1} = (\theta_i^{t*} - \theta_{fc_i}) \exp(-\alpha \Delta t) + \theta_{fc_i} \tag{6.41}$$

where

θ	=	soil layer water content ($cm^3\ cm^{-3}$)
θ_{fc}	=	water content at field capacity ($cm^3\ cm^{-3}$)
α	=	drainage rate parameter (day^{-1})

In this equation, t and t+1 denote beginning and end of time step values, respectively, and "*I*" is the soil layer index. The value t* denotes a value of time between the beginning and the end of the time step. The variable θ_i^{t*} denotes current storage plus any percolation from the next layer above, before the occurrence of any drainage from the current layer. Because Equation 6.41 is solved independently for each layer in the profile, there is a possibility of exceeding the storage capability (saturation water content, θ_s) of a low-permeability layer in the profile if a more permeable layer overlies it. At each time step, once redistribution is complete, the model searches the profile for any $\theta_i > \theta_{s_i}$. If this condition is found, the model redistributes water back into overlying layers, as if the percolation of additional water beyond that necessary to saturate the low-permeability layer had not occurred. This adjustment is necessary due to the nature of Equation 6.41 and the fact that these equations for each layer are not easily coupled. The difficulty in coupling the equations for the entire profile arises from the dichotomy that only one of two factors can limit percolation from any given stratum in the profile: either the rate at which that stratum can transmit water, or the ability of the stratum below it to store or transmit water. This dichotomy leads to an iterative (or at least corrective) approach to the explicit solution of a system of equations for θ_i represented by Equation 6.41. It should be noted, however, that the value of α selected by this approach is only relevant if the permeability of the soil materials, and not storage considerations in the profile (i.e., the presence of a water table), is the limiting factor for percolation of water.

6.3.3 Chemical Application and Foliar Washoff

The predecessor release of PRZM (PRZM-2.2) allowed for four different modes of pesticide application (input parameter FAM): (1) direct application to soil; (2) foliar application based on a linear crop growth model; (3) foliar application based on an exponential filtration model, and (4) chemical incorporation based on a uniform distribution of chemical residues to a user-defined depth. With the first three methods, chemical residues directly applied to soil (i.e., not intercepted by foliage) were uniformly distributed to a depth of 1 cm. Additionally, chemical residues from foliar washoff were placed into the first soil compartment.

PRZM-3 contains 8 application options. CAMs 1 through 3 are equivalent to the previous FAMs 1 through 3 in PRZM-2.2 except for the allocation of distributing residues in the soil profile from direct soil application and chemical washoff. CAM 4 is equivalent to the previous FAM 4. CAMs 5 through 8 are new options.

CAM=1	Recommended for direct surface applications. Residues are distributed to 4 cm, linearly decreasing with depth.
CAM=2	Application to foliage based on a crop canopy that varies linearly during the growing season. This is the same as the previous FAM=2 in PRZM-2.
CAM=3	Pesticide foliar application using nonlinear exponential filtration. This is the same as the

previous FAM=3 in PRZM-2.

CAM=4 Recommended for rototil incorporation. Uniform incorporation into the soil to a depth specified by the user. This is the same as the previous FAM=4 in PRZM-2. Specifying a depth of 1.0 cm will result in the same distribution used in the PRZM-2 for FAM=1.

CAM=5 Pesticide incorporation into an opened furrow that is then covered. Residues are distributed through the soil linearly, increasing to a user-defined depth.

CAM=6 Similar to CAM=1 except that residues are linearly decreasing to a user-defined depth.

CAM=7 Recommended for T-Band granular application. User defines the fraction of chemical to be applied in the top 2 cm, the remainder of the chemical is applied uniformly between 2 cm and a user-defined incorporation depth.

CAM=8 Recommended for shank injection. Residues are incorporated into a single compartment at a depth specified by the user.

CAM=9 Recommended for application to a linearly growing crop canopy. Chemical reaching the soil surface is incorporated to the depth given by DEPI (modified CAM 2).

CAM=10 Recommended for nonlinearly growing canopy using exponential filtration. Chemical reaching the soil surface is incorporated to the depth given by DEPI (modified CAM 3).

NOTE: DEPI must be set greater than 0.0 for CAM=4-10. If DEPI = 0, or DEPI < the depth of the first (top) surface soil layer, the chemical reaching the soil surface is distributed into the first (top) surface soil layer.

Residue distribution in the soil for each of these application methods is presented in **Figure 6.4**.

Pesticide washoff from foliage is calculated in the same manner as PRZM-2.2 except that the disposition of washed-off residues are processed differently. In PRZM-3, residues from washoff are distributed in the soil in the same manner as CAM =1, that is linearly decreasing with depth to a depth of 4 cm (**Figure 6.4**). This differs from PRZM-2.2 in which residues from washoff were distributed into the first soil compartment. In addition, IRTYPE 4 (under-canopy sprinklers/drip irrigation) no longer removes pesticide from the crop canopy.

6.3.4 Chemical Dissolved in Runoff

In the previous release of PRZM (PRZM-2.2), chemical residues in the dissolved phase were uniformly and completely available for runoff to a depth of 1 cm. Residues below 1 cm were unavailable for runoff. With the nonuniform extraction model in PRZM-3, residues have decreasing availability with depth (non-linear model) under the rationale that interaction between soil-pore water and excess precipitation (runoff) is diminished as a result of obstructions in the soil structure. This phenomenon has been discussed by numerous researchers (Bailey et al. 1974, Römkens and Nelson 1974, Bruce et al. 1975, Leonard et al. 1979, Ahuja et al. 1981, Sharpley et al. 1981, Ahuja and Lehman 1983, Heathman et al. 1986, Emmerich et al. 1989)

The nonuniform extraction model employs an exponential curve (**Figure 6.3**) to restrict the amount of dissolved phase chemical that is allowed to mix with runoff water as a function of soil depth according to:

$$DRI_i = 0.7\left(\frac{1}{\frac{2}{Midtot_i} + 0.9}\right)^2 \qquad \textbf{(6.42)}$$

in which DRI_i is the fraction of dissolved-phase chemical present in compartment i available for runoff, $Midtot_i$ is the

depth to the midpoint of compartment *i* (cm), 0.7 is an efficiency factor, and 0.9 = depth-reduction coefficient. Calculations are performed for all compartments (*i*) from the surface to a depth of 2 cm.

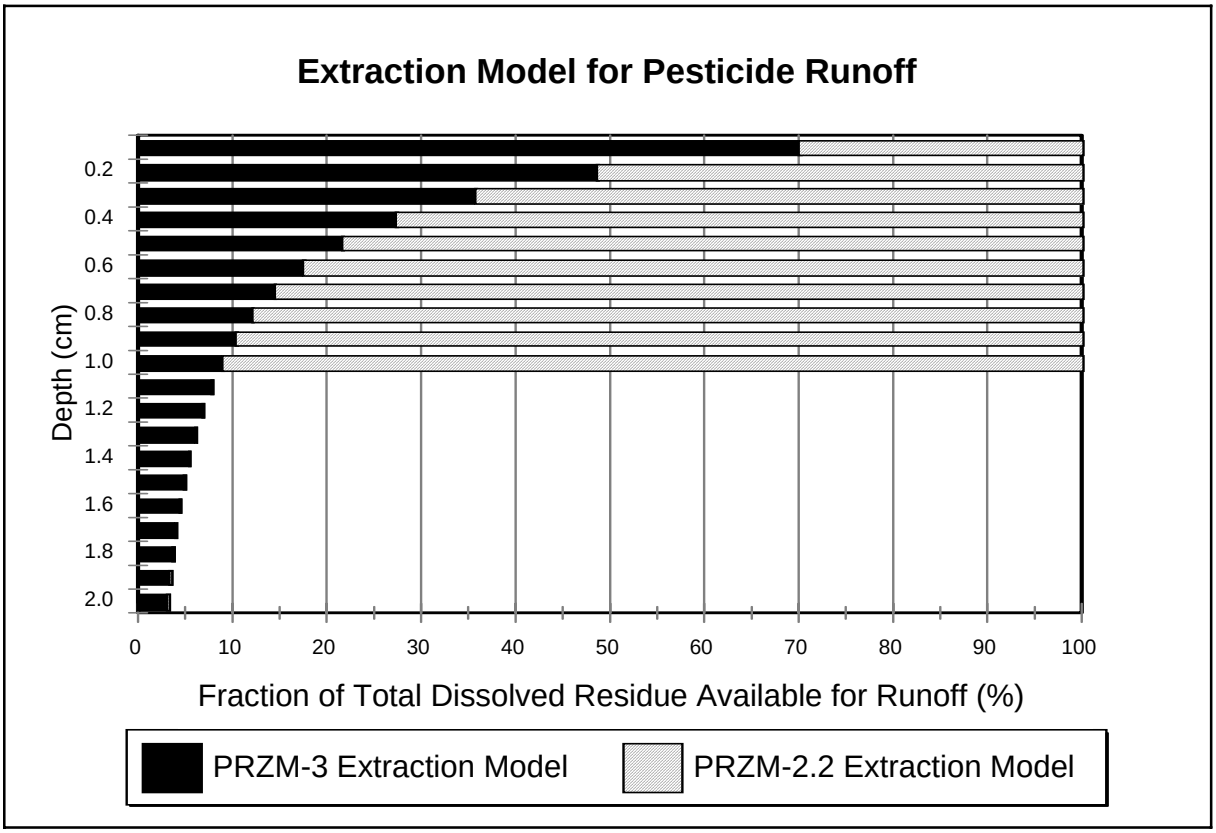


Figure 6.3 Extraction model for pesticide runoff.

The efficiency factor and the depth-reduction coefficient were derived empirically through model sensitivity runs and calibration during the application of the model to three field runoff study sites conducted for the herbicide atrazine in Georgia, Tennessee, and Iowa (discussed in more detail later in this section). The field studies used to derive the coefficients represent diverse climatology and soil textures.

Intuitively, the amount of decrease is likely to be dependent on several factors, including soil type, raindrop impact, and chemical *Kd*. Further analysis and calibration based on other field trials (including other chemicals) might yield further refinements to these factors or result in new equations and curves.

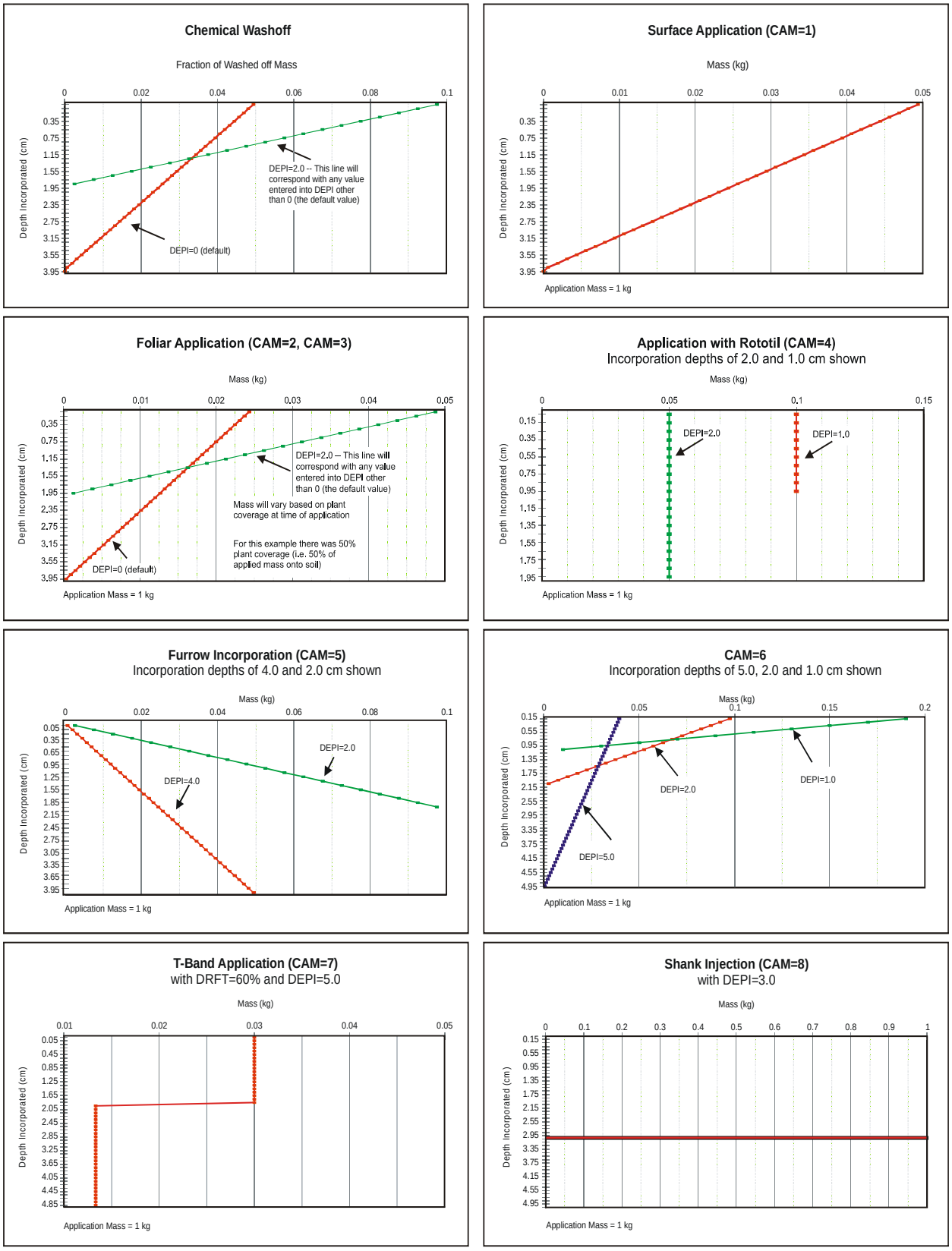


Figure 6.4 Illustration of chemical application methods.

6.3.5 Soil Erosion

Removal of sorbed pesticides on eroded sediments requires estimates for soil erosion. PRZM release 3 provides three methods to estimate soil erosion: the Modified Universal Soil Loss Equation (MUSLE) as developed by Williams (1975), contained in earlier versions of PRZM, plus two recent modifications, MUST and MUSS (Singh 1995):

$$\text{MUSLE,} \quad X_e = 1.586\ (V_r\ q_p)^{0.56} A^{0.12} K\ LS\ C\ P \tag{6.43}$$

$$\text{MUST,} \quad X_e = 2.50\ (V_r\ q_p)^{0.5} K\ LS\ C\ P \tag{6.44}$$

$$\text{MUSS,} \quad X_e = 0.79\ (V_r\ q_p)^{0.65} A^{0.009} K\ LS\ C\ P \tag{6.45}$$

in which

X_e	=	the event soil loss (metric tonnes day^{-1}),
V_r	=	volume of daily runoff event (mm),
q_p	=	peak storm runoff rate (mm/h),
A	=	field size (ha),
K	=	soil erodability factor (dimensionless),
LS	=	length-slope factor (dimensionless),
C	=	soil cover factor (dimensionless),
P	=	conservation practice factor (dimensionless).

MUST is a theoretical calculation and MUSS was specifically designed for small watersheds. The majority of parameter values for Equations 6.43 through 6.45 are determined from other calculations within PRZM (e.g., V_r) or are familiar terms readily available from handbooks.

Peak storm runoff rate, q_p, is calculated using the Graphical Peak Discharge Method (Soil Conservation Service, (Soil Conservation Service 1986):

$$q_p = a\ q_u\ A\ V_r\ F_p \tag{6.46}$$

in which

q_u	=	unit peak discharge rate, and
F_p	=	pond and swamp adjustment factor.

The parameter a is a units conversion factor. F_p has been preprogrammed to have a value of 1.0 in PRZM release 3. The unit peak discharge rate, q_u, is calculated by:

$$\log(q_u) = C_0 + C_1 \log(T_c) + C_2 [\log(T_c)]^2 \tag{6.47}$$

in which T_c is the time of concentration (hour) and C_0, C_1, and C_2 are regional coefficients that are related storm intensity and precipitation volume (See Soil Conservation Service 1986). The meteorological files that drive PRZM contain daily values of precipitation with no record of rainfall intensity over time. Therefore, rainfall intensity is assumed to occur according to design storm distributions (Type I, IA, II, and III) developed by the Soil Conservation Service from available National Weather Service duration-frequency data (Soil Conservation Service 1986). Distributions and associated regions are provided in **Figure 6.3** and **Figure 5.8**, respectively.

The SCS rainfall distributions were originally developed for flood control design and are biased to reflect intense, brief rainfalls. As a result, seasonal modifications to the SCS design storms were introduced to better represent periods that are characterized by longer duration precipitation events (e.g., frontal systems as opposed to thunderstorms). Regional peak discharge coefficients derived from the rainfall distributions are contained in Table 6.1.

The time of concentration, T_c, is defined as the time it takes water to flow from the furthest point in the watershed to a point of interest within the watershed, and is a function of basin shape, topography, and surface cover. T_c is calculated by summing the travel times for various designated flow segments within the watershed (Soil Conservation Service 1986). PRZM release 3 is configured with two flow segmentsto be summed : sheet flow for the first 100 meters and shallow, concentrated flow (unpaved) for the remaining portion of the hydraulic length. T_c is given by:

$$T_c = \underbrace{\frac{a\ 0.007\ (n\ L)^{0.8}}{P^{0.5} s^{0.4}}}_{\text{(sheet flow)}} + \underbrace{\frac{bL}{3600(16.1345 s^{0.5})}}_{\text{(shallow conc. flow)}} \qquad \textbf{(6.48)}$$

in which

n	=	Manning's roughness coefficient for the watershed,
L	=	hydraulic flow length (m),
P	=	daily precipitation (cm), and
s	=	slope of the hydraulic grade line(land slope, m/m).

Table 6.1 Coefficients for Calculation of Unit Peak Discharge

Rainfall Type	I_aP	C_0	C_1	C_2	Rainfall Type	I_aP	C_0	C_1	C_2
I	0.10	2.3055	-	-	II	0.10	2.55323	-	-0.16403
	0.20	2.2353	-	-		0.30	2.46532	-	-0.11657
	0.25	2.1821	-	-		0.35	2.41896	-	-0.08820
	0.30	2.1062	-	-		0.40	2.36409	-	-0.05621
	0.35	2.0030	-	0.01983		0.45	2.29238	-	-0.02281
	0.40	1.8773	-	0.05754		0.50	2.20282	-	-0.01259
	0.45	1.7631	-	0.00453	III	0.10	2.47317	-	-0.17083
	0.50	1.6788	-	0.0		0.30	2.39628	-	-0.13245
IA	0.10	2.0325	-	-		0.35	2.35477	-	-0.11985
	0.20	1.9197	-	-		0.40	2.30726	-	-0.11094
	0.25	1.8384	-	-		0.45	2.24876	-	-0.11508
	0.30	1.7265	-	0.02633		0.50	2.17772	-	-0.09525
	0.50	1.6341	-	0.0					

Coefficients *a* and *b* are unit conversion factors. The term for shallow, concentrated flow is derived from Manning's equation assuming a roughness coefficient, *n*, of 0.05 and a hydraulic radius of 0.2 (Soil Conservation Service 1986).

The enrichment ratio, r_{om}, is the remaining term that needs to be defined to estimate the removal of sorbed pesticides by erosion from the upper (top) soil layer. Because erosion is a selective process during runoff events, eroded sediments become "enriched" in smaller particles. The sediment transport theory available to describe this process requires substantially more hydraulic spatial and temporal resolution than is available in PRZM-3, leading to the adoption of an empirical approach (Menzel 1972). The enrichment ratio for organic matter is calculated from

$$\ln(r_{om}) = 2 - 0.2\ln(X_e/A_w) \quad \textbf{(6.49)}$$

6.3.6 Volatilization

Since volatilization was not included in the original release of PRZM, its theoretical basis is discussed in detail here. The following key processes have been identified as being important in deriving the volatilization algorithms to simulate vapor-phase pesticide transport within the soil/plant compartments:

- Vapor-phase movement of the pesticide in the soil profile
- Boundary layer transfer at the soil-air interface
- Vertical diffusion of pesticide vapor within the plant canopy
- Pesticide mass transfer between the plant (leaves) and the surrounding atmosphere
- Soil temperature effects on pesticide volatilization

The discussion of the volatilization algorithms is presented in four parts: influence of vapor phase pesticide in soil and volatilization flux, volatilization flux through the plant canopy, volatilization flux from plant surfaces, and soil temperature modeling and effects. **Figure 6.5** is a schematic of the pesticide vapor and volatilization processes considered in the PRZM-3 soil and plant compartments.

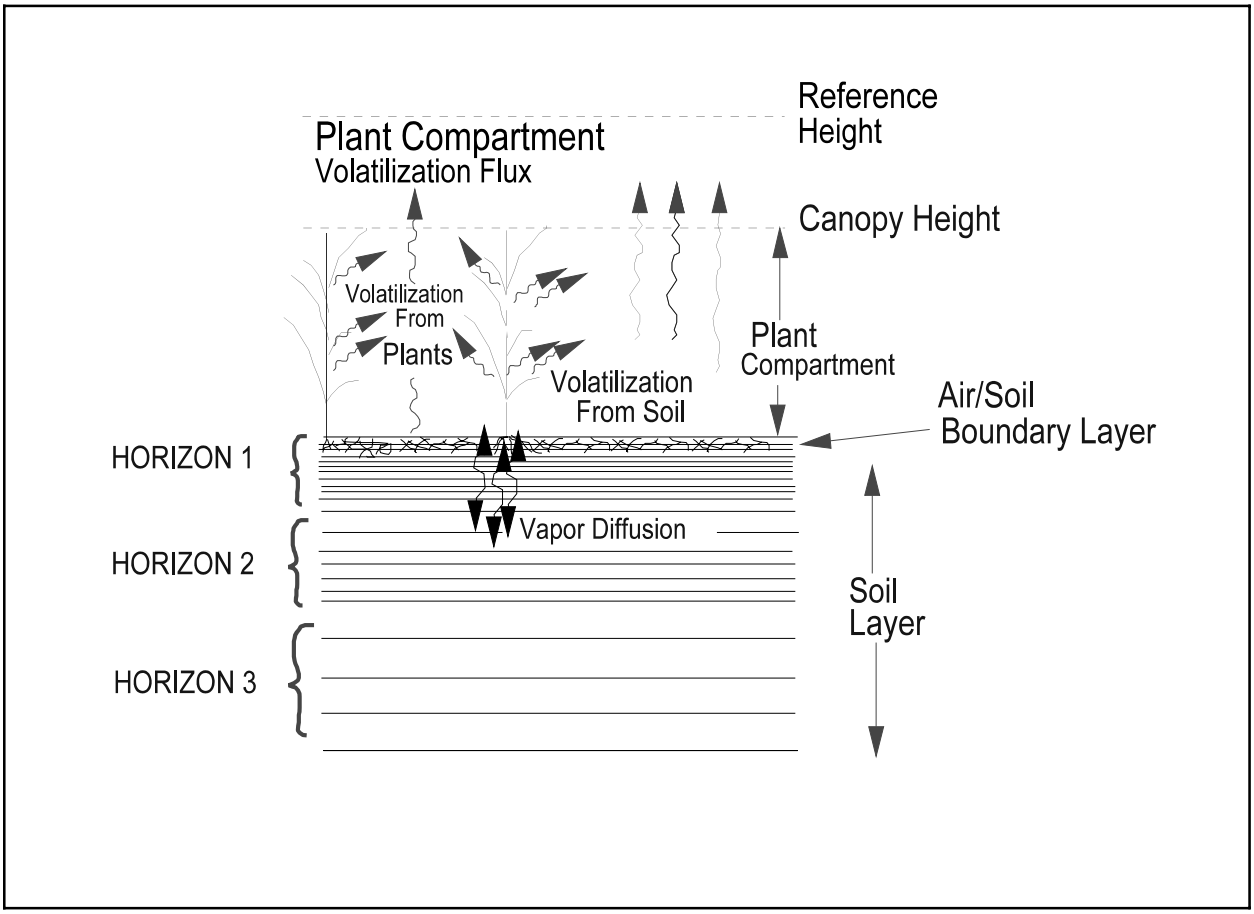


Figure 6.5 Schematic of pesticide vapor and volatilization processes.

6.3.6.1 Soil Vapor Phase and Volatilization Flux

The basic governing equations for chemical transport in the vapor phase were introduced previously in the description of transport in the soil. Fluxes from the soil column in the vapor phase are summarized in that discussion by Equations 6.3, 6.5, and 6.10. The terms in these equations are summed with the other flux terms to produce the overall pesticide transport Equation 6.20. In addition to these new terms, the upper boundary of PRZM-3 was changed from a zero-concentration boundary to a stagnant-layer boundary to allow diffusive transport upward from the soil to the overlying atmosphere. This enhancement is discussed in detail in the following.

Surface boundary condition – When a pesticide is incorporated into the soil, the initial volatilization rate is a function of the vapor pressure of the chemical at the surface as modified by adsorptive interactions with the soil. As the concentration at the surface of the soil changes, the volatilization rate can become more dependent on the rate of movement of the pesticide to the soil surface (Jury et al. 1983b).

The soil surface layer can be visualized as a membrane that allows water to pass through but keeps the solute behind. Experimental results show that, within the top centimeter of the soil surface, pesticide concentrations can increase as much as 10-fold due to the accumulation of chemical at the surface layer, resulting in higher vapor density. In order to describe these phenomena, Jury et al. (1983a, 1983b) proposed a boundary layer model that states that the controlling mechanism for pesticide volatilization is molecular diffusion through a stagnant surface boundary layer.

The layer of stagnant air may or may not form a significant barrier to volatilization loss for a given pesticide, depending on a variety of factors. In general, if the diffusion rate through the air layer is able to match the upward flux to the soil surface without having the surface concentration build up, then the stagnant layer is not acting as a barrier to loss and the volatilization flux will not depend strongly on the thickness of the boundary layer. Conversely, if the diffusion rate through the air is less than the flow to the surface by diffusion or mass flow, then the concentration at the soil surface will not be close to zero, and the thickness of the air layer will regulate the loss by volatilization. In other words, the significance of the boundary layer model depends on the ratio of the magnitudes between the upward soil pesticide flux and the boundary layer diffusion flux. Only downward, advective movement of water is treated in PRZM Release I. In this case, the sources that contribute to the upward soil pesticide flux are only the diffusion processes in the vapor and dissolved phases, but not upward water advection.

The zero chemical concentration upper boundary condition in the first release was modified in accordance with Jury's boundary layer model. The pesticide volatilization flux from the soil profile can be estimated as follows:

$$J_1 = \frac{D_a A}{d} (C_{g,1} - C^*_{g,d}) \qquad \textbf{(6.50)}$$

where

J_1	=	volatilization flux from soil (g day^{-1})
D_a	=	molecular diffusivity of the chemical in air (cm^2 day^{-1})
A	=	cross-sectional area of soil column (cm^2)
d	=	thickness of stagnant air boundary layer (cm)
$C_{g,1}$	=	vapor-phase concentration in the surface soil layer (g cm^{-3})
$C^*_{g,d}$	=	vapor-phase concentration above the stagnant air boundary layer (g cm^{-3})

The thickness of the stagnant boundary layer can be estimated using a water vapor transport approach (Jury et al. 1983a). However, Wagenet and Biggar (1987) assumed a constant value of 5 mm for this thickness, which is consistent with the values estimated by Jury. Consequently, the same assumption of a 5 mm thickness for the stagnant layer has been used here pending the results of further sensitivity analyses. The value of $C^*_{g,d}$ can take on a value of zero if the soil surface is bare or can be positive if a plant canopy exists.

6.3.6.2 Volatilization Flux Through the Plant Canopy

In pioneering work on this topic, Parmele et al. (1972) discuss a number of micrometeorological techniques for calculating pesticide volatilization flux from observed aerial pesticide concentrations. Their procedures are based on

the assumption that the vertical diffusivity coefficient (K_z) for pesticide vapor is analogous to the vertical diffusivity for water vapor, energy, or momentum. The pesticide volatilization flux can be computed by Fick's first law of diffusion, as follows

$$J_z(Z) = -K_z(Z)\,\frac{dP}{dZ} \tag{6.51}$$

where

$J_z(Z)$	=	pesticide gaseous phase flux at height Z (g m^{-2} s^{-1})
dP/dZ	=	pesticide gaseous phase concentration gradient (g m^{-2})
$K_z(Z)$	=	the vertical gaseous phase diffusivity at the height Z (m^2 s^{-1})

The value of K_z depends on the turbulence of the atmosphere into which the pesticide vapor is dissipated. Therefore, K_z is primarily a function of the prevailing meteorological conditions and not of any physical or chemical property of the pesticide.

In order to apply these concepts, vapor phase pesticide concentrations at two or more heights are required to estimate the pesticide gradient and the subsequent flux. For the estimation of vertical diffusivity, more extensive meteorological information is also required. These data requirements pose significant limitations for a predictive modeling approach.

In developing this PRZM-3 module, the following approaches circumvent the intensive data requirements. First, a relationship for K_z is derived as a function of height within the canopy. Then only the pesticide concentration gradient (or a suitable surrogate) is needed to compute the pesticide volatilization flux.

<u>Estimation of $K_z(Z)$</u> – Mehlenbacher and Whitfield (1977) present the following formula to compute K_z at various heights within a plant canopy.

$$K_z(Z) = K_z(Z_{CH})\,\exp\left[4.0\left(\frac{Z}{Z_{CH}} - 1.0\right)\right] \tag{6.52}$$

$$K_z(Z_{CH}) = \frac{U^*\,k(Z_{CH} - \underline{D})}{\phi_h} \tag{6.53}$$

$$U^* = \frac{k\,U_{CH}}{\ln[(Z_{CH} - \underline{D})/Z_o] + \psi_m\phi_m} \tag{6.54}$$

where

$K_z(Z)$	=	thermal eddy diffusivity at height Z (m^2 s^{-1})
$K_z(Z_{CH})$	=	thermal eddy diffusivity at canopy height (m^2 s^{-1})
Z_{CH}	=	canopy height (m)
Z_o	=	roughness length (m)
$\underline{D}$	=	zero plane displacement height (m)
k	=	von Karman's constant, 0.4
U^*	=	friction velocity (m s^{-1})
ϕ_h	=	stability function for sensible heat
$\psi_m(\phi_m)$	=	integrated momentum stability parameter
ϕ_m	=	stability function for momentum
U_{CH}	=	wind speed at the canopy height (m s^{-1})

For agricultural applications, the canopy height is used as a reference height for calculating U^*. The user must supply the wind speed and the height at which the measurement was made. The wind speed at the canopy height (U_{CH}) is

$$\frac{U_{CH}}{U_r} = \frac{\ln\left[\frac{Z_{CH} - \underline{D}_{CH}}{Z_{o,CH}}\right] - \psi_m(\phi_{m,CH})}{\ln\left[\frac{Z_r - \underline{D}_r}{Z_{o,r}}\right] - \psi_m(\phi_{m,r})} \tag{6.55}$$

where

U_r	=	wind speed (m s^{-1}) measured at the reference height Z_r (m)
D_r	=	zero plane displacement height (m) associated with the measurement
D_{CH}	=	zero plane displacement height (m) associated with the canopy
$Z_{o,r}$	=	roughness length (m) associated with the measurement
$Z_{o,CH}$	=	roughness length (m) associated with the canopy
$\phi_{m,CH}$	=	stability function for momentum associated with the canopy
$\phi_{m,r}$	=	stability function for momentum associated with the measurement

PRZM-3 assumes observations are made under neutrally stable atmospheric conditions. Under these conditions, $\psi_m(\phi_m)$ is equal to zero and Equation 6.55 reduces to the standard logarithmic wind velocity profile:

$$\frac{U_{CH}}{U_r} = \frac{\ln\left[\frac{Z_{CH} - \underline{D}_{CH}}{Z_{o,CH}}\right]}{\ln\left[\frac{Z_r - \underline{D}_r}{Z_{o,r}}\right]} \tag{6.56}$$

Aerodynamic parameters for several conditions are given in Table 6.2. PRZM assumes Open Flat Terrain parameters for wind speed computations. The user caan specify a reference height in the PRZM-3 input file (record 31, ZWIND).

Table 6.2 Aerodynamic parameters for wind speed computations. (Burns et al. 2005)

Surface	Reference height (m)	Roughness Length Z_0 (m)	Zero Plane Displacement $\underline{D}$ (m)	Reference
Open Flat Terrain (Used for Meteorological Stations)	10	0.03	None (few isolated obstacles)	(U.S. Environmental Protection Agency 2000)
Class A Pan Anemometer	0.6	0.01476	0.08	Assumed approx. same as FAO Short Grass
FAO Reference Short-Grass Crop	2	0.01476	0.08	(Allen et al. 1998)
Open sea, fetch > 5km	–	0.0002	Depends on sea state	(U.S. Environmental Protection Agency 2000)
Large Water Surfaces	–	0.0001-0.0006 0.000228	Depends on sea state	

The friction velocity U^* can be visualized as a characteristic of the flow regime within the uppermost part of the plant canopy in which the logarithmic velocity distribution law holds. In Equation 6.54, U^* is calculated as a

function of U_{CH}, Z_{CH}, Z_o, $\underline{D}$, and ψ_m. Rosenberg (1974) describes $Z_o + \underline{D}$ as the total height at which the velocity profile above the canopy extrapolates to zero wind velocity. For very short crops (lawns, for example), Z_o adequately describes the total roughness length, and little adjustment of the zero plane is necessary (i.e., $\underline{D} = 0$).

For tall crops, Z_o is related to canopy height (Z_{CH}) by

$$\log Z_o = 0.997 \log(Z_{CH}) - 0.883 \qquad \textbf{(6.57)}$$

In tall crops, Z_o is not an adequate description of the total roughness length; a value of $\underline{D}$, the zero plane displacement, is needed. For a wide range of crops and heights (0.02 m < Z_{CH} < 25 m), the following equation for $\underline{D}$ has been developed (Stanhill 1969).

$$\log \underline{D} = 0.9793 \log(Z_{CH}) - 0.1536 \qquad \textbf{(6.58)}$$

This equation results from a linear regression analysis based on published data for 19 different crops with limited data measured for the same crop at different growth stages. In the calculation of K_z, the PRZM-3 module uses these latter two equations for estimation of Z_o and $\underline{D}$, since there is no method available to justify any variations for crop type, row spacing, or canopy density.

In PRZM, when the canopy height is less than or equal to 5 cm, $\underline{D}$ is assumed to be zero and Z_o is set to the value given by Equation 6.57, evaluated at Z_{CH} = 0.05 m.

With estimates of Z_o and $\underline{D}$ in hand, U^* (friction velocity) can be estimated if the values of the stability parameters (ψ_m and ϕ_h) are known. These two variables are closely related to the Richardson number, *Ri*, which is the measure of the rate of conversion of convective turbulence to mechanical turbulence. It is defined as follows (Wark et al. 1998):

$$Ri = \frac{(g/T)\ (\partial T/\partial Z)}{(\partial U/\partial Z)^2} \qquad \textbf{(6.59)}$$

where

g = acceleration of gravity (9.8 m sec^{-2})
T = potential temperature (kelvin)
Z = height above ground surface (m)
U= wind velocity (m s^{-1})

Potential temperature is defined as the temperature that a parcel of dry air would acquire if brought adiabatically from its initial pressure to a saturated pressure of 1000 millibars (Perkins 1974). In application of this model, the measured temperature is used in the Richardson number calculation, as suggested by Rosenberg (1974).

The sign of *Ri* indicates the atmospheric condition, and its magnitude reflects the degree of the influence. There are several different formulas for relating *Ri* to the atmospheric stability parameters; for present purposes, the sign of *Ri* is of greater concern than its magnitude. When *Ri* is larger than 0.003, the atmosphere exhibits little vertical mixing, reflecting stable conditions; when the absolute value of *Ri*, |*Ri*|, is less than 0.003, neutral stability conditions exist (Oliver 1971); and when *Ri* is less than -0.003, convective mixing becomes dominant and atmospheric conditions are unstable.

The nominal range of the Richardson number is -2.0 < *Ri* < 0.2 (Thibodeaux 1996). If the Richardson number is outside this range PRZM will take a corrective action (described below) and resume execution.

To relate the atmospheric stability parameters to the Richardson number, Arya (1988) proposed the following formulas in terms of the dimensionless height ζ.

$$\zeta = \begin{cases} Ri & Ri > 0 \\ \dfrac{Ri}{1 - 5Ri} & 0 \le Ri \le 0.2 \end{cases} \tag{6.60}$$

The definition of ζ preserves the sign of the Richardson number (Ri), i.e., both quantities are positive, or both are negative, or both are equal to zero. Therefore atmospheric stability can also be deduced from the sign of ζ. When the estimated $Ri \geq 0.2$, PRZM-3 sets Ri to 0.19 and continues execution. For neutral conditions ($Ri = 0$ or $\zeta = 0$), $\phi_m = \phi_h = 1$, and $\psi_m = 0$.

The stability functions for momentum (ϕ_m) and sensible heat (ϕ_h) are given by:

$$\phi_m(\zeta) = \begin{cases} (1 - 15\zeta)^{-1/4} & \zeta < 0 \\ 1 + 5\zeta & \zeta \ge 0 \end{cases} \tag{6.61}$$

$$\phi_h(\zeta) = \begin{cases} \phi_m^2(\zeta) & \zeta < 0 \\ \phi_m(\zeta) & \zeta \ge 0 \end{cases} \tag{6.62}$$

The integrated momentum stability parameter, ψ_m, is given by Thibodeaux (1996):

$$\psi_m(\zeta) = \begin{cases} \dfrac{\pi}{2} - 2\tan^{-1}(\phi_m) + \ln\left[\left(\dfrac{1+\phi_m^2}{2}\right)\left(\dfrac{1+\phi_m}{2}\right)^2\right] & \zeta < 0 \\ -5\zeta & \zeta \ge 0 \end{cases} \tag{6.63}$$

<u>The resistance approach for the estimation of volatilization flux from soil</u> – The calculation of the chemical volatilization flux from the soil is based on a resistance-type approach. For pre-plant pesticides, and time periods just after emergence and post-harvest, transport by volatilization from plant surfaces is much less than vapor phase transport by other mechanisms. For those conditions in which the plant leaves do not act as significant sources or sinks for pesticide vapor, the resistances of the air column over the whole plant compartment can be estimated as follows (Mehlenbacher and Whitfield 1977).

$$\Sigma R = R_{bd} + R_{pc} \tag{6.64}$$

$$R_{bd} = \frac{D}{D_a} \tag{6.65}$$

$$R_{pc} = \int_{D}^{z_{CH}} \frac{dz}{K_z(Z)} \tag{6.66}$$

where

ΣR	=	total vertical vapor transfer resistance (day cm^{-1})
R_{bd}	=	boundary layer resistance (day cm^{-1})
R_{pc}	=	plant canopy resistance (day cm^{-1})

The flux is calculated as follows

$$J_{pc} = \frac{C_{g,l}}{\Sigma R} \tag{6.67}$$

where

J_{pc}	=	volatilization flux from plant canopy (g cm^{-2} day^{-1})

$C_{g,1}$ = pesticide vapor concentration in top soil layer (g cm^{-3})

For those conditions in which plants can act as significant pesticide sources or sinks, another approach must be taken. The influences of plant canopy require the formulation for the surface boundary condition as described in the following two sections.

6.3.6.3 Volatilization Flux from Plant Surfaces

A detailed description of the controlling factors for volatilization from plant surfaces has been presented by Taylor (1978). He indicated that the distribution of the pesticide residues over the plant surface appeared to be the dominant factor. This, together with the influence of the microscale climate at the plant surface, makes accurate simulation of plant volatilization processes very difficult.

For organophosphate insecticides, Stamper et al. (1979) have shown that the disappearance rates from leaf surfaces can be estimated by a logarithmic or a first-order kinetics approach. Similar observations of first-order kinetics were found for volatilization of 2,4-D iso-octyl ester from leaf surfaces by Grover et al. (1985). Thus, a simple rate constant approach is possible that requires the user to input the first-order loss rate constant for volatilization. The plant leaf volatilization flux can be estimated as follows.

$$J_{pl} = M_{Z_{CH}} K_f = \int_{0.5\,Z_{CH}} \frac{dz}{K_z(Z)} \qquad \textbf{(6.68)}$$

where

J_{pl} = pesticide volatilization flux from the leaf (g cm^{-2} day^{-1})
M = foliar pesticide mass (g cm^{-2})
K_f = first-order volatilization loss rate constant (day^{-1})

A resistance type approach is also applicable for volatilization flux estimation from plant leaves. The current code employs the first-order kinetics approach to calculate pesticide volatilization flux from plant leaf surfaces described above. This approach, that requires the user to specify the first-order rate constants for plant leaf volatilization, was selected because it is consistent with the foliar fate model in PRZM Release I.

Average pesticide concentration in plant canopy – Volatilization flux from plant leaves (J_{pl}) will be calculated only if pesticide application to the plant foliage has been specified in the model input. Whenever a plant canopy exists, the averagepesricide concentration in the air within the plant canopy can be estimated as follows.

$$C_g^* = (J_{pc} + J_{pl})\ \Sigma\ R_{0.5} \qquad \textbf{(6.69)}$$

where

C_g^* = average concentration in the air between the ground surface and the plant canopy height (g cm^{-3})
$\Sigma R_{0.5}$ = canopy resistance from half canopy height to the top of the canopy

.3.6.4 Soil Temperature Simulation

Soil temperature is modeled in PRZM release 3 to correct the Henry's law constant, K_H, for temperature effects, to simulate temperature dependent degradation, and to limit infiltration during snowmelt and precipitation when the soil is frozen. The interaction of its microclimate with the soil surface that results in a given soil temperature regime is complex and dynamic. Soil surface configuration and plant residue cover, both affected by tillage, have significant impacts on soil heat flux and, therefore, soil temperature. Studies of tillage and residue effects on soil temperature have been dominated by qualitative observations and site-specific measurements. The lack of mathematical evaluation and supporting field data has limited the ability of researchers to predict, beyond qualitative terms, the

tillage and residue effect on soil temperature for soil and climatic conditions other than those under which data have been collected.

The objective of the soil temperature model is to provide a scientifically sound and usable approach: (i) to predict with reasonable accuracy the daily average soil temperatures at the soil surface and in and below the root zone, utilizing basic soil physical and thermal properties, and daily climatic measurements taken at weather stations; and (ii) to allow consideration of the residue, canopy, and tillage effects on soil temperature.

Several models are available to predict soil temperature under various soil surface conditions, but there are restrictions to the general use of these models because either they need large data bases that are not available at many places, or they are site-specific. Existing soil temperature models form two general groups: (1) process-oriented models, which require detailed information on soil and surface characteristics, initial and boundary conditions, and inputs, and (2) semi- or non-process-oriented models, which often utilize weather station information and soil temperature information at one depth to develop empirical relationships for extrapolation to other locations.

Table 6.3 summarizes the key characteristics of the soil temperature models reviewed in this work. For both the process and semi-process oriented models, the two primary components are estimation of soil surface (or upper boundary) temperatures and soil profile temperature utilizing the calculated or estimated surface temperature as the upper boundary condition. A number of the models utilize the same procedure for calculating temperature in the soil profile (Gupta et al. 1981, Wagenet and Hutson 1987) and differ only in the procedures for specifying the surface boundary condition.

Van Bavel and Hillel (1976b, 1976a) developed a dynamic numerical procedure to link the process-oriented simulations of heat movement in the soil and the partition of heat and energy at the soil surface. Soil surface temperature, T_o, is calculated as a factor in predicting evaporation from a bare soil. Their technique utilized simultaneous solutions of seven equations with seven unknowns: net radiative flux, evaporation rate, air sensible heat flux, soil sensible heat flux, surface soil temperature, Richardson's number, and the saturation humidity at the surface soil temperature. Heat and water (liquid) flows are each coupled at the soil surface. An iterative procedure was used at each update to find the proper soil surface temperature. Soil profile temperatures were then estimated (Wierenga and de Wit 1970) by using these estimates of T_o as the surface boundary condition. Inputs required for this model include solar radiation, air and dewpoint temperature, wind speed, initial soil temperature profile, and the surface roughness evaluated by its effect on the aerodynamic roughness parameter. No comparisons were made between predicted and measured soil temperatures. Thibodeaux (1979) describes a similar energy-balance procedure for calculating soil surface temperatures.

For modeling soil profile temperatures, Hanks et al. (1971) used a numerical approximation for the one-dimensional soil-heat flow equation. This method requires the input of initial and boundary conditions, as well as the soil thermal conductivity and heat capacity as a function of depth and time. Predicted root zone soil temperature profiles were within 1°C of observed values for a 3-day period, but this model needs estimated or measured soil surface temperatures as its upper boundary condition.

Using the Hanks et al. (1971) procedure for the root zone, Gupta et al. (1981, 1982, 1983, 1984) developed a model for estimating hourly soil temperature by depth from meteorologic data. Inputs needed for this model include hourly air temperature at the 2-m height; daily maximum and minimum soil temperatures; initial soil temperature with depth; and soil thermal diffusivity, that can be estimated from soil mineral composition, organic matter percentage, bulk density, and soil water content. The upper boundary temperature is estimated by a sine function. The amplitude of the function is equal to the difference between daily maximum temperatures of air and soil surface or daily minimum temperatures of air and soil surface. Empirical curves, relating daily maximum air temperature to daily maximum soil surface temperature and daily minimum air temperature to daily minimum soil surface temperature, were developed for different residue and tillage conditions for the specific application site. These relationships provided a means of accounting for residue and tillage effects on soil temperature, but require site-specific data.

The correction for temperature dependent degradation is based on the Q_{10} equation (similar to an Arrhenius equation).

$$Q10FAC = QFAC^{(T - T_{BASE})/10} \quad \textbf{(6.70)}$$

where

$Q10FAC$	=	correction factor for biodegradation based on the actual temperature
$QFAC$	=	factor for rate increase when temperature increases by 10°C
T	=	actual soil temperature
T_{BASE}	=	temperature during the test of biodegradation

The soil temperature model in PRZM-3 is derived from a combination of the work by van Bavel and Hillel (1976b) and Thibodeaux (1979) for estimating the soil surface/upper boundary temperature. The soil profile temperature procedures are those developed by Hanks et al. (1971) and applied by Gupta et al. (1981, 1982, 1983)and Wagenet and Hutson (1987).

Table 6.3 Summary of Soil Temperature Model Characteristics

Model/Author(s)	van Bavel and Hillel (1976a)	Thibodeaux (1979)	Gupta et al. (1981, 1982, 1983)	Parton (1984)	Cruse et al. (1980)	Hasfurther and Burman (1974)	Williams et al. (1984)	Wagenet and Hutson (1987)	Chen et al. (1983)
1) Type of Model:									
a)Process-Oriented	X	X					X	X	X
b)Semi-Process-Oriented			X	X					
c)Non-Process-Oriented					X	X			
2)Heat Flow Process									
a)Conduction	X		X	X			X	X	X
b)Convection									X
c)Radiation	X	X			X		X		AT
3)Upper Boundary Temperature									
a)Est. by Energy Partitioning	X	X							
b)Est. by Empirical Relationship			X	X	X		ME	AVE	
4)Soil Temperature Profile: (Solving 1-D Heat Flow Eqn. Using the Procedure of:)									
a) Hanks et al. (1971)			X	EX				X	
b) Wierenga and de Wit (1970)	X*								
c)Curve Fitting					X**	X	DD		
5)Input Data Required									
a)Daily Max and Min Air Temp.			X	X	X	X	X		

Table 6.3 Summary of Soil Temperature Model Characteristics

Model/Author(s)	van Bavel and Hillel (1976a)	Thibodeaux (1979)	Gupta et al. (1981, 1982, 1983)	Parton (1984)	Cruse et al. (1980)	Hasfurther and Burman (1974)	Williams et al. (1984)	Wagenet and Hutson (1987)	Chen et al. (1983)
b)Daily Max and Min Soil			X						
Surface Temperature									
c)Hourly Air Temperature	X	X	X						X
d)Hourly Solar Radiation	X	X		XX	XX		XX		
e)Surface Albedo	X	X			X		X		
f)Wind Velocity	X	X			X				
g)Humidity/Dewpoint Temp.	X	X							
h)Canopy Shadow/Ht. of Veg.	X	X							
i)Soil Water Content	X		X		at 5 cm		X	X	X
j)Soil Bulk Density	X		X		X		X	X	X
k)Soil Mineral Composition	X		X		X			X	X
l)Percentage Organic Matter	X		X		X			X	X
6)Soil Surface Condition									
a)Residue Cover	X		X		X			X	100%
b)Tillage Condition			X		X		X		
c) Crop Canopy	X	X	X	X			X		
7)Time Step									

Table 6.3 Summary of Soil Temperature Model Characteristics

Model/Author(s)	van Bavel and Hillel (1976a)	Thibodeaux (1979)	Gupta et al. (1981, 1982, 1983)	Parton (1984)	Cruse et al. (1980)	Hasfurther and Burman (1974)	Williams et al. (1984)	Wagenet and Hutson (1987)	Chen et al. (1983)
a)Hourly	X	X	X	X				X	X
b)Daily					X	X	X	X	X

* - Horton et al. (1984) used a 2-D heat flow equation.
** - Regression equation is fitted for soil temp at 5-cm depth.
AVE - "Average" measured soil surface temperatures are used.
AT - Ambient air temperature is used as upper boundary temperature.
DD - Damping depth parameter is used to predict soil temperature at different depths.
XX - Total daily solar radiation.
EX - Explicit Finite Difference Scheme.
ME - Simplified mathematical relationship involving solar radiation, surface albedo, and daily min and max air temperatures.

Estimating upper boundary temperature – An energy balance procedure is used in PRZM-3 to estimate soil surface temperature (van Bavel and Hillel 1976b, Thibodeaux 1979). The same procedure is used in the POSSM model (Brown and Boutwell 1986), that employed PRZM-2 as a framework for PCB fate simulation.

The basic energy-balance equation with terms having units of cal cm^{-2} day^{-1} at the air/soil interface is described as:

$$R_n - H_s - LE_s - G_s = \Delta TH \qquad \textbf{(6.71)}$$

where

R_n	=	net radiation (positive downward)
H_s	=	sensible air heat flux (positive upward)
LE_s	=	latent heat flux (positive upward)
G_s	=	soil heat flux (positive downward)
ΔTH	=	change in thermal energy storage in the thin surface soil layer (cal cm^{-2} day^{-1})

The term ΔTH is also given by:

$$\Delta TH = (\rho_b d)\ s\ (T_{i+1} - T_i) \qquad \textbf{(6.72)}$$

where

ρ_b	=	bulk density of soil (g cm^{-3})
d	=	thickness of a thin, surface soil layer (cm)
s	=	the specific heat capacity of soil (cal g^{-1} $°C^{-1}$)
T_i, T_{i+1}	=	the representative temperature for the surface layer at two consecutive time steps and can be represented as the average of the temperatures at the top and bottom of thethin, surface soil layer ($°C^{-1}$/day).

For evaluating the heat exchange across the air/soil interface, the top soil layer thickness, d, can be set to a small value so that ΔTH may be neglected. As a result, the right side of Equation 6.71 can be set equal to zero.

Net radiation flux at any surface can be represented as:

$$R_n = (R_s - R_{sr}) + (R_{la} - R_{lar}) - R_{ls} \qquad \textbf{(6.73)}$$

where

R_n	=	the net radiation flux (cal cm^{-2} day^{-1})
R_s	=	incident short-wave solar radiation (cal cm^{-2} day^{-1})
R_{sr}	=	reflected short-wave solar radiation (cal cm^{-2} day^{-1})
R_{la}	=	incident long-wave atmospheric radiation (cal cm^{-2} day^{-1})
R_{lar}	=	reflected long-wave atmospheric radiation (cal cm^{-2} day^{-1})
R_{ls}	=	long-wave radiation emitted by the soil (cal cm^{-2} day^{-1})

The terms R_s and R_{sr} include both the direct and diffuse short-wave radiation, and are related as follows.

$$R_{sr} = \alpha R_s \qquad \textbf{(6.74)}$$

where

α	=	the albedo of the surface (dimensionless)

Therefore, the short-wave radiation component of the energy balance is

$$R_s - R_{sr} = R_s(1 - \alpha) \qquad \textbf{(6.75)}$$

The incident short-wave radiation can either be measured directly using pyranometers or calculated using a variety of available empirical relationships or nomographs. PRZM-3requires input of radiation daily time series, whether measured or calculated, in order to simulate soil temperature.

The albedo of a canopy-covered land surface can be estimated as:

$$\alpha(t) = \alpha_c C(t) + \alpha_s [1 - C(t)] \tag{6.76}$$

where

$\alpha(t)$	=	albedo on day t
α_c	=	albedo of canopy cover (0.23 for vegetation)
$C(t)$	=	canopy cover on day t (fraction)
α_s	=	albedo of soil surface (dimensionless)

Since the albedo of a soil surface changes with the soil surface condition, its value must be defined by the user as 12 monthly values corresponding to the first day of each month; the albedo value for each day is interpolated between the neighboring monthly values. For snow cover less than 0.5 cm, the surface albedo is estimated using Equation 6.76, and for snow cover above 0.5 cm, the surface albedo is set equal to the snow albedo value (0.80).

The incident long-wave atmospheric radiation, R_{la}, is represented as

$$R_{la} = e_a \sigma T_a^4 \tag{6.77}$$

where

e_a	=	emissivity of the atmosphere (dimensionless)
σ	=	the Stefan-Boltzmann constant (11.7×10^{-8} cal cm^{-2} K^{-4} day^{-1})
T_a	=	the air temperature (K)

Wunderlich (1972) proposed a correction to Equation 6.77 for the effects of cloud cover, that can increase R_{la} by up to 25 percent under overcast conditions. However, this correction is not included in the model because it would require input of a cloud cover time series, and the effect on the calculated soil surface temperature would be small.

The emissivity of the atmosphere varies from a low of 0.7 to almost unity. Numerous empirical relationships for estimating e_a have been proposed (Salhotra 1986). A simple, reliable method is the use of Swinbank's formula:

$$e_a = 0.936\times10^{-5} T_a^2 \tag{6.78}$$

The reflected long-wave radiation, R_{lar}, can be expressed as:

$$R_{lar} = R_{la} (1 - \gamma) \tag{6.79}$$

where

γ	=	the reflectivity of the surface for long-wave radiation (dimensionless)

The resulting net atmospheric long-wave radiation component becomes:

$$R_{la} - R_{lar} = R_{la}(1 - \gamma) = 0.936\times10^{-5} T_a^6 \sigma (1 - \gamma) \tag{6.80}$$

The long-wave radiation component emitted by the soil surface is represented in an analogous equation to the atmospheric component, as follows

$$R_{ls} = e_s \sigma T_s^4 \tag{6.81}$$

where

e_s	=	infrared emissivity of soil (dimensionless)
σ	=	the Stefan-Boltzmann constant (11.7×10^{-8} cal cm^{-2} K^{-4} day^{-1})
T_s	=	soil surface temperature (K)

Since the soil emissivity and reflectivity are related as $e_s = 1-\gamma$, we can replace $(1 - \gamma)$ in Equation 6.80 with e_s.

Combining the radiation components from Equations 6.75, 6.80, and 6.81, the net radiation flux is calculated as

follows.

$$R_n = (1 - \alpha) R_s + 0.936 \times 10^{-5} \sigma T_a^6 e_s - e_s \sigma T_s^4 \quad \textbf{(6.82)}$$

The evaporative heat flux, LE_s, is estimated by:

$$LE_s = \mu E \rho_w \quad \textbf{(6.83)}$$

where

μ	=	latent heat of vaporization/unit quantity of water (580.0 cal g^{-1})
E	=	evaporation rate (cm day^{-1})
ρ_w	=	density of water (1.0 g cm^{-3})

The evaporation rate , E, is obtained from the evapotranspiration (EVPOTR) subroutine of PRZM. It is assumed that the calculated evapotranspiration from the top 5 cm of soil represents the potential evaporation energy loss at the air/soil interface. However, only a fraction of the evapotranspiration loss calculated by PRZM contributes to this heat flux. This fraction is estimated as the portion of the land surface not covered by vegetation, (i.e., 1.0 - canopy cover).

The sensible air heat flux, H_s, is given by:

$$H_s = \rho_a C_{pa} h (T_s - T_a) \quad \textbf{(6.84)}$$

where

ρ_a	=	air density (g cm^{-3}), estimated by $\rho_a = (-0.0042\ T_a + 1.292) \times 10^{-3}$ (Thibodeaux (1979))
C_{pa}	=	specific heat of air at constant pressure (0.2402 cal g^{-1} K^{-1})
h	=	heat transfer coefficient at air-soil interface (cm day^{-1})
T_a	=	the air temperature (°C)

The heat transfer coefficient is given by:

$$h = K_1^2 V_z \ln\left(\frac{Z_{RH} - \underline{D}}{Z_o}\right) \quad \textbf{(6.85)}$$

where

K_1	=	Von Karman's number (0.4)
V_z	=	wind velocity (cm day^{-1})
Z_{RH}	=	reference height at which V_z is measured (m)
$\underline{D}$	=	zero plane displacement (m)
Z_o	=	roughness height (m)

Equation 6.85 is valid only when the air temperature does not vary greatly with height, as is often the case near sunrise or sunset or under cloudy skies or when canopy heights are relatively small. It appears to be a reasonable approximation for most agricultural crops. Correlations have been developed relating Z_o and $\underline{D}$ to the canopy height as described previously in this section by Equations 6.57 and 6.58, respectively.

From the fundamental equation of heat conduction, the soil heat flux, G_s, is given by:

$$G_s = (T_s - T_1) \lambda_1 / D_1 \quad \textbf{(6.86)}$$

where

T_1	=	temperature of the soil at bottom of layer 1 (K)
T_s	=	soil surface temperature (K)
λ_1	=	thermal conductivity of layer 1 (cal cm^{-1} day^{-1} K^{-1})
D_1	=	thickness of layer 1 (cm)

Substituting Equations 6.82, 6.83, 6.84, and 6.86 into Equation 6.71 produces a polynomial in T_s :

$$e_s \sigma T_s^4 + [\rho_a C_{pa} h + \lambda_1 / D_1] T_s - [(1-\alpha) R_s + 0.936 \times 10^{-5} \sigma T_a^6 e_s + \rho_a C_{pa} h T_a - \mu E \rho_w + T_1 \lambda_1 / D_1] = 0 \quad \textbf{(6.87)}$$

The value of T_s at each time step is estimated by solving the above equation using an iterative solution based on the Newton-Raphson method. The initial estimate of soil surface temperature is taken to equal to the measured air temperature. The value for T_1 is obtained from the previous time step. These calculations are repeated until the difference between two consecutive estimates for soil surface temperature is less than the preset convergence criteria (set to 0.1°C).

Simulation of heat flow through the soil profile – The soil profile temperature model is based on the one-dimensional partial differential equation describing heat flow in soils:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(d \frac{\partial T}{\partial z} \right) \quad \textbf{(6.88)}$$

where

d = the soil thermal diffusivity.

The thermal diffusivity is equal to the ratio of thermal conductivity and heat capacity of the soil. The procedures used to estimate soil thermal conductivity and heat capacity are taken from de Vries (1963). They are calculated from basic soil properties – soil water content, mineral composition, texture, and thermal conductivity of the individual soil particles. These parameters are either input or supplied by the model in the simulation. The thermal diffusivity is given by:

$$d = \lambda / C \quad \textbf{(6.89)}$$

where

d = thermal diffusivity of the soil layer ($cm^2\ day^{-1}$)
λ = thermal conductivity of the soil layer ($cal\ cm^{-1}\ day^{-1}\ °C^{-1}$)
C = heat capacity per unit volume of the soil layer ($cal\ cm^{-3}\ °C^{-1}$)

Temperature effect – A detailed discussion of the temperature effect on the volatilization behavior of pesticides is presented by Streile (1984). Two parameters that influence the vapor-phase transport in the soil profile are Henry's constant and the vapor diffusion coefficient.

The equation used to correct Henry's constant for temperature effects is (Streile 1984):

$$K_H(T) = K_{H,1} \exp\left[\frac{-\Delta H_{vap} a}{R} \left(\frac{1}{T} - \frac{1}{T_1} \right) \right] \quad \textbf{(6.90)}$$

where

$K_{H,1}$ = Henry's constant at the reference temperature T_1
$\Delta H'_{vap}$ = partial molar enthalpy of vaporization from solution ($J\ mole^{-1}$)

The temperature effect on the vapor phase diffusion coefficient can be estimated from the Fuller correlation as presented in Liley and Gambill (1973). However, it is not implemented in the PRZM-3 code due to the general lack of information required to use it.

6.3.7 Irrigation Equations

PRZM-3 irrigation algorithms determine depths of irrigation water to be applied at the soil surface. These depths are computed based on the available soil water deficit, and are added as infiltration to the first (uppermost) PRZM soil compartment. Above- and below-canopy sprinklers, flooding, and furrow irrigation can be simulated. Methods for

computing water application depths/amounts for each type of irrigation are described in the following paragraphs.

6.3.7.1 Soil Moisture Deficit

Irrigation is triggered in PRZM-3 when the soil moisture volume in the active root zone (whose depth increases during crop development) falls to a user-defined fraction (with permissible range of 0.0 to 0.9) of the available water capacity (θ_{fc}-θ_{wp}). The soil moisture deficit, *D*, is then given by:

$$D = (\theta_{fc} - \theta_z)\, Z_r \qquad \textbf{(6.91)}$$

where

D	=	soil moisture deficit (cm)
θ_z	=	active root-zone soil moisture content (cm^3cm^{-3}) on the current day
θ_{fc}	=	active root-zone soil moisture content at field capacity (cm^3cm^{-3})
Z_r	=	active root zone depth (cm) (varies with crop stage)

D is the depth of water over the unit area that must be added to the soil by irrigation to bring the soil water content up to field capacity.

Rainfall can also occur on the same day as irrigation water has been applied: PRZM assumes that the decision to irrigate has been made and implemented prior to the beginning of the rain event. This behavior probably imitates most agricultural practice, i.e., apparent crop needs are likely in most instances to weigh more heavily than do uncertain weather forecasts in a decision to irrigate the crop. This rather conservative, although not unreasonable, assumption can lead to significant runoff and erosion producing events, for example, from a field that has been irrigated in the morning and then receives an additional soaking from an afternoon convective storm.

6.3.7.2 Sprinkler Irrigation

Irrigation water from sprinklers can be applied either above or below the crop canopy. When applied above the crop canopy, irrigation water is intercepted by the canopy and may or may not run off when it reaches the soil surface. (At the user's option, however, runoff can be prevented, thereby invoking an assumption that irrigation rates are generally controlled intentionally to avoid exceeding the infiltration rate.) The depth of water applied during a daily PRZM-3 time step by overcanopy sprinklers is estimated from the soil moisture deficit as:

$$Da = D\,(1 + LF) + I_f \qquad \textbf{(6.92)}$$

where

Da	=	depth of irrigation water applied to the field (cm)
LF	=	a factor specified by the user to allow for the practice in saline soils of adding water to leach salts out of the root zone (fraction of *Da*)
I_f	=	crop canopy interception capacity (cm)

The water depth *Da* is applied as “precipitation” above the crop canopy, and canopy interception is computed for the current crop situation in the PRZM-3 crop growth subroutines. Unless the user specifies that irrigation is controlled to prevent runoff, sprinkler runoff from the soil surface is estimated using the SCS curve number approach, assuming that runoff characteristics of sprinkler water are similar to those of precipitation. Water that does not run off infiltrates into the first (uppermost) PRZM-3 soil compartment.

Irrigation water applied below the crop canopy is not subject to canopy interception losses. The depth of water applied by undercanopy sprinklers is therefore, is given by:

$$Da = D\,(1 + LF) \qquad \textbf{(6.93)}$$

The irrigation water depth APDEP is applied as throughfall to the soil surface; potential sprinkler runoff is also estimated using the SCS curve number approach.

In some instances, the sprinkler system may be unable, due to hydraulic limitations, to deliver water at the rate needed to meet the required daily application depth. In these cases, the sprinkler application depth *Da* is set equal to the maximum depth that the system can deliver. The user, therefore, is required to input the maximum water application rate R_{max} (cm hr^{-1}) for the particular sprinkler system to be used.

6.3.7.3 Flood Irrigation

Flood irrigation, in this case, refers to the practice of flooding entire fields with irrigation water. Flood-irrigated fields are diked around the edges to allow water to pond and infiltrate into the soil. In the PRZM irrigation algorithm, it is assumed that this water ponds uniformly over the entire field. The amount of water applied to the soil surface is then:

$$Da = D\ (1 + LF) \qquad \textbf{(6.94)}$$

Since the field is assumed to be diked around the edges, no water is allowed to run off from the field.

6.3.7.4 Furrow Irrigation

Furrow irrigation involves the release of water into numerous small channels that cut across the planted field. Infiltration depths within furrows vary due to differences in times at which water reaches various locations down the furrow, with less water infiltrating at the downstream end (**Figure 6.6**). Hydraulic characteristics of the furrow determine how quickly water moves down the channel, while soil characteristics determine the rate of infiltration once water reaches a location in the furrow.

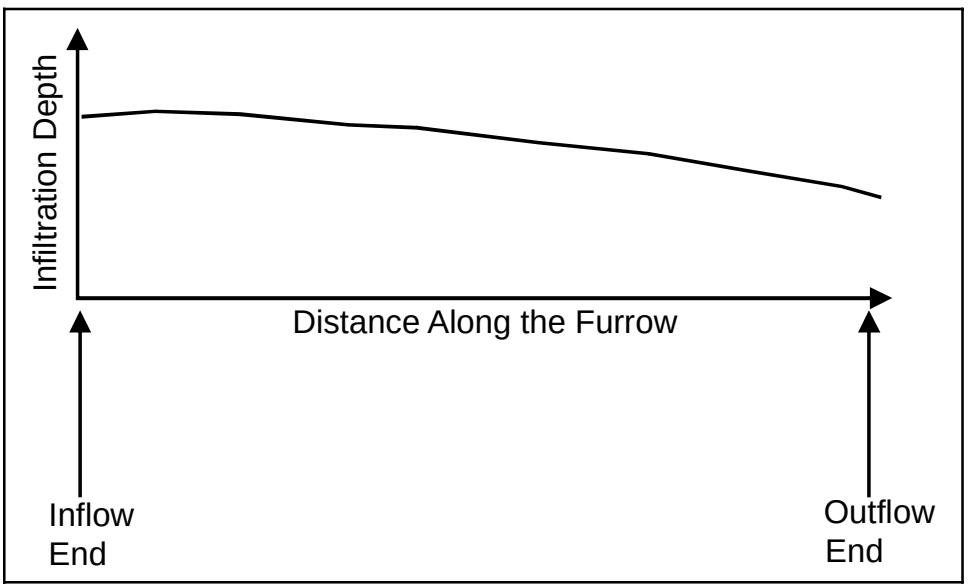


Figure 6.6 Variability of infiltration depths within an irrigation furrow.

The PRZM-3 furrow irrigation model computes daily infiltration depths at various locations down the length of the furrow. This requires solution of the open channel flow equations of motion coupled with a soil infiltration model. Model developers have made numerous attempts to solve the furrow-irrigation advance problem, ranging in complexity from empirical volume-balance solutions (Fok and Bishop 1965, Wilke and Smerdon 1965) to numerical solutions of the full open channel flow equations of motion (Bassett and Fitzsimmons 1974). In general, solutions of the full equations of motion are too computationally intensive for this application, while simpler empirical models involve infiltration parameters that are not easily related to physical soil characteristics.

The PRZM-3 furrow advance model uses the kinematic wave simplification of the equations of motion coupled with the Green-Ampt infiltration model to determine furrow infiltration depths. Kinematic-wave theory neglects inertial

accelerations and assumes that the water surface slope is equal to the ground slope. The equations of motion then reduce to:

$$\frac{\partial Q}{\partial z} + \frac{\partial A}{\partial t} = -\frac{\partial q}{\partial t} \qquad \textbf{(6.95)}$$

where

Q	=	flow rate in the channel ($m^3\ s^{-1}$)
A	=	cross-sectional area of flow (m^2)
z	=	distance down the furrow (m)
q	=	lateral flow infiltrated per unit length of channel (m^3 /m s))

The flow area A is related to the flow rate Q by Manning's equation:

$$Q = \frac{1}{n} AR^{2/3}\ S^{1/2} \qquad \textbf{(6.96)}$$

where

n	=	Manning's roughness coefficient
R	=	the hydraulic radius of flow (m)
S	=	the channel slope (vertical/horizontal)

Section 6.4.4 explains how the solution of the horizontal furrow irrigation equation is applied in PRZM-3.

6.3.8 Nitrogen Species Algorithms

Nitrogen species reactions can be divided between those that are chemical in nature and those that are a combination of chemical and biological reactions. The adsorption and desorption of ammonium is a chemical process. The user has the option of simulating ammonium adsorption and desorption by first order kinetics with subroutine FIRORD or by the Freundlich isotherm method with subroutine SV (discussed in the following).

The other nitrogen species reactions are a combination of biological and chemical transformations. They all can be simulated with first order kinetics, but plant uptake can optionally use another algorithm (described later). The optimum first order kinetic rate constant is corrected for soil temperatures below 35°C by the generalized equation:

$$KK = K \times TH^{T-35} \qquad \textbf{(6.97)}$$

where:

KK	=	temperature corrected first order transformation rate constant (per day)
K	=	optimum first order reaction rate constant (per day)
TH	=	temperature coefficient for reaction rate correction (dimensionless) (typically about 1.06)
T	=	soil layer temperature (°C)

Soil temperature must also be simulated when nitrogen species transformation processes are being simulated with PRZM-3. When temperatures are greater than 35°C, the rate is considered optimum, that is, *KK* is set equal to *K*. When the temperature of the soil layer is below 4°C or the layer is dry, no biochemical transformations occur. Identifiers with a leading "K" (e.g., KDNI) are the optimum rates; those for corrected rates have both a leading and trailing "K" (e.g., KDNIK). The corrected reaction rate constants are determined every day and multiplied by the respective storages as shown in **Figure 6.7** to obtain the reaction fluxes.

Denitrification is also modeled as a first-order rate, but it is dependent on soil moisture levels following procedures used in GLEAMS (Knisel et al. 1994). The user controls the starting point of denitrification by specifying the initial “% saturation” soil moisture level, the denitrification rate then increases linearly to a maximum at saturation (at the current soil temperature value).

The biochemical reaction rate fluxes that are shown in **Figure 6.7** are coupled, that is, added to and subtracted from the storages simultaneously. The coupling of the fluxes is efficient in use of computer time but has a tendency to produce unrealistic negative storages when large reaction intervals and large reaction rates are used jointly. A method has been introduced into PRZM-3 that modies the reaction fluxes so that they do not produce negative storages. A warning message is issued when this modification occurs.

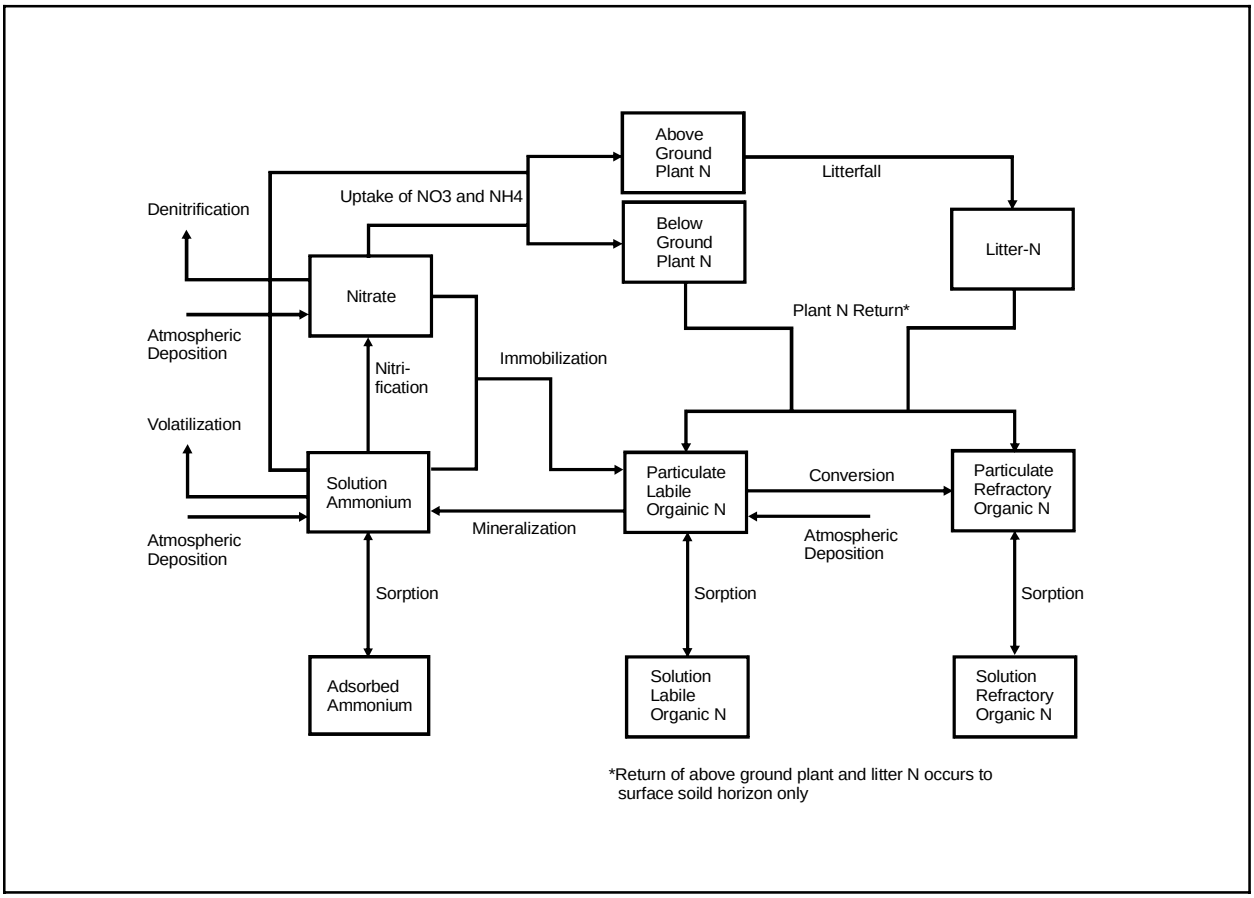


Figure 6.7 PRZM-3 soil/plant nitrogen transformations.

6.3.8.1 Ammonia Volatilization

Ammonia volatilization is included to allow large concentrations of ammonia in the soil resulting from OSWDS (On-site Wastewater Disposal System, i.e., septic systems) inputs, animal waste, and fertilizer applications to be attenuated by losses to the atmosphere. A simple, first-order rate expression is used in PRZM-3 with an adjustment for air temperature. The original formulation (Reddy et al. 1979) was adjusted for the soil cation exchange capacity (CEC) and wind speed, and automatically turned off after seven days. In the PRZM-3 implementation, we assume that the constant CEC factor is incorporated into the first-order rate constant, and the wind speed (air flow) is always large enough to result in maximum loss (Reddy's equation reduced volatilization only when wind was less than 1.4 km/day). Also, we calculate the volatilization rates for each soil horizon such that the rates decrease as the ammonia moves down through the soil column. The volatilization flux in each layer is computed as:

$$AMVOL = AMSU \cdot KVOL \cdot TCVOL^{T-20} \qquad \textbf{(6.98)}$$

where:

$AMVOL$ = loss of ammonia (mg l^{-1} day^{-1})
$AMSU$ = dissolved ammonia concentration (mg/l)

KVOL = rate constant at 20°C (day^{-1})
TCVOL = temperature correction coefficient (dimensionless)
T = air temperature (°C)

The temperature correction for volatilization of ammonia is slightly different than that described for the other first-order rate processes. The reference temperature can be user-specified; since rates in the literature are often given at a temperature of 20°C, we use this value as the default. Also, the rate will be adjusted upwards when the soil temperature exceeds the reference temperature.

6.3.8.2 Sorption/Desorption of Ammonium

When FORAFG = 0, the adsorption and desorption reaction fluxes of ammonium chemicals are simulated with the FIRORD subroutine using temperature-dependent first-order kinetics. The calculation of these fluxes by first-order kinetics for soil temperatures less than 35°C takes the form:

$$DES = CMAD \cdot KDS \cdot THKDS^{TMP-35} \quad \textbf{(6.99)}$$

$$ADS = CMSU \cdot KAD \cdot THKAD^{TMP-35} \quad \textbf{(6.100)}$$

where:
DES = current desorption flux of chemical (mass/area per time interval)
CMAD = storage of adsorbed chemical (mass/area)
KDS = first-order desorption rate constant (per time interval)
THKDS = temperature correction coefficient for desorption
TMP = soil layer temperature (°C)
ADS = current adsorption flux of chemical (mass/area per time interval)
CMSU = storage of chemical in solution (mass/area)
KAD = first-order adsorption rate constant (per time interval)
THKAD = temperature correction coefficient for adsorption; *THKDS* and *THKAD* are typically about 1.06.

All of the variables except the temperature coefficients can vary with the layer of the soil being simulated. As noted previously, soil temperature must be simulated when nitrogen is being simulated. The temperature correction of the reaction rate constant is based on the Arrhenius equation. At temperatures of 35°C or above, no correction is made. When the temperature is at 0°C or below or the soil layer is dry, no adsorption and desorption occurs.

When FORAFG = 1, subroutine SV simulates sorption/desorption based on the Freundlich isotherm that unlike first-order kinetics, assumes instantaneous equilibrium. That is, no matter how much chemical is added to a particular phase, equilibrium is assumed to be established between the solution and adsorbed phase of the chemical. This method also assumes that for any given amount of chemical in the soil, the equilibrium distribution of the chemical between the soil solution and on the soil particle can be found from an isotherm.

The adsorbed and solution phases of ammonium in this subroutine are related by a modification of the standard Freundlich equation. When the amount of chemical is less than the capacity of the soil particle lattice to permanently bind the chemical (*XFIX*), then all the material is consider fixed. All the fixed chemical is contained in the adsorbed phase of the soil layer storage. Otherwise, the Freundlich equation is used to determine ammonium/chemical partitioning between into the adsorbed and solution phases is:

$$X = KF1 \times C^{1/N1} + XFIX \quad \textbf{(6.101)}$$

where:
X = chemical adsorbed on soil (ppm of soil)
KF1 = single value Freundlich *K* coefficient
C = equilibrium chemical concentration in solution (ppm of solution)
N1 = single value Freundlich exponent
XFIX = chemical that is permanently fixed (ppm of soil)

This equation is solved in subroutine ITER by an iteration technique. The parameters used in the computation can differ for each soil horizon.

6.3.8.3 Nitrogen Inputs

Inputs of nitrogen to the surface and subsurface soil horizons can include OSWDS (On-site Wastewater Disposal System, i.e., septic system effluent) loadings, atmospheric deposition, and nitrogen additions through fertilizer and/or manure applications. All nitrogen inputs are defined in their elemental forms as NO_3-N, NH_4-N, and organic N; for each of the three input forms further restrictions apply on the form and species of the applied amounts (discussed in the following).

OSWDS loadings can be input as user-defined WDM files, or as output files generated by either or both of the treatment options included in the OSWDS module; they are then input to a specific PRZM soil horizon defined by the user (see Section 4.2.3 for a complete discussion).

Two basic types of atmospheric deposition are simulated. Dry deposition is considered to be a flux input over the land surface independent of rainfall. Wet deposition is considered to be a concentration of a nitrogen species dissolved in the input precipitation. If data is available as a total flux only, it should be input as dry deposition. All deposition inputs are added to the surface soil horizon, and are assumed to be input as NO_3-N, adsorbed NH_4-N, and particulate labile organic N. See Section 4.2.2 for a discussion of input methods.

When atmospheric deposition is being simulated, the soil storage in the surface horizon is updated for each of these three species of nitrogen using the formula:

$$N(I+1) = N(I) + ADFX + PREC \times ADCN \qquad \textbf{(6.102)}$$

where:

N(I)	=	storage of nitrogen species in the soil surface layer on day *I*, in mass/area
ADFX	=	dry or total atmospheric deposition flux in mass/area per time interval
PREC	=	precipitation depth
ADCN	=	concentration of nitrogen species in wet atmospheric deposition in mass/volume

Nitrogen applications with fertilizers or manure is accomplished in a manner analogous to pesticide applications. Application dates are specified for the entire simulation period, along with the specific amounts of each N form, NO_3-N, NH_4-N, and organic N, the depth of incorporation for each application, and the labile fraction of the applied organic N. See Section 4 for a discussion of input methods.

6.3.8.4 Plant Uptake

Plant uptake of soil nutrients in PRZM-3 can be modeled by two alternative methods using the NITR module. When NUPTFG = 0, plant uptake is represented as a first-order rate process with an Arrhenius temperature correction adjustment based on simulated soil temperatures. The first-order plant uptake rates are defined by the user, can be specified separately for each soil horizon within PRZM, and can vary for each month to approximate the monthly pattern of crop growth and nutrient uptake. The rates are adjusted during calibration to mimic the expected annual nutrient uptake and the seasonal pattern for the specific crop and practice. Plant uptake can be distributed between nitrate and ammonium by input parameters intended to designate the fraction of plant uptake from each species.

Because this option uses first-order monthly uptake rates to represent time-varying plant nutrient uptake, the calculated uptake amounts are highly sensitive to, and a direct function of, the available nutrients in the soil profile and the specific nutrient input/application rates. This causes a problem when application rates are changed, such as under nutrient reduction alternatives, because the uptake amounts are not a function of expected crop yields and associated nutrient uptake; thus, even though sufficient nutrients may be available to satisfy crop needs under the reduced application rates, the calculated uptake may be less than the crop needs because of the first-order formulation.

The situation just described and other issues related to the plant uptake algorithms in the AGCHEM modules of HSPF have been reviewed, along with the primary alternative algorithms used in a number of other current agricultural nutrient models (Donigian et al. 1995). Based on that review and the compatibility of alternative functions with the AGCHEM and HSPF soil profile representation, the conceptual approach of the plant uptake formulation in the NLEAP model (Shaffer et al. 1991) was selected for incorporation into AGCHEM/HSPF Version No. 11 (Bicknell et al. 1995). This selection was based on the following characteristics of the NLEAP plant nutrient uptake function:

- Calculates crop nutrient needs as a function of expected crop yield
- Allows seasonal uptake variation based on expected crop growth patterns
- Accommodates (or can be modified to accommodate) time steps less than one day
- Considers both NO_3-N and NH_4-N as available for N uptake
- Considers N fixation, double cropping, and uptake from different soil layers
- Except for N fixation, the N uptake functions can be adapted for P uptake in AGCHEM
- Overall level of detail is consistent and compatible with AGCHEM

Due to differing hydrology, soil moisture, and soil profile simulation procedures among NLEAP, AGCHEM, and PRZM, the NLEAP plant N uptake functions required adaptation. The changes made primarily provided greater user flexibility in defining the timing and distribution of plant uptake from the individual soil layers, whose depths are also user-specified in both AGCHEM and PRZM, and to represent a wider potential range of land surface conditions. The details of the changes are discussed by Donigian et al. (1995).

The yield-based plant nitrogen uptake formulation is selected when NUPTFG = 1, and is essentially the same in PRZM-3 and AGCHEM/HSPF Version No. 11. A total annual nitogen uptake target, NUPTGT, is specified by the user, and is then divided into monthly targets during the crop growing season for each soil horizon. The monthly target for each horizon is calculated as:

$$MONTGT = NUPTGT \times NUPTFM(MON) \times NUPTM(MON) \times CRPFRC(MON,ICROP) \qquad \textbf{(6.103)}$$

where:

MONTGT	=	monthly plant uptake target for current crop, mass N/area
NUPTGT	=	total annual uptake target, mass N/area
NUPTFM	=	monthly fraction of total annual uptake target (dimensionless)
NUPTM	=	soil horizon fraction of monthly uptake target (dimensionless)
CRPFRC	=	fraction of monthly uptake target for current crop (dimensionless). Default value is 1.0, unless the month contains parts of two or more crop seasons, in which case the monthly uptake target is divided among the crops according to the number of days of the month belonging to each crop season.
MON	=	current month
ICROP	=	index for current crop

Planting and harvesting dates can be specified for up to three separate crops during the year. Plant uptake is assumed to occur only during its growing season, defined as the time period between planting and harvest. As stated previously, When portions of two growing seasons are contained within one month, the total monthly target is divided between the two crops in proportion to the number of days in each season in that month. The daily target is calculated by starting at zero at the beginning of a crop season and using a trapezoidal rule to solve for monthly boundaries; linear interpolation is used to solve for daily values between the monthly boundaries, and between a monthly boundary and a planting or harvest date.

Yield-based plant uptake values only occur when the soil moisture is above the wilting point, specified by the user for each soil horizon, and sufficient nutrients are available. No temperature rate adjustment is performed, but all uptake is stopped when soil temperature is below 4°C. If the uptake target is not met during a given time interval, whether due to nutrient, temperature, or moisture stress, then a deficit is accumulated and applied to the next time interval's target. If uptake later becomes possible, the program will attempt to make-up the deficit by taking-up nitrogen at a rate higher than the normal daily target, up to a user-specified maximum defined as a multiple of the

target rate. The deficit is tracked for each soil layer, and is reset to zero at harvest, i.e. it does not carryover from one crop season to the next.

When using the yield-based plant uptake option, it is also possible to represent leguminous plants (e.g. soybeans) that will fix nitrogen from the atmosphere. The algorithm is designed to allow N fixation only to make up any shortfall in soil nitrogen, i.e. fixation is only allowed if the available soil nitrogen (i.e. nitrate and solution ammonium) is insufficient to satisfy the target uptake. The maximum daily nitrogen fixation rate is subject to the same limits as the uptake under deficit conditions noted above.

6.3.8.5 Soil and Plant Nitrogen, and Litter Compartments

In the previous version of the NITR module in HSPF AGCHEM, plant N was a single "state variable" that represented the cumulative amount of N taken up by plants from each soil layer. This material continues to "build up" during the simulation, i.e., it is not converted to any other species in the soil. In AGCHEM Version 11 and PRZM-3 a pathway has been added in each layer so that plant N can be converted (by first-order rate) to organic N (labile particulate) to represent the return of plant N to the soil through leaf fall or crop residues, and root decay. This rate can be either constant or monthly variable.

Nitrogen that is taken up by the plants can be divided between above-ground and below-ground fractions (using a simple fraction of the total uptake). The above-ground plant N return would first fall into a litter compartment before returning to the soil organic N. Both of these rates - from above-ground N to litter and from litter to organic N - can be either constant or monthly variable. The above-ground plant N and litter N are single compartments, while the below-ground plant N storage will be maintained for each of the soil compartments. Note that under this option, the old definition of plant N as the nitrogen that has been derived from a particular layer will not be correct since some of the plant N derived from a layer will be allocated to the above-ground storage.

When ALPNFG = 1, plant nitrogen is divided into above-ground, litter, and below-ground compartments. Above-ground plant N returns to the litter compartment, and litter N returns to particulate organic N (with labile and refractory fractions) in the surface soil horizon. Both of these reactions are simulated using first-order kinetics. No other reactions affect these nitrogen storages except for plant uptake to the above-ground compartment, as calculated in subroutine NITRXN.

Return of litter and below-ground plant N to particulate organic N is divided into labile and refractory fractions, which can be constant or monthly variable. Regardless of the option used to simulate plant uptake, if the above-ground and litter compartments are being simulated, then the user can specify the fraction of uptake from each layer that goes to the above-ground storage. The rest is assumed to remain within the below-ground plant N compartment for that soil layer.

6.3.8.6 Organic Nitrogen Compartments and Reactions

The previous NITR module of AGCHEM contained a single organic N state variable in each soil layer. This material was assumed to be a particulate species that is increased from immobilization of nitrate and ammonia, and is converted back to ammonia by mineralization in the soil. It also is transported on the surface by association with sediment. In PRZM-3, this species is described as a "particulate labile" fraction of organic N; it will undergo conversion by first order rate to a "particulate refractory" fraction, and it will partition to a "soluble labile" fraction. The "particulate refractory" species will also partition to a "soluble refractory" fraction. The two soluble species will therefore be available for transport as runoff and leaching within the soil profile, and likewise, the new particulate fraction will be transported on the surface with sediment. The partitioning reactions are described by a simple ratio of particulate concentration to solution concentration, i.e. a standard linear partition coefficient. The four fractions and their assorted reactions are illustrated in **Figure 6.7**. Note that the storages and transformations in this figure are repeated in each soil horizon except for the aboveground plant N and the litter compartments.

6.4 Numerical Solution Techniques

This section describes the numerical techniques that are used to solve the differential equations introduced in the preceding section. Section 6.4.1 discusses the two numerical techniques available to solve the chemical transport equations – a backwards-difference implicit scheme and a method of characteristics algorithm. The additional terms and the adjustment in the upper soil boundary that are added into these transport equations to simulate volatilization are described in Section 6.4.2. The numerical approximations used to calculate soil temperature are presented in Section 6.4.3 and the numerical solution for furrow infiltration depths are presented in Section 6.4.4.

6.4.1 Chemical Transport Equations

The second-order partial differential equation outlined in Section 6.3 must be solved with appropriate boundary conditions. The calculations for moisture contents, air contents, pore velocities, erosion, and runoff are decoupled from, and solved in advance of, the transport equation. The resulting values, treated as constant for each specific time step, are then used as coefficients in a discretized numerical approximation of the chemical transport equation.

Two techniques are currently available to solve the discretized chemical transport equation for the new dissolved pesticide concentration at the end of the time step. The available techniques are:

- A backward-difference, implicit scheme to simulate all chemical transport processes
- A method of characteristics (MOC) algorithm that simulates diffusion, decay, erosion, runoff, and uptake by the backward-difference technique, but uses the method of characteristics to simulate advective transport

The user is allowed to select the desired solution technique in the input sequence. Details of these techniques are provided below. Results from test simulations are provided in Section 6.5.1.

Identical discretizations and initial and boundary conditions are used with both numerical simulation techniques. A spatial and temporal discretization step is used equal to those applied in the water balance equations. For boundary conditions at the base of the soil column, the numerical technique uses

$$\frac{C_{w_{i+1}}\theta_{i+1} - C_{w_i}\theta_i}{\Delta z} = 0 \qquad \textbf{(6.104)}$$

in which the subscripts "*i*" refer to soil layer numbers.

This condition corresponds to a zero concentration gradient at the bottom of the soil profile. The upper boundary condition is discussed in more detail in Section 6.4.2.

A backwards-difference solution algorithm was the only solution option available in the original PRZM model. In this method, the first derivative in space, the advection term, is written as a backward difference (i.e., involves the difference *C[i,j]-C[i-1,j]*). The second spatial derivative, the diffusion term, is centered in space (i.e., based on the terms *C[i-1,j]+C[i+1,j]-2C[i,j]*). The time derivative is also calculated as a backward difference in the original code, (*C[i,j]-C[i,j-1]*). The equations are then made implicit by writing each concentration for the (*j*+1)th time step. The advantage of this numerical scheme is that it is unconditionally stable and convergent. However, the terms truncated in the Taylor's series expansion from which the finite difference expression are formulated lead to errors that, in the advection terms, appear identical to the expressions for hydrodynamic dispersion. In the simulation results, these terms manifest themselves as "numerical dispersion," which is difficult to separate from the physical dispersion that is intentionally simulated. In systems exhibiting significant advection (i.e., high Peclet number), the artificial numerical diffusion may dominate the physical dispersion. It can be larger by orders of magnitude, leading to difficulty in the interpretation of simulation results.

To minimize the effects of numerical dispersion in systems having high Peclet numbers, a method of characteristics

solution was added as an option to PRZM-3. This solution method avoids the backwards-difference approximation for the advection term and the associated numerical dispersion by decomposing the governing transport equation. In advection-dominated systems, as the dispersion term becomes small with respect to the advection term, the advection-dispersion equation approaches a hyperbolic equation. According to the MOC theory, advection of the solute can be simulated separately from the other processes governing the fate of that advected solute. Baptista et al. (1984) state that no error is introduced by this decomposition provided that the advection equation is solved first by an explicit procedure, and the diffusion equation is solved next by an implicit technique. This order was preserved in the PRZM-3 model by utilizing a new explicit algorithm for advection that is always called first, and is immediately followed by execution of a modified version of the existing implicit algorithm for simulation of other processes. The advection algorithm employed was adapted from those described by Khalell and Reddell (1986) and Konikow and Bredehoeft (1978). These techniques were modified to allow simulation of changes in saturation and adsorption of the pesticide and variable compartment size.

In the new explicit advection algorithm, in addition to the fixed grid system, a set of moving points is introduced. These points can be visualized as carrying the chemical mass contained within a small region in space surrounding the point. Initially, these points are uniformly distributed throughout the flow domain. At each time interval, these moving points are redistributed according to the local solute velocity in each compartment. New points may enter the top of the flow domain, while old points may move out the bottom. When the moving points are transported in horizons where the compartment size is larger and numerical resolution is less, the points may be consolidated to conserve computational effort. After the new locations have been assigned to each point, the average concentration in each compartment is computed based on the number and mass carried by the points contained within the compartment at that time. This temporary average concentration is returned to the main program, and a subroutine that assembles the terms in the transport equation (without advection) is called. Changes in concentration due to all other transport and transformation processes (diffusion, decay, sources, etc.) are calculated for each compartment exactly as in the original version of PRZM. These values are then returned to the main program, and one transport step is complete.

When the MOC algorithm is called during the next time step, the exact location of each moving point has been saved. The first task is to update the masses carried by each moving point using the changes calculated during the last time step. Increases in mass are simply added equally to each point in the compartment, while decreases are weighted by the actual value at each point before subtraction to avoid simulating negative masses. The updated moving points are then relocated and the two-step process is repeated again until the end of the simulation.

Regardless of which method (backwards-difference or MOC) is selected to approximate the governing equation(s) for transport, a tri-diagonal matrix solution (Thomas algorithm) is utilized by the model code. The key elements of the tri-diagonal matrix are the lower diagonal element (A), the diagonal element (B), the upper diagonal element (C), and the vector of source terms (F). The elements of the solution matrix for the transport equation are determined based on the values supplied for numerous input parameters as identified below.

<u>'A' Term</u>

- DISP - dispersion/diffusion coefficient ($cm^2\ day^{-1}$)
- HENRYK - Henry's constant ($cm^3\ cm^{-3}$)
- DAIR - molecular diffusivity in the air ($cm^2\ day^{-1}$)

<u>'B' Term</u>

- DISP - dispersion/diffusion coefficient ($cm^2\ day^{-1}$)
- HENRYK - Henry's constant ($cm^3\ cm^{-3}$)
- DAIR - molecular diffusivity in the air ($cm^2\ day^{-1}$)
- DWRATE - solution phase degradation rate constant (day^{-1})
- DSRATE - adsorbed phase degradation rate constant (day^{-1})
- DGRATE - vapor phase degradation rate constant (day^{-1})
- KD - adsorption/partition coefficient for soil ($cm^3\ g^{-1}$)
- BD - mineral soil bulk density ($g\ cm^{-3}$)
- UPTKF - plant pesticide uptake efficiency factor

- PEVP - pan evaporation data (cm day^{-1})
- DKRT12 - transformation rate from parent pesticide to first daughter product (day^{-1})
- DKRT13 - transformation rate from parent pesticide to second daughter product (day^{-1})
- DKRT23 - transformation rate from first daughter product to second daughter product (day^{-1})
- ELTERM - erosion loss term, calculated from erosion input parameters
- DKBIO - biodegradation term, calculated from biodegradation input parameters

'C' Term

- DISP - dispersion/diffusion coefficient (cm^2 day^{-1})
- HENRYK - Henry's constant (cm^3 cm^{-3})
- DAIR - molecular diffusivity in the air (cm^2 day^{-1})

'F' Term

- KD - adsorption/partition coefficient for soil (cm^3 g^{-1})
- BD - mineral soil bulk density (g cm^{-3})
- HENRYK - Henry's constant (cm^3 cm^{-3})
- DKRT12 - transformation rate from parent pesticide to first daughter product (day^{-1})
- DKRT13 - transformation rate from parent pesticide to second daughter product (day^{-1})
- DKRT23 - transformation rate from first daughter product to second daughter product (day^{-1})
- FEXTRC - foliar extraction coefficient for foliar washoff model (cm^{-1})

6.4.2 Volatilization

The numerical techniques discussed in Section 6.4.1 are the basis of the simulation of chemical transport in all phases. However, some modifications have been made to the upper boundary condition in order to model volatilization of chemical from the soil surface.

In order to simulate vapor-phase pesticide movement past the soil surface, the zero concentration upper boundary conditions used in the original PRZM code has to be modified. Jury's boundary layer model (Jury et al. 1983a, Jury et al. 1983b) has been incorporated into the PRZM-3 code. The model states that the controlling mechanism for pesticide volatilization is molecular diffusion through the stagnant surface boundary layer. The volatilization flux from soil profile can be estimated by:

$$J_1 = \frac{D_a A}{\underline{d}} (C_{g,1} - C^*_{g,d}) \qquad \textbf{(6.105)}$$

where

J_1	=	volatilization flux from soil (g day^{-1})
D_a	=	molecular diffusivity of the chemical in air ($cm^2 day^{-1}$)
$C_{g,1}$	=	vapor-phase concentration in the surface soil layer (g cm^{-3})
$C^*_{g,d}$	=	vapor-phase concentration above the stagnant air boundary layer (= 0, for the no-canopy field condition) (g cm^{-3})
$\underline{d}$	=	thickness of stagnant air boundary layer (cm)

This equation defines the new flux-type boundary condition for the volatilization simulation. In order to incorporate the new flux-type boundary condition into the PRZM-3 code, new mass balance equations were derived for the surface soil and stagnant air layers. **Figure 6.8(a)** is a schematic of the top two soil layers and the stagnant surface boundary layer when no plant canopy exists. Zero concentration is assumed for $C^*_{g,d}$ under the no-canopy field condition.

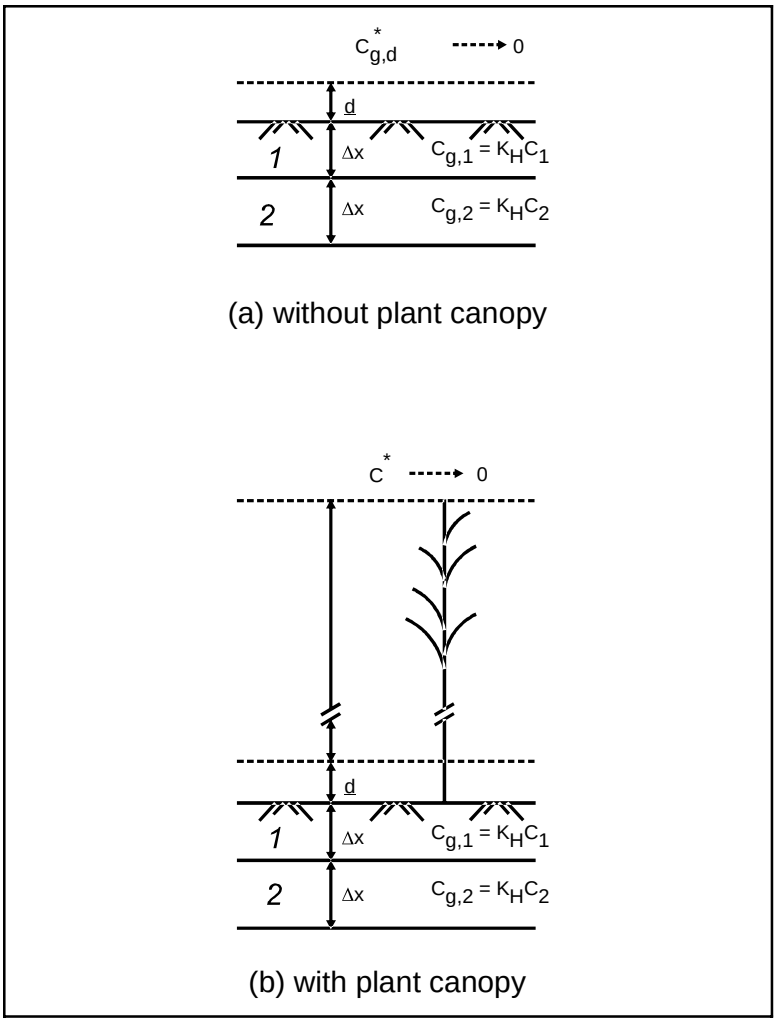


Figure 6.8 Schematic of the top two soil compartments and the overlaying surface compartment (a) without plant canopy, (b) with plant canopy.

A mass balance equation for the uppermost soil compartment is

$$V\frac{\Delta(a\ C_{g,1})}{\Delta t} = AD_g\frac{\Delta C_g}{\Delta z} - A\frac{D_a}{d}C_{g,1} - VK_g a C_{g,1} \qquad \textbf{(6.106)}$$

where

D_g	=	molecular diffusivity of pesticide in air filled pore space ($cm^2 day^{-1}$)
V	=	volume of the compartment (cm^3)
A	=	area of the compartment (cm^2)
a	=	volumetric air content ($cm^3\ cm^{-3}$)
K_g	=	first-order reaction rate constant (day^{-1})

By substituting Equation 6.108 into the overall (i.e., all phases) mass balance equation for the uppermost soil layer, a flux-type upper boundary condition is obtained. **Figure 6.8(b)** reflects the field situation when a plant canopy exists. Zero concentration is now assumed to exist above the top of the canopy compartment. The volatilization flux from the plant canopy is defined as follows.

$$J_{pc} = \left(\frac{1}{\frac{d}{D_a} + \Sigma R} \right) (C_{g,1} - C^*) \tag{6.107}$$

where

J_{pc}	=	volatilization flux through the plant canopy (g cm^{-2} day^{-1})
ΣR	=	vertical transfer resistance (day cm^{-1}), described in Section 6.3.6.3)
C^*	=	concentration above the plant canopy (assumed to be zero)

The first term of the right side of Equation 6.106 represents the gas diffusive flux into the surface soil layer, and the second term denotes the gas diffusive output as governed by the stagnant boundary layer above the soil surface. By using backward implicit finite differencing, the following is derived.

$$a[1,n-1]\ K_H\ C_w[1,n-1] = -\frac{\Delta t}{\Delta z^2} D_g[2,n]\ K_H\ C_w[2,n] + \left(\frac{\Delta t}{\Delta z^2} D_g[1,n] K_H + a[1,n] K_H (1 + K_g) + \frac{\Delta t\ D_a}{\Delta z\ d} K_H \right) C_w[1,n] \tag{6.108}$$

where

n	=	time index

By carrying out a similar mass balance using finite differences, the boundary condition that describes the field with canopy existing is obtained.

6.4.3 Soil Temperature

Soil temperature is solved for numerically. Section 6.3.6.4 describes the theoretical basis for the simulation of soil temperature. The distribution of temperature within the soil profile is summarized by Equation 6.88. This equation is solved numerically for soil temperature, T, as a function of depth, Z, and time, t, based on the input thermal diffusivity, d, for each soil compartment, and the following initial and boundary conditions.

Initial Condition:

$$T_{z,o} = T(z) \tag{6.109}$$

Boundary Conditions:

$$T_{o,t} = T_s(t) \tag{6.110}$$

$$T_{L,t} = T_L(t) \tag{6.111}$$

where

$T(z)$	=	initial soil temperature in each soil compartment (°C)
$T_s(t)$	=	calculated soil surface temperature for each time step (°C)
$T_L(t)$	=	lower boundary temperature condition at the bottom of the soil core (°C)

The lower boundary temperature is defined by the user as 12 monthly values corresponding to the first day of each month; the value for each day is interpolated between the neighboring monthly values.

The following numerical approximation used in the model is taken from Hanks et al. (1971)

$$\frac{T_{i,j} - T_{i,j-1}}{\Delta t} = \frac{(T_{i-1,j} - T_{i,j})\, d_{i-1/2,j} - (T_{i,j} - T_{i+1,j})\, d_{i+1/2,j}}{\Delta z^2} \tag{6.112}$$

Equation 6.107 is solved using a modified numerical solution procedure of Hanks et al. (1971), the same finite difference technique and tridiagonal matrix solver (Thomas algorithm) used in PRZM (Carsel et al. 1984).

6.4.4 Furrow Irrigation

To simplify the algebra required to calculate the furrow infiltration volume as Manning's equation is substituted into the kinematic wave model (Equation 6.95), Manning's equation is approximated as follows:

$$A = \alpha\, Q^m \tag{6.113}$$

α and m are constants that are estimated by the model from the parameters of Manning's equation as follows:

$$m = \frac{\ln(A_2/A_1)}{\ln(Q_2/Q_1)} \tag{6.114}$$

$$\alpha = \frac{A_1}{Q_1^m} \tag{6.115}$$

where

A_1, A_2	=	cross-sectional areas (m^2) at depths y_1 and y_2
Q_1, Q_2	=	flow rates ($m^3\ s^{-1}$) computed from Manning's equation (Equation 6.96) at depths y_1 and y_2
y_1	=	1 cm
y_2	=	10 cm

The depths y_1 and y_2 were chosen to represent the range of depths likely to occur in furrows.

Substituting Equation 6.113 into Equation 6.95 produces:

$$\frac{\partial Q}{\partial z} + \frac{\partial(\alpha\, Q^m)}{\partial t} = -\frac{\partial q}{\partial t} \tag{6.116}$$

No closed-form solution to the above equation is known when infiltration is time-variable. Equation 6.116 therefore, is, solved for Q using the backwards-space, backwards-time finite-difference solution described by Li et al. (Li et al. 1975). Writing Equation 6.116 in finite-difference form produces:

$$\frac{Q_{i+1}^{k+1} - Q_i^{k+1}}{\Delta z} + \frac{\alpha(Q_{i+1}^{k+1})^m - \alpha(Q_{i+1}^{k})^m}{\Delta t} = -\frac{q_{i+1}^{k+1} - q_{i+1}^{k}}{\Delta t} \tag{6.117}$$

where

Q_i^k	=	flow rate at time k, station i
Δz	=	spatial step
Δt	=	time step

Infiltration volumes are computed using the Green-Ampt model:

$$\frac{\partial I_i^k}{\partial t} = K_s \left(1 + \frac{(H + H_s)\theta}{I}\right) \tag{6.118}$$

where

I_i^k	=	infiltration depth (m) at time k, station i
K_s	=	saturated hydraulic conductivity of the soil ($m\ s^{-1}$)

H	=	ponded water depth (m)
H_s	=	suction parameter (m)
θ	=	available porosity (fraction)
I	=	total volume of infiltrated water (m)

The solution of Equation 6.118, subject to the initial condition $I(t_0) = 0$, is

$$K_s\,(t - t_0) = I - h \ln\left(1 + \frac{I}{h}\right) \tag{6.119}$$

where

$$h = (H + H_s)\,\theta \tag{6.120}$$

This solution assumes I is a function of time only. Equation 6.119 has an explicit solution in terms of the Lambert W function (Barry et al. 1995a, Barry et al. 1995b, Corless et al. 1996),

$$I(t) = -h\,[1 + \mathrm{W}_{-1}(z)] \tag{6.121}$$

where

$$z = -\mathrm{Exp}\left[-1 - \frac{K_s(t - t_0)}{h}\right] \tag{6.122}$$

and $\mathrm{W}_{-1}(z)$ represents the branch of the Lambert W function with domain $-\mathrm{Exp}(-1) \le z < 0$ and range $\mathrm{W}_{-1}(z) \le -1$.

The Green-Ampt model has long been accepted as a model of the advance of the wetting front through the soil column, and involves parameters that can be related to well-known soil properties. The volume of infiltration is computed assuming I_i^k is an average infiltration depth for the channel at location i:

$$q_i^k = W_i^k\, I_i^k \tag{6.123}$$

where

q_i^k	=	volume infiltrated at location i ($m^3\ m^{-1}$)
W_i^k	=	current flow width at location i (m)

Furrow channels are assumed to be trapezoidal in shape. Equation 6.96 is solved at each station at the end of each time step for the new flow rate Q_{i+1}^{k+1}. Because the equation is non-linear with respect to Q, the new value of flow is found using second-order Taylor series iteration. Given the flow rate in the furrow, infiltration depths at each location are then computed using the Green-Ampt model (Equation 6.106).

The PRZM-3 furrow irrigation model determines infiltration depths at various locations in the furrow. Irrigation continues until the depth of water infiltrated at the downstream end of the furrow is sufficient to meet the soil moisture deficit SMDEF. The depth of water applied as irrigation to the first PRZM-3 soil compartment is then set equal to either the average furrow infiltration depth or the infiltration depth at a specific location in the furrow, depending on options selected by the user. This depth of water then infiltrates through the root zone as determined by the PRZM-3 soil hydraulic algorithms.

6.5 Results of PRZM Testing Simulations

This section includes the results of testing the two solute transport solution techniques and the volatilization algorithm. Simulated results are compared with those from analytic solutions. Sensitivity analyses also were performed to evaluate the effects of key model parameters on the prediction of volatilization rates. A test comparison

of the model with field data from Georgia (soybeans) concludes the section.

The PRZM model has undergone additional performance testing with field data in New York and Wisconsin (potatoes), Florida (citrus), and Georgia (corn) (Jones 1983, Jones et al. 1983, Carsel et al. 1985). The results of these tests demonstrate that PRZM is a useful tool for evaluating groundwater threats from pesticide use. Please refer to these references for information regarding the further testing of PRZM under field conditions.

6.5.1 Transport Equation Solution Options

Currently, two numerical solution options are available to the PRZM-3 user for the chemical transport equation. As discussed in Section 6.4.1, the finite difference option (utilizing subroutine SLPST0) is unconditionally stable and convergent, but may result in excessive numerical dispersion in high Peclet number systems. The method of characteristics algorithm (utilizing subroutines MOC and SLPST1) eliminates or reduces that numerical dispersion. Two examples are provided that compare the alternate solutions methods at high Peclet number (greater than 5.0) and at low Peclet number (less than 0.5).

6.5.1.1 High Peclet Number

Figure 6.9 presents the analytical solution (Hunt 1978) together with the SLPST0 and MOC/SLPST1 solutions at 6 days for the transport of a 69 mg cm^{-3} pesticide application in the uppermost compartment. The physical parameters are as presented in the figure – notably the Peclet number is 5.1. The following table details pertinent features of the simulation:

Method	**Location of Peak**	**Value of Peak (mg/cm^3)**	**% Error at Peak**	**Runtime (sec)**
Analytical	5.8	11.2	–	–
SLPSTO	4.5	5.07	-54	88.5
MOC/SLPST1	5.5	12.09	+7	112.4

At this relatively high Peclet number, the SLPST0 algorithm shows excessive numerical dispersion, capturing only about half the amplitude of the peak concentration, while showing excessive mass in both tails. In addition, the SLPST0 algorithm does not predict the location of the peak precisely. (It is lagged behind the location of the peak given by the analytical solution and the MOC/SLPST1 solution.) The MOC/SLPST1 algorithm requires 27% more runtime, but errs by only 7% in the peak and shows good agreement in the tails.

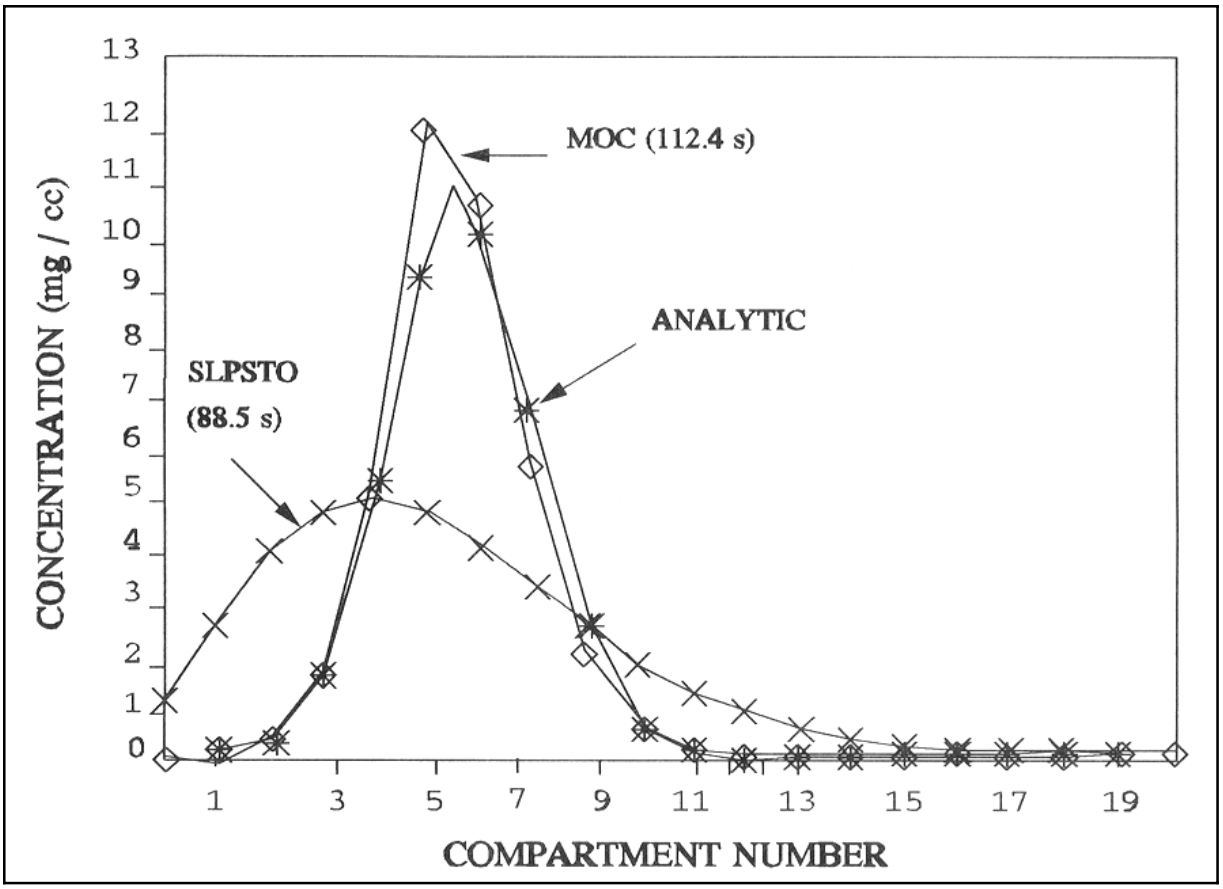


Figure 6.9 Comparison of simulation results at high Peclet number.

6.5.1.2 Low Peclet Number

Figure 6.10 illustrates the results of a SLPST0 and MOC/SLPST1 simulation 8 days after an incorporation of 69 mg/cm^3 in the sixth compartment using the parameters listed. The predicted concentrations at this lower Peclet number, 0.46, are very similar in the peaks and the tails, and apparently little additional resolution is gained from utilizing the MOC algorithm. However, the additional computational burden associated with the MOC algorithm is only 7%.

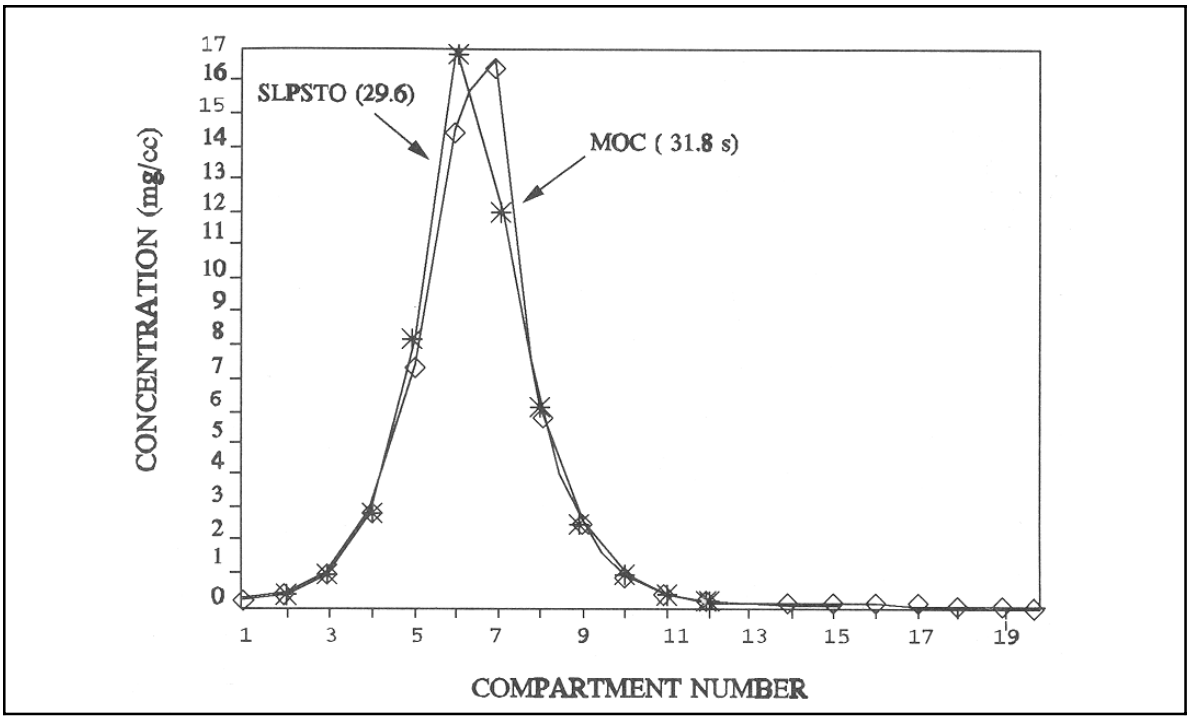


Figure 6.10 Comparison of simulation results at low Peclet number.

6.5.2 Testing Results of Volatilization Subroutines

To test and validate the operation of the volatilization algorithms, model results were compared with Jury's analytical solution (Jury et al. 1983a), and against field data for trifluralin from Watkinsville, GA. Sensitivity analyses were also performed to evaluate effects of key parameters on model predictions. The intent of this preliminary model testing was to evaluate model operation by comparing the results for the volatilization flux from a soil surface application.

6.5.2.1 Comparison with Analytical Solution

Jury et al. (1983a) presented a mathematical model for describing volatile loss and movement of soil-applied organic chemicals. By making the following assumptions, they derived an analytical solution for evaluating the chemical concentration profile within the soil and the volatilization flux at the soil surface:

- Uniform soil properties consisting of a constant water content, bulk density, liquid water flux (either upward, downward, or zero), and a constant organic carbon fraction
- Linear equilibrium adsorption isotherm
- Linear equilibrium liquid-vapor partitioning (Henry's law)
- Uniform incorporation of a quantity of chemical to a specified depth below the surface
- Pesticide loss by volatilization through a stagnant air boundary layer at the soil surface
- Infinite depth of uniform soil below the depth of incorporation

The second through fifth assumptions are satisfied by the current PRZM-3 code. The sixth assumption defines zero concentration for the bottom layer, which is somewhat different from PRZM's zero gradient bottom boundary condition. However, as long as no chemical reaches the bottom layer, these two types of boundary conditions produce identical results. Our test runs for volatilization were designed to satisfy this requirement. In order to comply with the first assumption, the hydrological computation subroutines in PRZM were bypassed and replaced

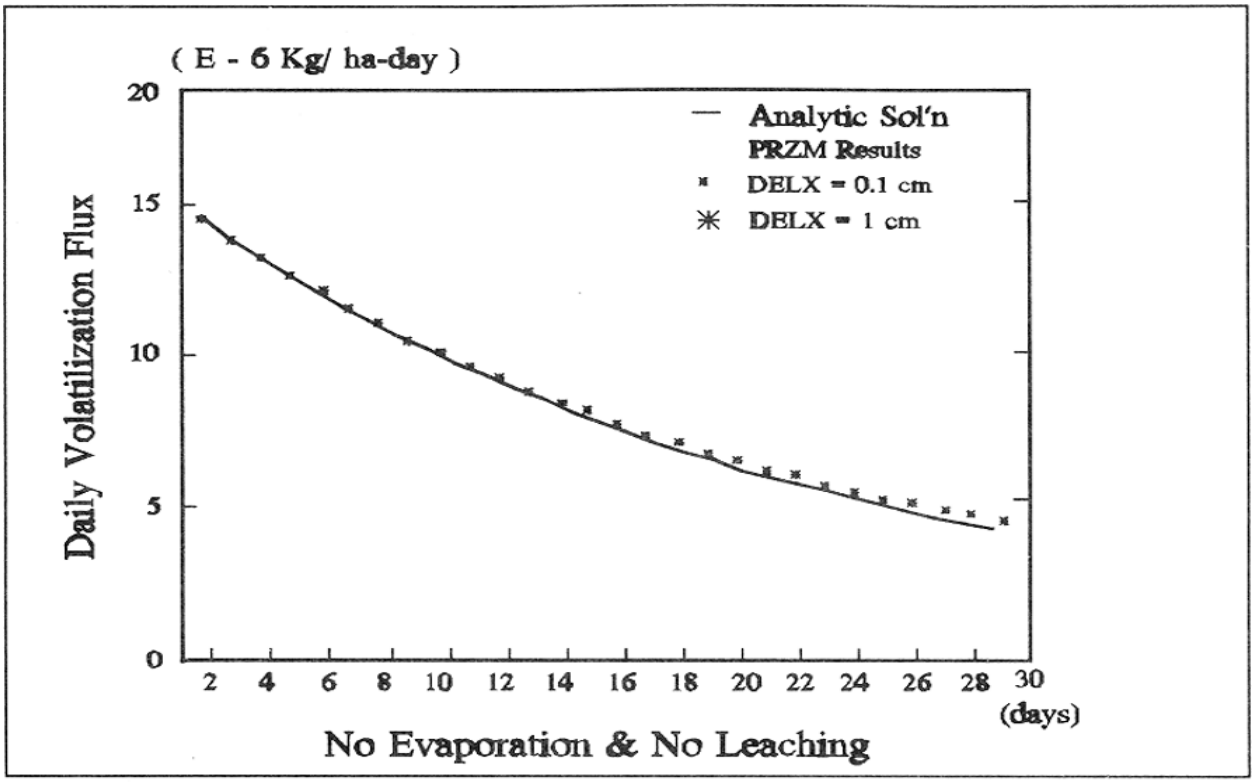
with a constant value for water flux. A positive flux value indicates a leaching condition, whereas a negative flux value indicates an evaporating condition. The hydrological subroutines in PRZM-3 are based on a moisture-routing method in which daily accounting of water inflow and outflow is recorded. One limitation of the moisture-routing method is that it is unable to properly describe the upward movement of evaporating water. Evaporation loss is removed from specific surface soil layers without accounting for movement between layers.

The pesticide 2,4-D was chosen as the test compound for our simulation; the input parameters are listed in Table 6.4 and were obtained from Jury et al. (1983a). The test run results for daily volatilization flux are presented in **Figure 6.11(a)**, **Figure 6.11(b)**, **Figure 6.12(a)**, and **Figure 6.12(b)**, corresponding to the four test cases listed at the bottom of Table 6.4. Two different soil compartment depths (DELX) of 1.0 and 0.1 cm were used to investigate the sensitivity of the volatilization algorithms to the spatial discretization in the surface soil horizon.

Figure 6.11(a) shows the steady state situation (i.e., no evaporation and no leaching) without any advective movement. The daily volatilization flux values predicted by the two different DELXs are almost identical. In this case, the magnitude of DELX is relatively unimportant. The simulation results with a leaching rate of 0.01 cm day^{-1} are shown in **Figure 6.11(b)**. Because of the leaching influence, the predicted daily flux is smaller than the corresponding daily value shown in **Figure 6.11(a)**. The differences between the analytical solution and the PRZM-3 predictions are due to the finite difference solution technique and the occurrence of advective movement by leaching. The simulation results using the smaller DELX (0.1 cm) more closely match the analytical solution results, and an even smaller DELX would have improved the agreement further. The slope of both DELX curves is the same as the analytical solution, and the maximum differences (for the 1.0 cm DELX) from the analytical solution are 10% or less.

Figure 6.12 shows the simulation results under evaporating conditions with the upward advective velocity at 0.01 (**Figure 6.12(a)**) and 0.25 (**Figure 6.12(b)**) cm day^{-1}. The "wick effect" phenomenon (described in Section 6.3.6) leading to enhanced upward movement of the pesticide can be observed in these two figures. The maximum daily flux occurs on the first day for the leaching conditions. Depending on the magnitude of the evaporating water velocity, the maximum daily flux no longer occurs on the first day of the pesticide application. Also the magnitude of the maximum daily flux is enhanced by the magnitude of the evaporating water velocity. The effect of DELX becomes more critical as the influence of advective movement increases. For simulations using a 1.0-cm DELX, **Figure 6.12(a)** shows stable numerical behavior with a small discrepancy when compared to the analytical solution result. As the advective movement becomes larger, the numerical behavior becomes more unstable, as shown in **Figure 6.12(b)**. The smaller 0.1-cm DELX showed good agreement with the analytical solution for both test cases shown in **Figure 6.12**.

Based on these test cases, it appears that a finer DELX, in the range of 0.1 to 0.5 cm, is needed for top soil layers when volatilization processes are simulated with PRZM-3. However, this finer DELX requirements poses an additional computational burden for PRZM-3 applications due to the increase in the number of soil compartments. To circumvent this burden, the PRZM-3 code was modified to allow a variable compartment depth, which allows the user to select a smaller DELX for the top horizon (or any other horizon) and a bigger DELX for the rest of the soil profile. By selecting this variable compartment depth capability, a significant saving in CPU time may be achieved while a better representation is provided for calculation of the surface volatilization flux. In conjunction with field data comparisons (presented below), the results of model runs and CPU time are presented for simulation runs both uniform and variable compartment depth.



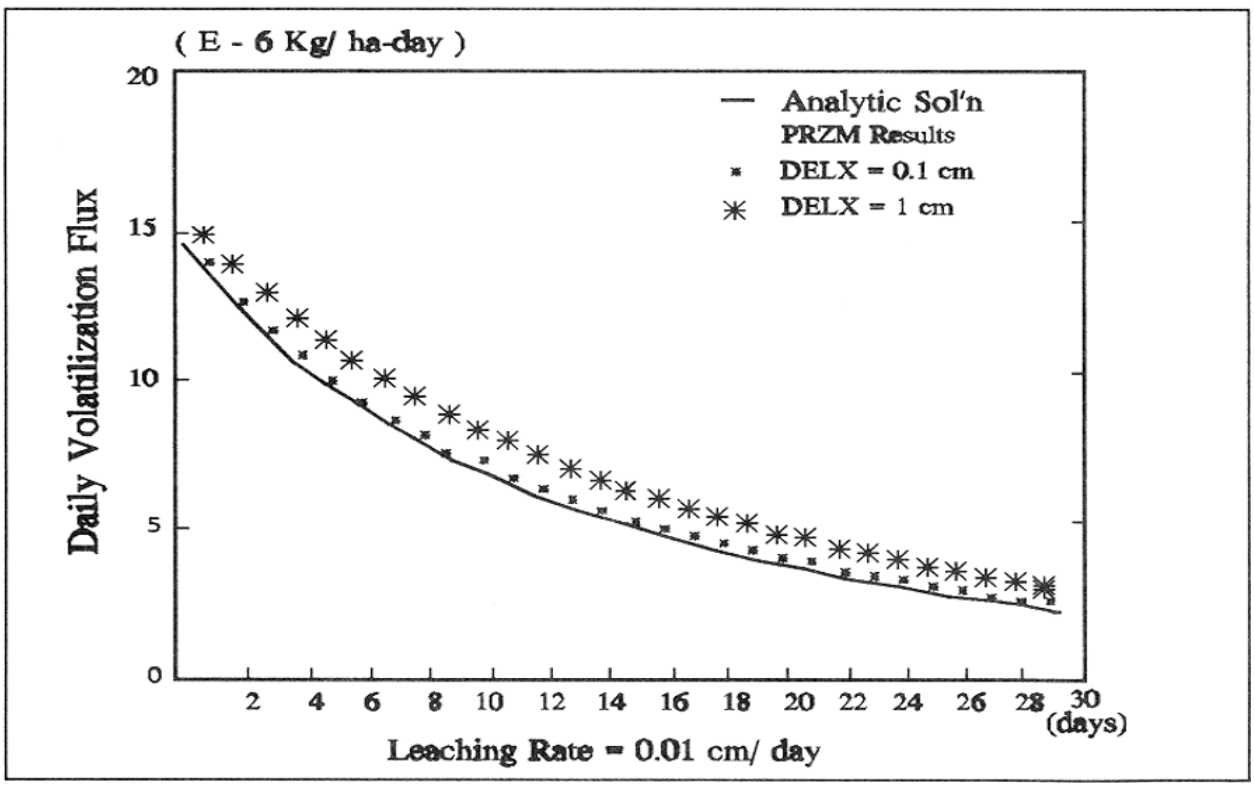


Figure 6.11 Comparison of volatilization flux predicted by PRZM and Jury's analytical solution: Test cases #1 and #2

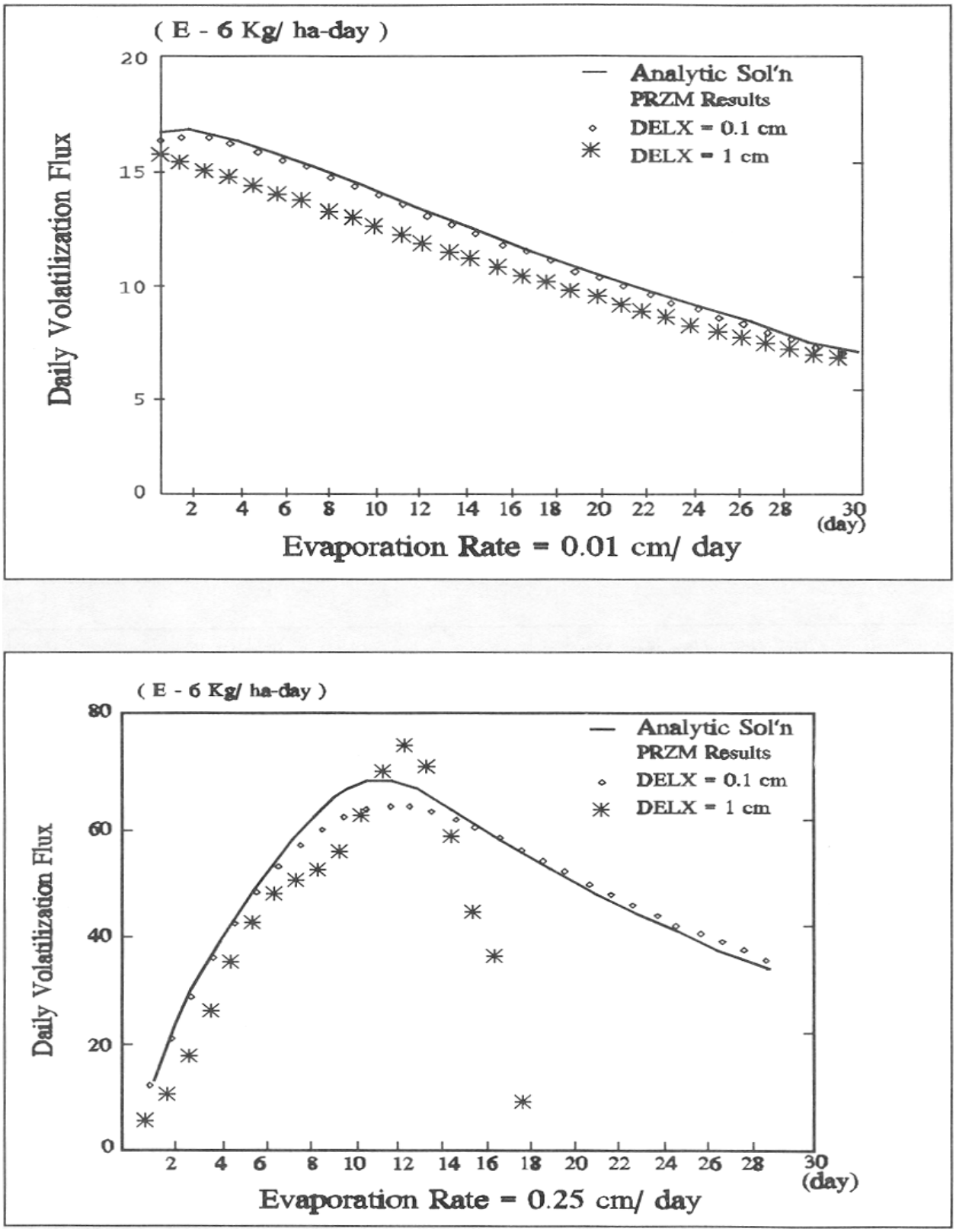


Figure 6.12 Comparison of volatilization flux predicted by PRZM and Jury's Analytical solution. Test cases #3 and #4

6.5.2.2 Comparison with Field Data

Preliminary model testing with field observations also was performed to assess the ability to predict the general magnitude of volatilization losses and daily fluxes under field conditions. Based on a review of available volatilization field data sets, a USDA experimental watershed site in north-central Georgia was selected because of its use of a volatile pesticide (trifluralin), surface-applied to a major crop (soybeans), with a comprehensive micrometeorological and soil sampling plan.

The study site was located at Watkinsville, GA, on a 1.26-ha watershed comprised of Cecil soil (63.9% sand, 23.6% silt, and 12.5% clay) with 0.55% organic carbon, a pH of 6.5, and a slope of 3.0%. Harper et al. (1976) present a detailed description of the site, the equipment, and the installation procedures required for collecting microclimate data. They also summarize the method, assumptions, and calculations used for determining pesticide volatilization flux rates. Trifluralin was surface-applied as a spray to a bare soil surface, using a ground sprayer equipped with flat-fan nozzles, at a rate of 1.12 kg/ha between 1220 and 1247 eastern daylight time (EDT) on 15 June 1973.

The field results shown in Table 6.5 were obtained from White et al. (1977). The values in columns 2, 4 and 5 of Table 6.5 provide the cumulative volatilization flux, remaining pesticide in soil, and total cumulative decay losses, respectively. A discrepancy is noted for the data in column 4 of Table 6.5; the pesticide remaining in soil at the 35th day is smaller than that at the 49th day.

This discrepancy is most likely due to sampling variations, although data were not available to establish accuracy limits on the data points. Meteorological data required for applying PRZM to the site, which include daily precipitation and pan evaporation, were obtained from Smith et al. (1978).

The PRZM-3 input parameters for trifluralin and the Watkinsville site are listed in Table 6.6. Two additional key parameters which influence the volatilization results are the decay rate and the adsorption partition coefficient. The magnitude of the decay rate can be estimated from the data in column 5 of Table 6.5, assuming that decay accounts for all losses from the soil other than volatilization. A value of 0.0206 per day for the first-order decay rate constant obtained from these data points is consistent with the value of 0.0198 per day used by Donigian et al. (Donigian et al. 1986) after reviewing the literature. An initial value for K_d was obtained from the organic carbon content of 0.55% and an organic-carbon partition coefficient (Koc) value of 13,700, resulting in a K_d of 75 ml/g. **Figure 6.13** shows the results of sensitivity analyses runs for K_d and the decay rate; the observed data for trifluralin from Table 6.5 are also included for comparison. **Figure 6.13(a)** shows a good representation of the observed cumulative volatilization curve. **Figure 6.13(b)** shows that a value of 40 for K_d, and a decay rate of 0.02 per day provides the best representation of the decay rate values analyzed.

The simulation results for cumulative volatilization flux and cumulative pesticide decay are shown in **Figure 6.14** for four different DELX combinations. For these simulations, DELX values of 1.0, 0.5, 0.25, and 0.1 cm were chosen for the first horizon and 5-cm DELX for the rest of the profile. The field data are also included in the figures for comparison. Table 6.7 shows the total volatilization flux for each of the four combinations using variable DELX, as well as for a simulation using simulations, a constant 1.0-cm DELX throughout the whole soil profile. The CPU requirements for each run are also included in Table 6.7. The predicted total volatilization flux using the smallest DELX of 0.1 cm is closest to the field-measured value; the values for DELX of 0.25 cm and 0.50 cm are also quite close to the field value. The saving of CPU time can be observed from Table 6.7.The simulation requires 129 seconds using 1.0 cm DELX for the whole soil profile, compared with only 39 seconds for the simulation using 1.0 cm for the top horizon and 5.0 cm for the rest of the profile. The results in Table 6.7 indicate that a DELX of 0.25 to 0.50 cm for the top horizon may be a reasonable compromise between simulation accuracy and CPU costs.

Velocity = 1.82 cm/day	Delta x = 1 cm
Diff coef = 4.0 cm^2/day	Delta t = 1 day
Retardation Coef = 11.74	Core Length = 20 cm
Decay = 0.1/day	Peclet = 0.46

Table 6.4	Input Parameters for the Test Cases - Analytical Solution	
D_G	Air diffusion coefficient	0.43 (m^2 day^{-1})
D_L	Water diffusion coefficient	4.3×10^{-5} (m^2 day^{-1})
ϕ	Porosity	0.5
ρ	Bulk density	1.35 (kg m_{-3})
T	Temperature	25°C
f_{oc}	Organic carbon fraction	0.0125
θ	Water content	0.3
a	Air content	0.2
M	Pesticide applied	1 (kg ha^{-1})
L	Depth of incorporation	0.1 m
K_H	Henry's constant for 2,4-D	5.5×10^{-9}
K_{oc}	Organic carbon partition coefficient for 2,4-D	0.02 (m^3 kg^{-1})
u	Decay coefficient for 2,4-D	4.62×10^{-2} (day^{-1})
l	Total depth of soil column	0.3 m
t	Simulation period	30 days
J_w	Water flux	
E	Evaporation flux	

Test case #1: no evaporation and no leaching (J_w = E = 0)
Test case #2: with leaching (J_w = 0.01 cm day^{-1})
Test case #3: with evaporation (E = 0.01 cm day^{-1})
Test case #4: with evaporation (E = 0.25 cm day^{-1})

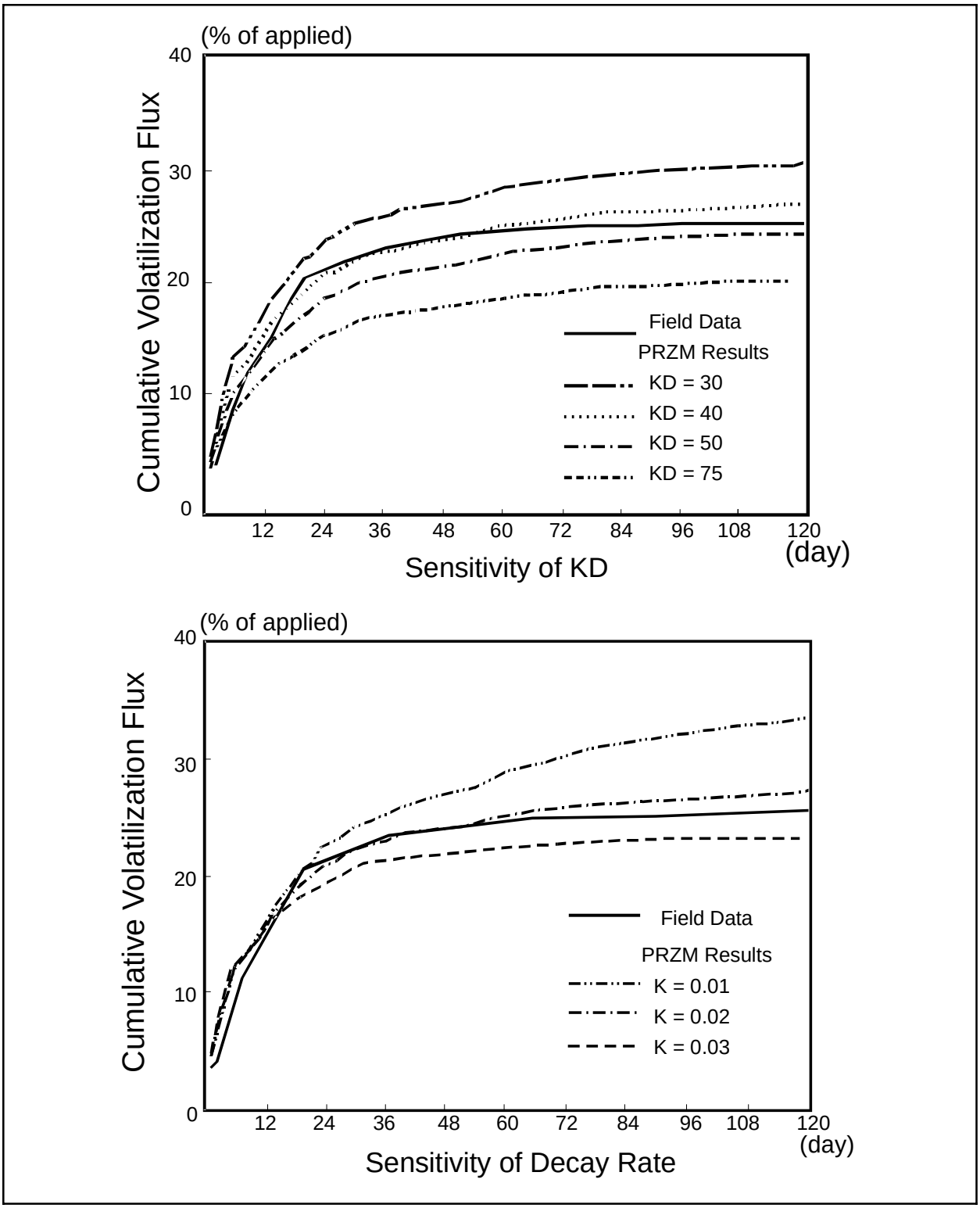


Figure 6.13 Sensitivity of cumulative volatilization flux to K_d and decay rate.

Table 6.5 Trifluralin Volatilization Losses, Amounts Remaining in Soil, and Estimated Losses via Other Pathways for the 120-day Field Test

Time, (day)	Cumulative Volatilized		Remaining* in Soil, % Applied	Estimated Other Losses, % of Applied
	% of Total Applied	% of Total Applied		
Application	3.5	13.3	–	–
1	3.8	14.8	89	7.2
2	5.3	20.3	72	22.7
6	10.9	42.2	64	25.1
18	20.5	79.1	51	28.5
35	23.4	90.2	33	43.6
49	24.4	94.1	35	40.6
63	25.1	96.9	23	48.9
76	25.4	98.2	20	54.6
120	25.9	100.0	11	63.1

Source: White et al. (1977).
* Based on amount remaining in soil at a 0 cm to 7.5 cm depth as compared with an initial 1.0 µg/g level at application (rate was 1.12 kg/ha).

Table 6.6 Input Parameters for the Test Cases - Watkinsville Site

Simulation start date					14 June 1973
Simulation end date					31 December 1973
Trifluralin:	**Henry's constant**				6.7×10^{-3}
	Diffusion coefficient in air				0.43 m^2 day^{-1}
	Application date				15 June 1973
	Amount applied				1.12 kg ha^{-1}
	Incorporation depth				5 cm
Horizon	**Thickness (cm)**	**DELX (cm)**	**Field Capacity**	**Wilting Point**	**Initial Water Content**
1	5	0.1	0.207	0.095	0.166
2	10	5.0	0.207	0.095	0.217
3	15	5.0	0.339	0.239	0.318

Horizon	Thickness (cm)	DELX (cm)	Field Capacity	Wilting Point	Initial Water Content
4	60	5.0	0.320	0.239	0.394

Table 6.7 Simulation Results Using Different Compartment Depth (DELX)

Horizon	Constant DELX		Variable DELX				
	Depth (cm)	DELX (cm)	DELX (cm)	DELX (cm)	DELX (cm)	DELX (cm)	
1	5	1.0	1.0	0.5	0.25	0.1	
2	10	1.0	5.0	5.0	5.0	5.0	
3	15	1.0	5.0	5.0	5.0	5.0	Field
4	60	1.0	5.0	5.0	5.0	5.0	Value
Total Volatilization Flux (kg/ha)		0.393	0.398	0.338	0.317	0.316	0.290
CPU (Sec)		129	39	46	67	106	

Figure 6.15(a) reveals significant differences between the observed pesticide decay and the simulated values during the first few weeks following application. In fact, the observed data appear to indicate a much higher attenuation rate during the first few days following application, with a lower rate for the remaining period. To better match the decay characteristics, and evaluate the potential impact on the volatilization simulation, a two-step decay procedure was used with a rate of 0.1 per day for 5 days following application and a rate of 0.01 per day for the remaining period. The results of these simulations in terms of pesticide remaining in the soil, shown in **Figure 6.15**, indicate a much better agreement with the observed field values in **Figure 6.15(b)**. The impact of the two-step decay on both cumulative decay and volatilization flux is shown in **Figure 6.16**. The cumulative pesticide decay shown in **Figure 6.16(a)** improves considerably (compared to **Figure 6.14(b)**), while the results for cumulative volatilization flux (**Figure 6.16(b)**) are slightly better than those in **Figure 6.14(a)**.

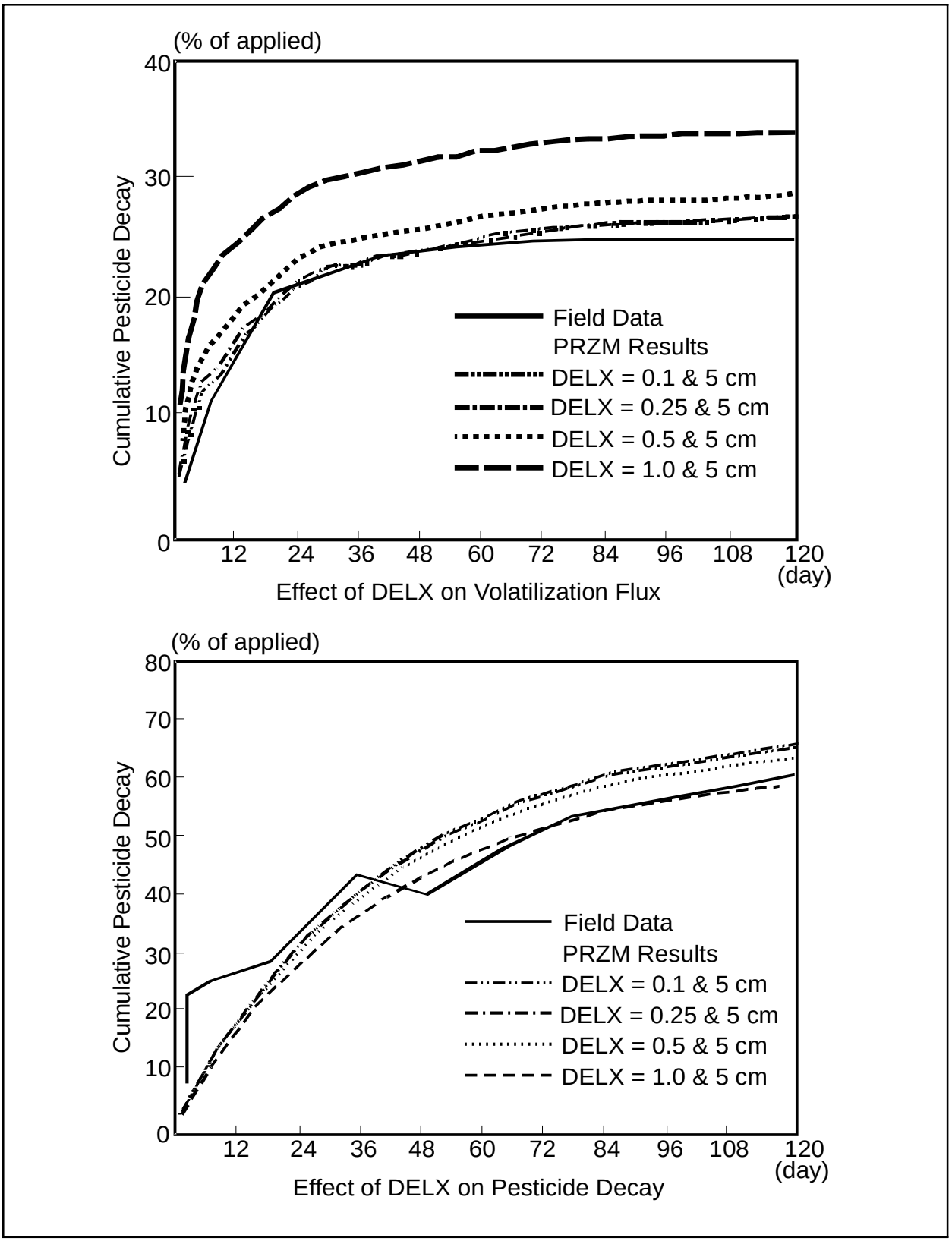


Figure 6.14 Effects of DELX on volatilization flux and pesticide decay.

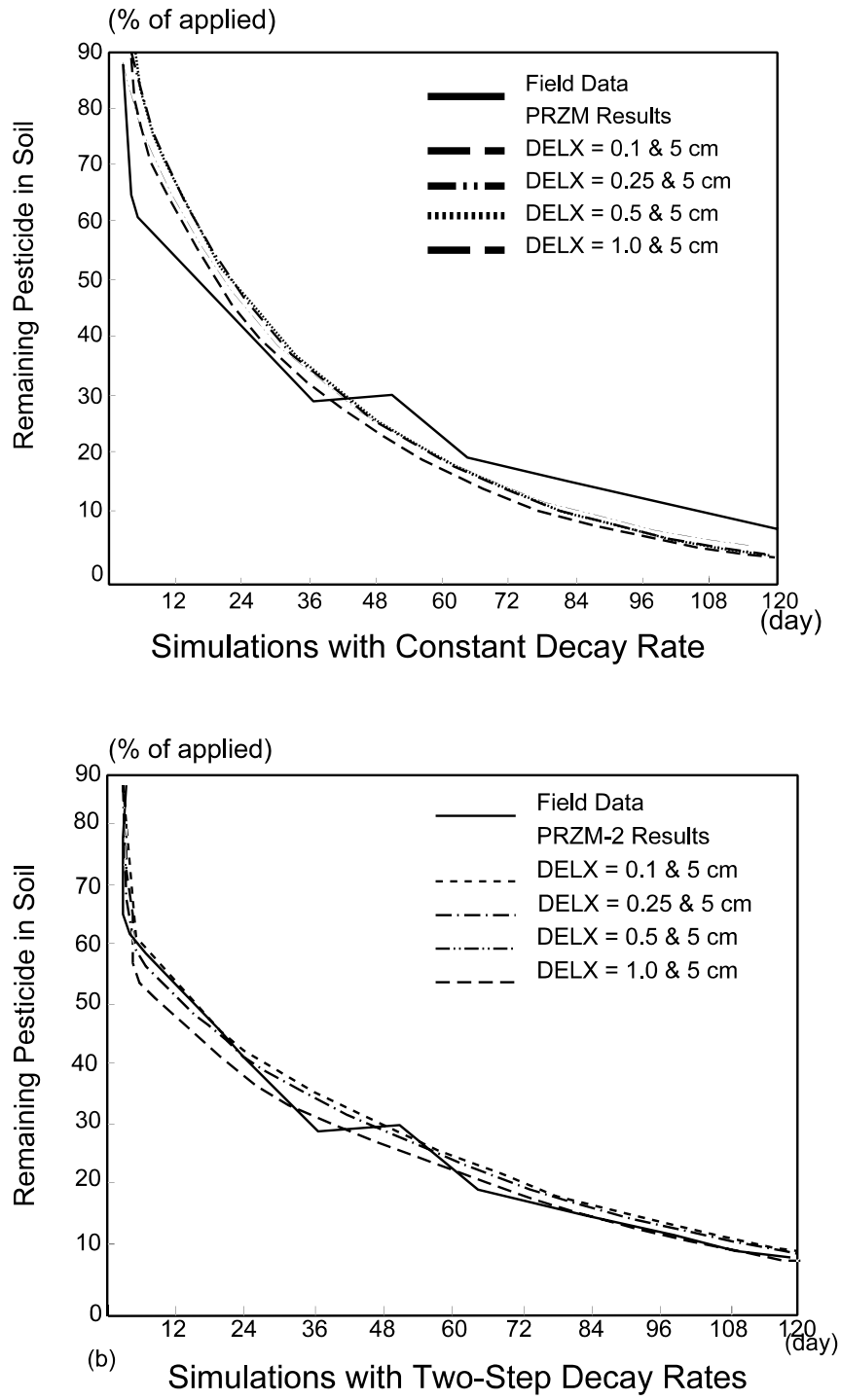


Figure 6.15 Comparison of constant and two-step decay rates.

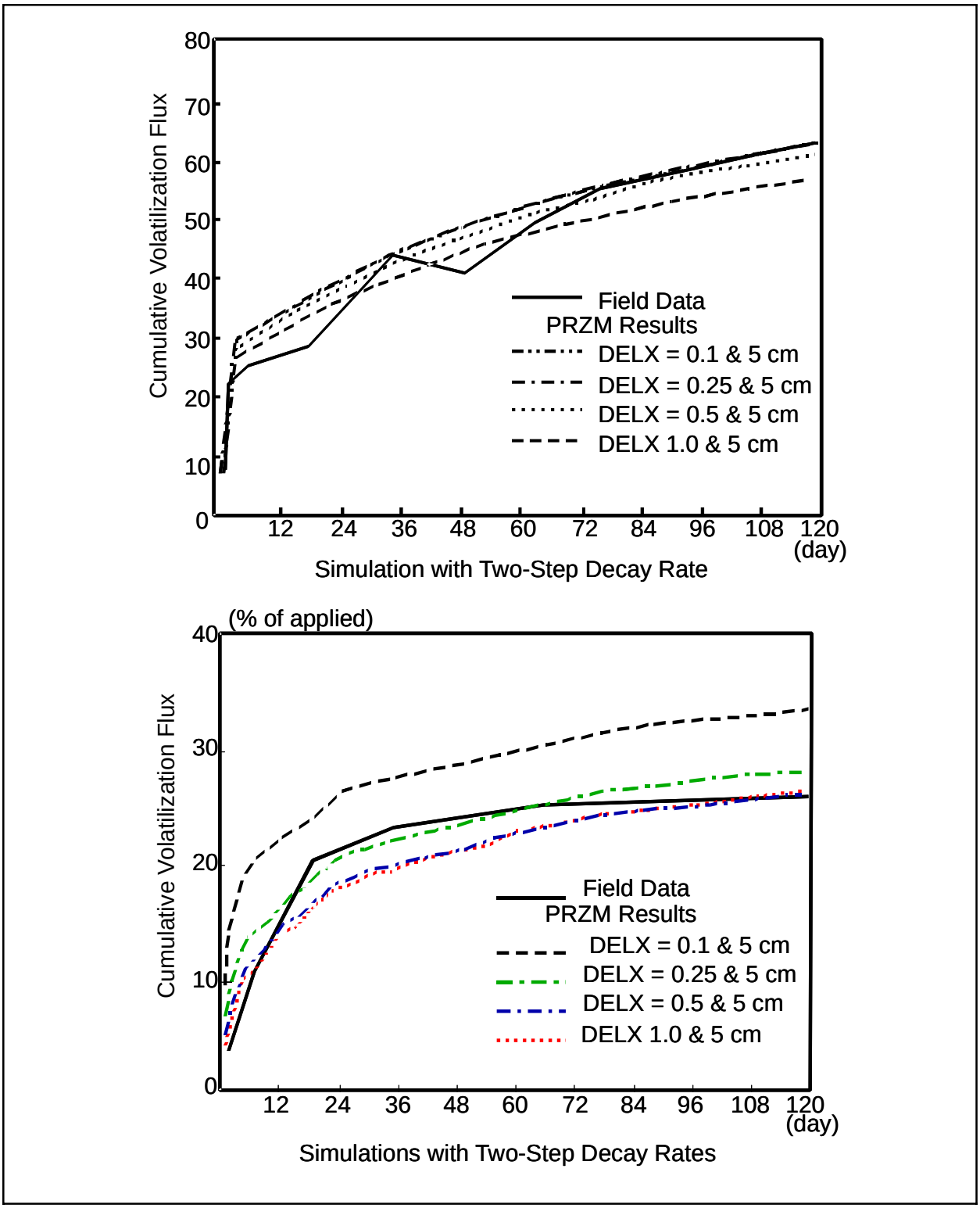


Figure 6.16 Effects of two-step decay rates on volatilization flux and pesticide decay.

6.5.2.3 Conclusions from Volatilization Model Testing

The primary conclusions derived from this preliminary model testing are as follows.

1) Comparisons with Jury's analytical solution indicate that the volatilization algorithms are operating correctly, and that, with a very small DELX (0.1 cm or less), the results are in excellent agreement.

2) The preliminary field testing results with trifluralin in Watkinsville, GA, indicate good agreement between measured and predicted volatilization flux when measured decay rates and adjusted K_D values are used.

3) Small soil layer depths (in the range of 0.25 and 0.50 cm) are needed to provide the best presentation of volatilization flux at reasonable CPU times, based on the Watkinsville testing.

4) A two-step decay rate best represents the attenuation behavior of trifluralin using a higher rate for the period immediately following application and a lower rate for the remaining period.

Further testing of the volatilization model should be performed to evaluate its capabilities for different compounds, different regions, and other crops. In addition, the vapor transport and concentration calculations for the plant compartment should be tested with the additional data available from the Watkinsville site and from other field data sets (e.g., Grover et al. (1985) and Willis et al. (1983)).

6.5.3 Testing Results of Soil Temperature Simulation Subroutine

Preliminary testing of the simulation subroutine for the soil profile temperature was performed by comparing predicted values with values obtained by an analytical solution to the governing heat flow equation. These testing results are discussed in this section. Testing of the soil surface/upper boundary temperature simulation, estimated by the energy balance procedure in the model, was not performed due to problems in obtaining observed meteorological and soil temperature data for the Watkinsville, GA, test site.

An analytical solution presented in Kreysig (1972) for the classical one-dimensional heat flow partial differential equation (described in Section 6.3.6.4) was used to calculate changes in the soil temperature profile with time, due to a change in the upper boundary temperature. In order to develop a valid comparison between the analytical and finite difference methods, three assumptions were made:

a) Uniform properties throughout the soil profile
b) Constant lower-boundary temperature
c) Uniform initial temperatures throughout the profile

To compare the results of the analytical solution with the finite difference solution from the soil temperature model, the following parameters were used.

Depth of the soil profile	= 100 cm
Compartment thickness (DELX)	= 1.0 cm
Diffusivity of the soil profile	= 864 cm^2 day^{-1}
Upper-boundary temperature, $T_{(o,t)}$	= 30°C
Lower-boundary temperature, $T_{(L,t)}$	= 20°C
Initial temperature, $T_{(x,o)}$	= 20°C

Figure 6.17 and **Figure 6.18** show the comparison of soil temperature profiles predicted by both the analytical solution and the finite difference soil temperature model after 1 day and 5 days of simulation. In **Figure 6.17** the finite difference solution is obtained by using a 1-hour time step, while in **Figure 6.18** a 1-day time step is used. The following observations are evident from these testing results.

1) Comparison of the soil temperature profiles predicted by both methods indicate excellent agreement when the smaller, 1-hour time step is used in the finite difference procedure, as shown

in **Figure 6.17**.

2) The finite difference solution obtained by using the daily time steps deviates from the analytical solution by about 1°C, in the upper and middle portions of the soil profile (**Figure 6.18**). This deviation is due to the assumption of a constant initial temperature profile and the abrupt change in the upper-boundary temperature from 20°C to 30°C for the first daily time step.

3) As the steady-state condition is approached, irrespective of the time step used in the finite difference solution, the soil temperature profiles predicted by both methods are in good agreement (**Figure 6.17(b)** and **Figure 6.18(b)**).

Table 6.8 shows that reducing the depth of the compartment from 1 cm to 0.1 cm does not produce any significant change in the finite difference solution. These depths bracket the range of values for DELX (i.e., compartment thickness) likely to be used for the surface soil horizon.

These test results show that, for smaller time steps, the finite difference solution will be in complete agreement with the analytical solution. For a daily time step as used in PRZM-3, under expected environmental conditions, with a non-uniform initial temperature profile, non-uniform soil characteristics, and smaller daily changes in the upper-boundary temperature, the soil temperature profile estimated by the finite difference method used in the model is expected to be capable of providing close agreement with observed temperature profile data. In addition to further testing of the soil profile temperature model with field data, the procedure to estimate the upper-boundary temperature should be tested to evaluate and demonstrate the validity of the entire soil temperature simulation model.

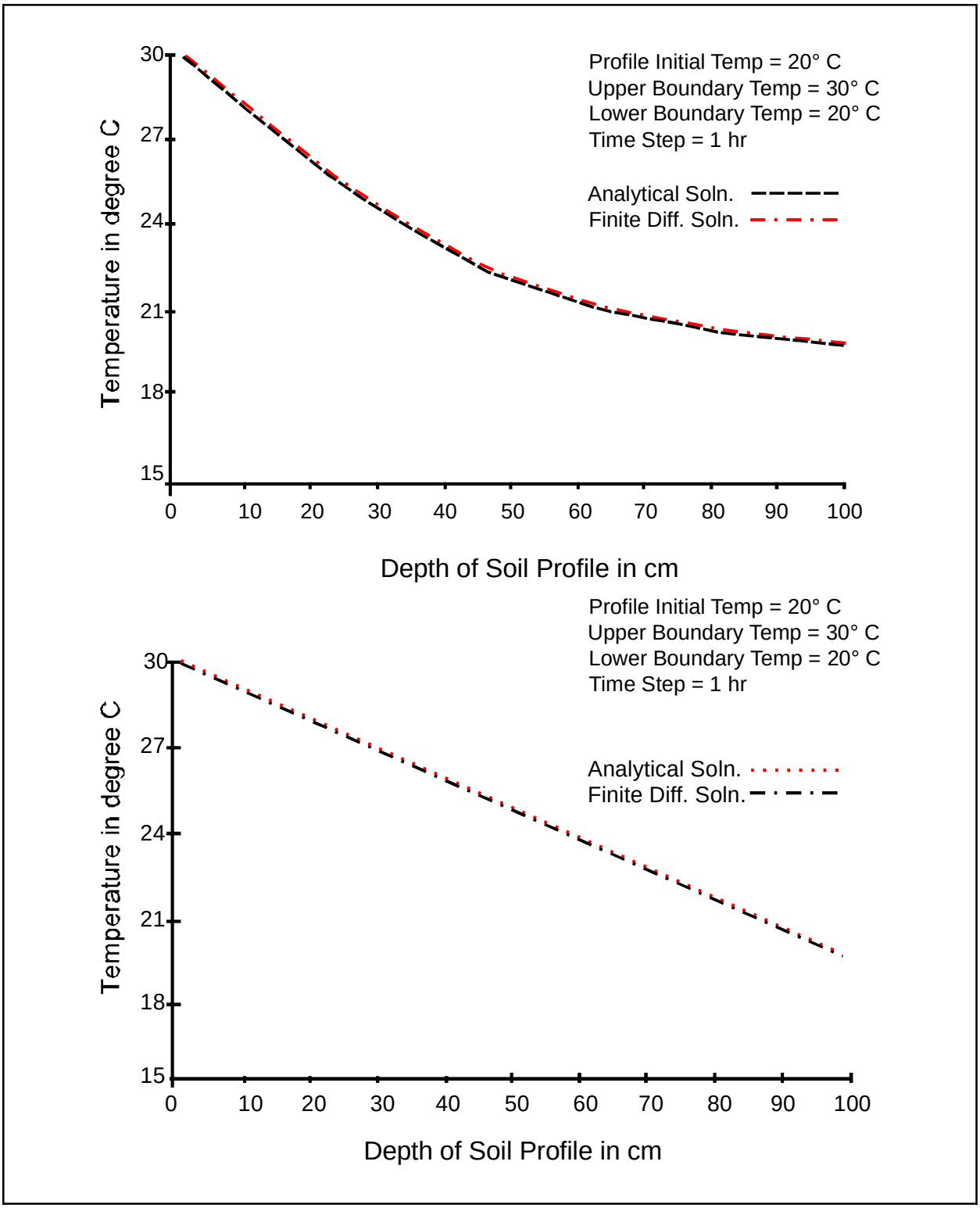


Figure 6.17 Comparison of soil temperature profiles predicted by analytical and finite difference solutions (Time Step=1 HR).

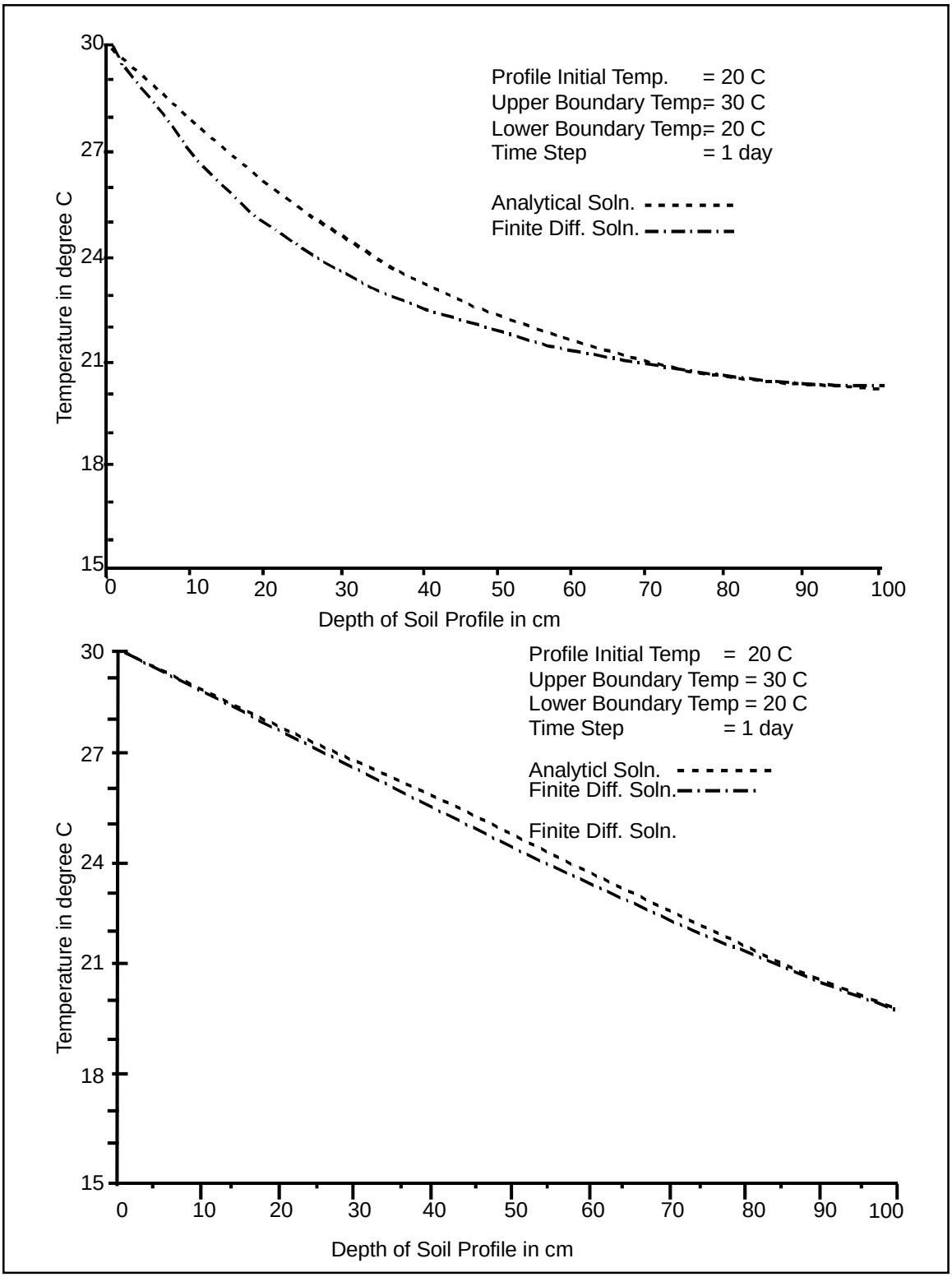


Figure 6.18 Comparison of soil temperature profiles predicted by analytical and finite difference solutions (Time Step=1 day).

Table 6.8 Simulated Soil Temperature Profile after One Day for Different Compartment Thicknesses (Time Step = 1 Day)		
Depth (cm)	**DELX = 1 cm**	**DELX = 0.1 cm**
0.0	30.000	30.000
1.0	29.665	29.664
2.0	29.341	29.340
3.0	29.028	29.026
4.0	28.725	28.723
5.0	28.432	28.431
10.0	27.109	27.106
20.0	25.048	25.045
30.0	23.577	23.574
40.0	22.524	22.520
50.0	21.766	21.760
60.0	21.215	21.206
75.0	20.638	20.627
99.0	20.023	20.020
100.0	20.000	20.000

6.5.4 Testing of Daughter Products Simulation

The fate of pesticides in soils is a complex issue. Many processes (i.e., volatilization, degradation, etc.) must be considered in order to adequately address this issue. One of these processes, which has been largely neglected in pesticide leaching models, is that of the transformation of the parent compound to various toxic daughter products. The tendency has been to lump all the toxic family into a "total toxic residue" and to model the fate of this composite as a single chemical. This assumption may not be acceptable, especially if the daughters have very different decay rates or adsorption partition coefficients from the parent or from each other.

Algorithms have been included in PRZM-3 to simulate parent/daughter relationships. An analytical solution to the decay and transformation model was derived to check the numerical model.

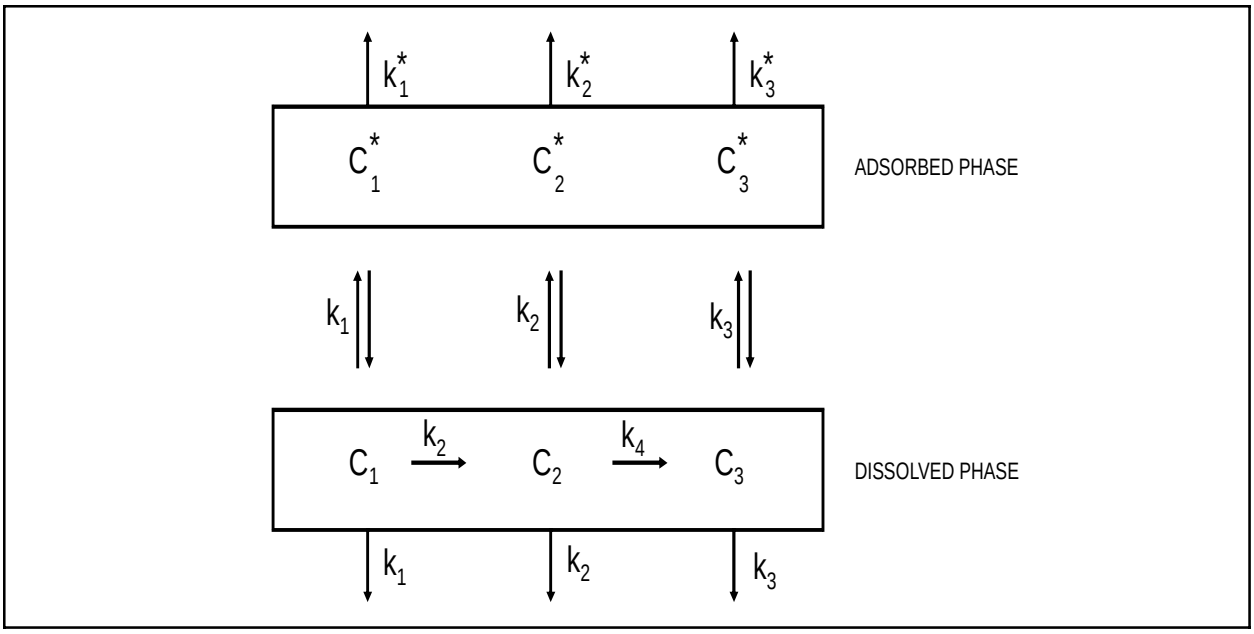


Figure 6.19 Schematic of a system of parent and daughter pesticide relationships.

The system that was modeled is shown in **Figure 6.19**. The C_i are dissolved concentrations and the C_i^* are adsorbed concentrations. The K_i are adsorption partition coefficients, the k_j are decay and transformation rates in the dissolved species, the k_i^* are adsorbed phase decay coefficients and θ and ρ are the water content and soil bulk densities, respectively. Notice that only the dissolved forms may be transformed from one toxic form to another. A system of first order differential equations describing this system can be written as:

$$\frac{dC_1\theta}{dt} = -(k_1 + k_2)\, C_1\theta \qquad \textbf{(6.124)}$$

$$\frac{d\, C_2\theta}{dt} = -(k_3 + k_4)\, C_2\theta + k_2\, C_1\theta \qquad \textbf{(6.125)}$$

$$\frac{d\, C_3\theta}{dt} = -k_5\, C_3\theta + k_4\, C_2\theta \qquad \textbf{(6.126)}$$

$$\frac{d\, C_1^*\rho}{dt} = -K_1^*\, C_1^*\, \rho \qquad \textbf{(6.127)}$$

$$\frac{d\, C_2^*\rho}{dt} = -k_2^*\, C_2^*\, \rho \qquad \textbf{(6.128)}$$

$$\frac{d\, C_3^*\rho}{dt} = -K_3^*\, C_3^*\, \rho \qquad \textbf{(6.129)}$$

Making use of $C_i\, K_i = C_i^*$ we can reduce the six equations above to three equations in three unknowns, namely:

$$\frac{d\ C_1}{dt} = a_1\ C_1 \tag{6.130}$$

$$\frac{d\ C_2}{dt} = a_2\ C_1 + a_3\ C_2 \tag{6.131}$$

$$\frac{d\ C_3}{dt} = a_4\ C_2 + a_5\ C_3 \tag{6.132}$$

in which

$$a_1 = -\frac{\theta(k_1 + k_2) - k_1^*\ K_1\rho}{\theta + K_1\ \rho} \tag{6.133}$$

$$a_2 = \frac{k_2\theta}{\theta + K_2\rho} \tag{6.134}$$

$$a_3 = -\frac{\theta(k_3 + k_4) - k_2^*\ K_2\rho}{\theta + K_2\ \rho} \tag{6.135}$$

$$a_4 = \frac{k_4\theta}{\theta + K_3\rho} \tag{6.136}$$

$$a_5 = -\frac{\theta k_5 - k_3^*\ K_3\rho}{\theta + K_3\ \rho} \tag{6.137}$$

These ordinary differential equations with constant coefficients can be solved analytically for C_1, C_2 and C_3 using the initial conditions $C_1 = C_1'$ when $t = 0$ and $C_2 = C_3 = 0$ at $t = 0$. The solution is:

$$C_1(t) = C_1'\ e^{a_1 t} \tag{6.138}$$

$$C_2(t) = \frac{a_2 C_1' [e^{a_1 t} - e^{a_3 t}]}{a_1 - a_3} \tag{6.139}$$

$$C_3(t) = \frac{a_2 a_4 C_1' [(a_3 - a_5)e^{a_1 t} + (a_5 - a_1)e^{a_3 t} + (a_1 - a_3)e^{a_5 t}]}{(a_1 - a_3)\ (a_1 - a_5)\ (a_3 - a_5)} \tag{6.140}$$

In PRZM-3, the equations are solved numerically as part of the general advection-dispersion equation for a solute in a porous medium by using an implicit scheme. A new subroutine was added to set up the transformation (source and sink) terms for the system. The relationship $C_1 \rightarrow C_2 \rightarrow C_3$ may be modeled or the system can be configured for $C_1 \rightarrow C_2$ and $C_1 \rightarrow C_3$ or for independent C_1, C_2 and C_3 simply by selecting zero or positive values for the appropriate transformation rate constants.

Figure 6.20 and **Figure 6.21** show the results of a series of tests performed on the numerical model and checked by the analytical model. In these figures, the solid line represents the "true" or analytical solution, and the dashed line

represents the approximate numerical solution. In **Figure 6.20**, there was no decay of the dissolved phase chemicals and no adsorption of any species. The rate of transformation from C_1 to C_2 was 0.2 day^{-1} and that from C_2 to C_3 was 0.5 day^{-1}. After 20 days nearly all the chemical is in form C_3. The numerical model traces the decay and formation of each constituent closely, being poorer in those regions where the rate of change of the concentrations are more rapid. **Figure 6.21** shows the same system with a decay rate of 0.01 day^{-1} in the dissolved phase.

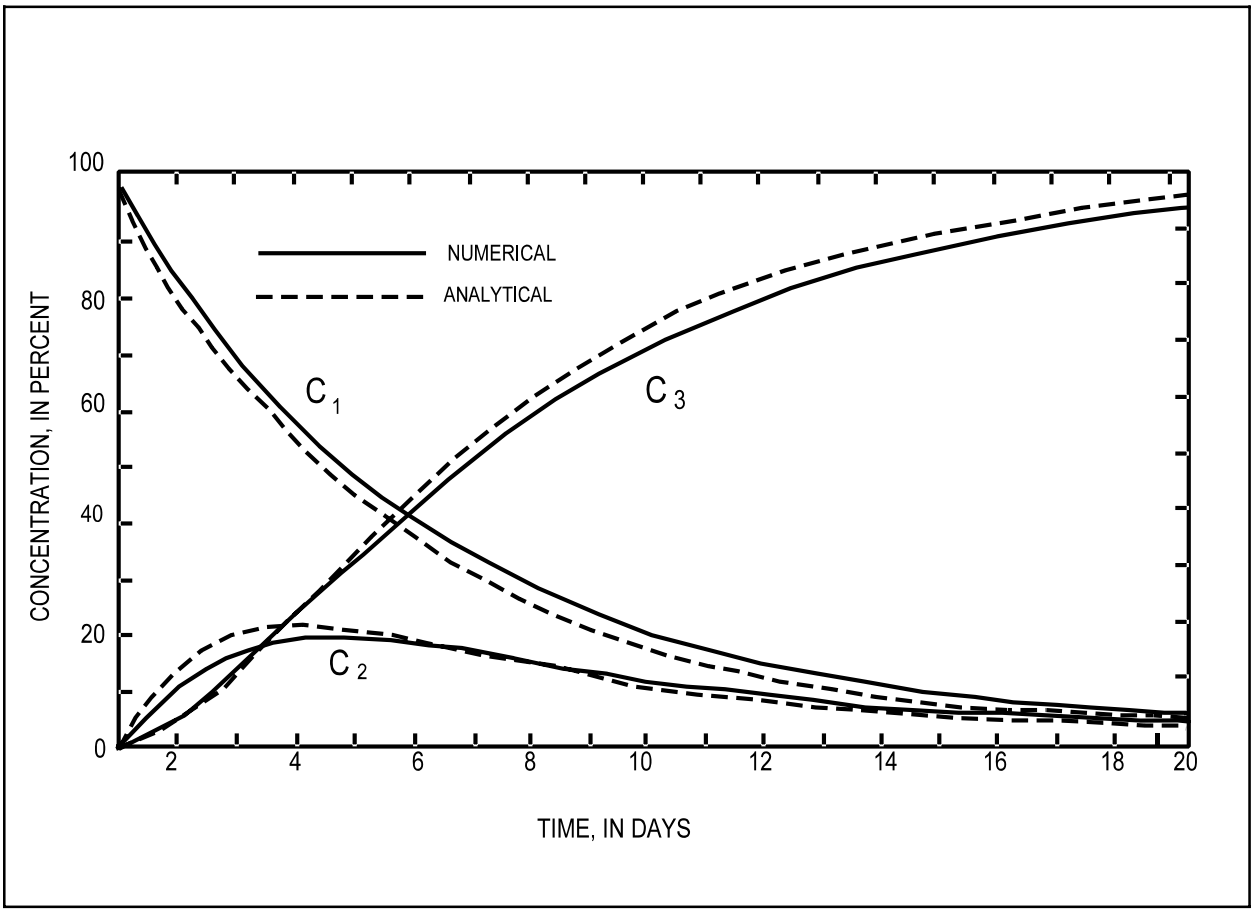


Figure 6.20 Conversion of C_1 to C_2 to C_3 with no adsorption without decay.

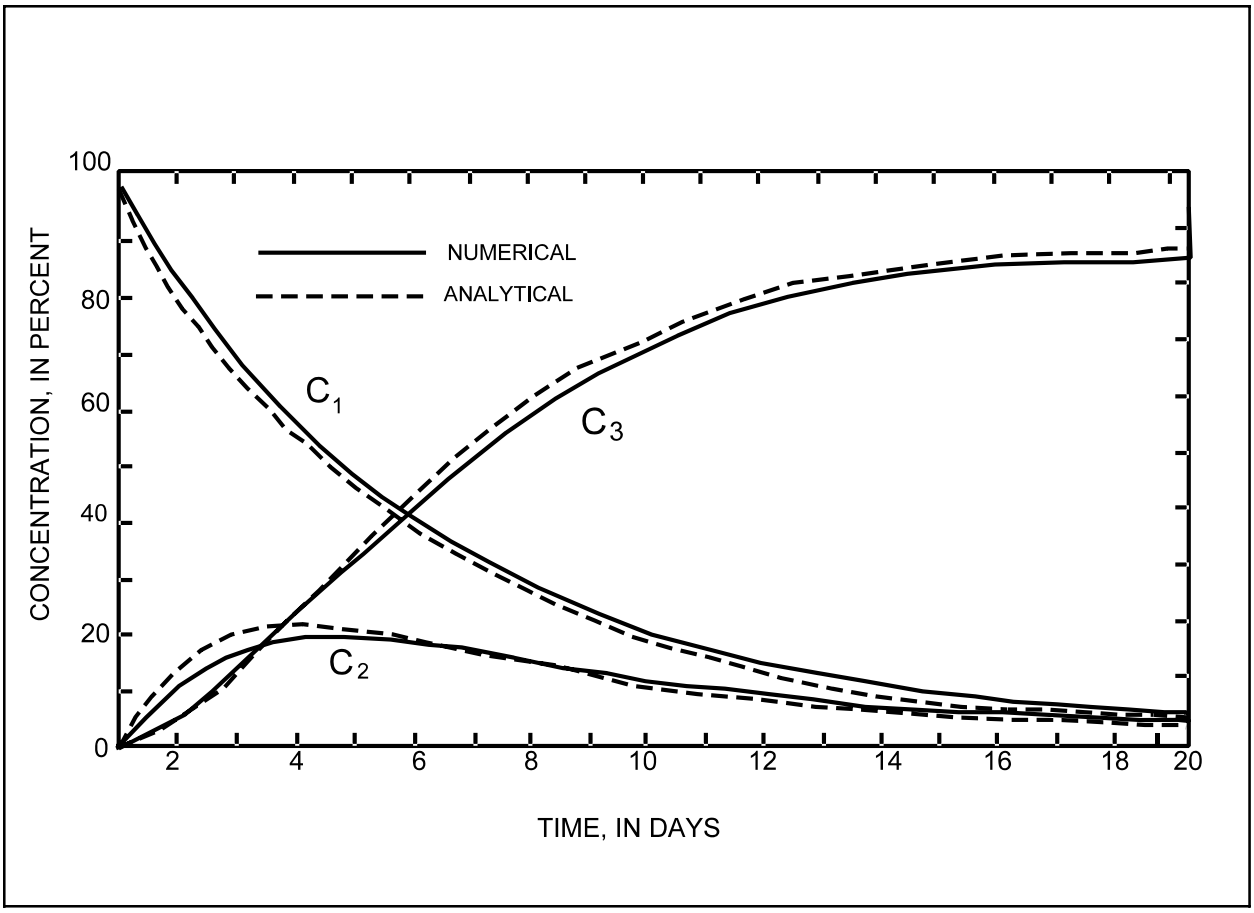


Figure 6.21 Conversion of C_1 to C_2 to C_3 with no adsorption without decay.

Using the analytical model, the assumption of modeling the "total toxic residue" decay as a first-order process was tested. Adsorption coefficients for aldicarb, aldicarb sulfoxide and aldicarb sulfone in a Woburn sandy loam (K_1 = 0.55, K_2 = 0.16 and K_3 = 0.185) and decay and transformation rate constants (k_1 = 0.07, k_2 = 0.55, k_3 = 0.01, k_4 = 0.031 and k_5 = 0.0152) were taken from Bromilow et al. (1980). A soil bulk density of 1.45, a water content of 0.27 $cm^3\ cm^{-3}$ and an initial aldicarb parent mass of 100 mg were also used. The model was run for 90 days and the results are shown in **Figure 6.22**.

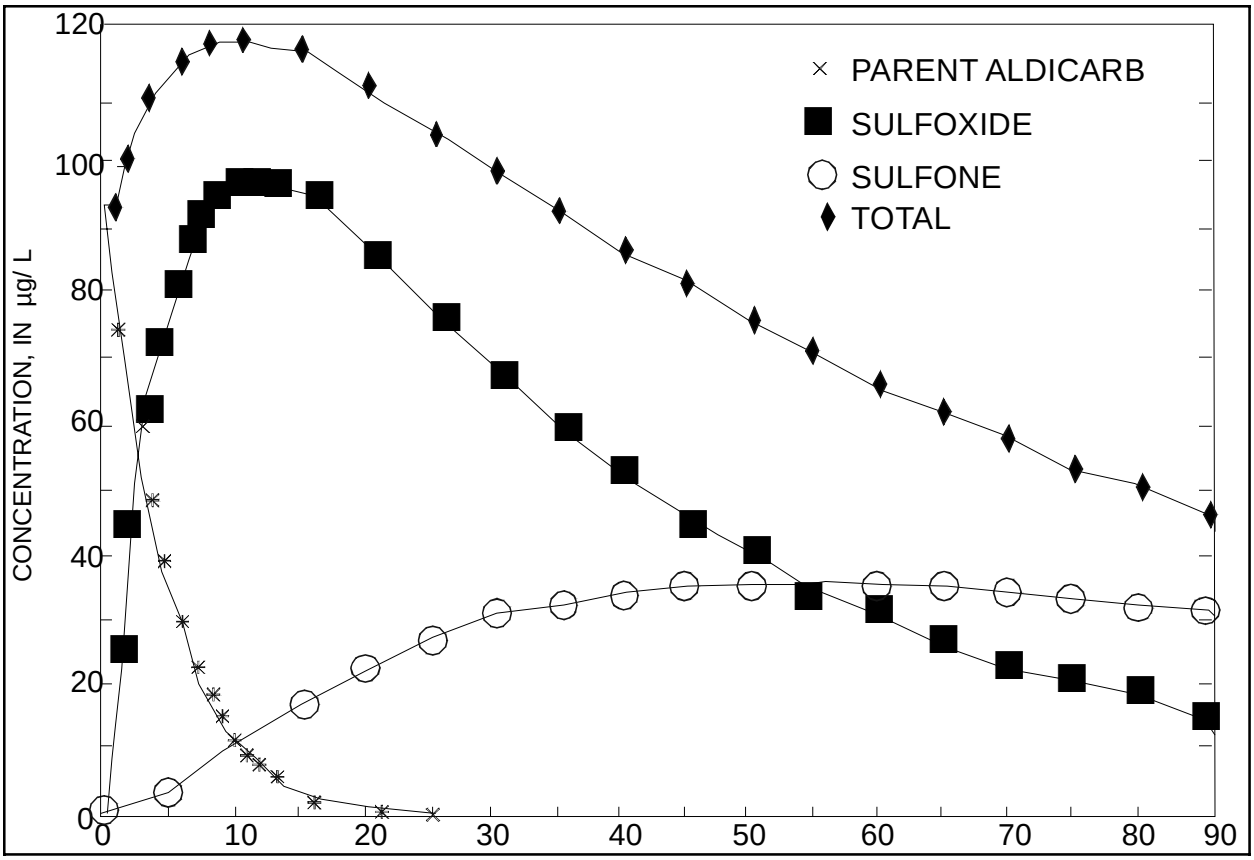


Figure 6.22 Conversion of aldicarb to aldicarb sulfoxide to aldicarb sulfone.

The results show that the decay of the sum of the dissolved aldicarb concentrations does not follow first-order kinetics. The reason for this is the conversion of aldicarb parent to aldicarb sulfoxide. Because the sulfoxide has a lower partition coefficient, the dissolved concentration increases until most of this conversion is complete. Once this happens, however, the sum of the sulfoxide and the sulfone concentrations does follow a first-order decay curve.

6.5.5 Testing of Nonuniform Extraction Model for Runoff and Revisions in the Distribution of Residues

The nonuniform extraction model for runoff and revisions in the distribution of residues following washoff and application (CAM=1) first appeared in an unofficial release of PRZM-2, developed by Waterborne Environmental, Inc., referred to as PRZM-2.3 (Waterborne Environmental 1995). PRZM-2.3 was developed in response to data indicating that PRZM-2.2 was over-predicting pesticide runoff for the herbicide atrazine by about an order of magnitude at the Georgia, Tennessee, and Iowa study sites (Solomon et al. 1996). PRZM-2.3 provided significantly better estimates of atrazine runoff compared at all three field sites; results comparisons for the Georgia and Tennessee sites are shown in **Figure 6.23** and **Figure 6.24**, respectively. Sites consisted of different geographical areas, soil times, and climatological conditions.

- Shelby County, Tennessee. This study was conducted by Memphis State University and consisted of 18 hectares. The upper 8 hectares were in pasture and the lower 10 hectares were planted in corn (Klaine et al. 1988). Soils consisted of the Falaya silt loam, having a 1 to 2 percent slope and classified as Hydrologic Soil Group D. Atrazine was applied at 0.92 kg a.i./ha

- Watkinsville, Georgia. Site monitored by the U. S. Environmental Protection Agency and U. S. Department of Agriculture in 1972 through 1973 (Smith et al. 1978). The study was conducted on

a 1.3-ha drainage area planted in corn. Soils consisted of the Cecil sandy loam (Hydrologic Soil Group B) having a slope of 1 to 3 percent. Atrazine application at 3.36 kg a.i./ha

- Monona County, Iowa. This study was conducted by Iowa State University as part of an evaluation of the effect of tillage practices on the movement of pesticides and nutrients with water and sediment (Baker and Johnson 1978). The study site consisted of a 0.78-ha drainage area planted in corn. The predominant soil was the Ida silt loam having a slope of 12 to 18 percent and classified as Hydrologic Soil Group C. Atrazine application at 2.24 kg a.i./ha

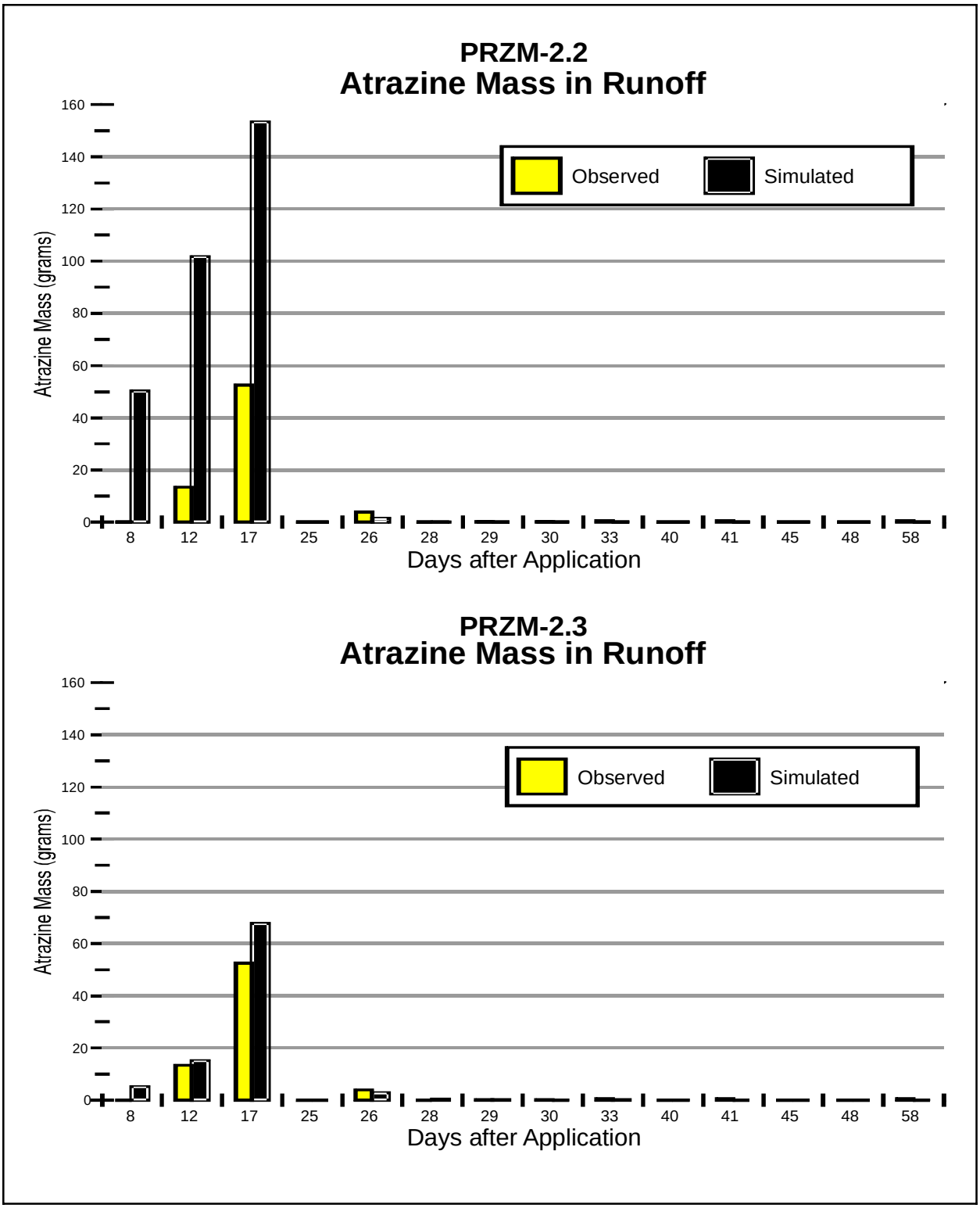


Figure 6.23 Comparison of PRZM-2.2 and PRZM-3 at Georgia study site. (PRZM-3 results are the same as those generated by the experimental version 2.3)

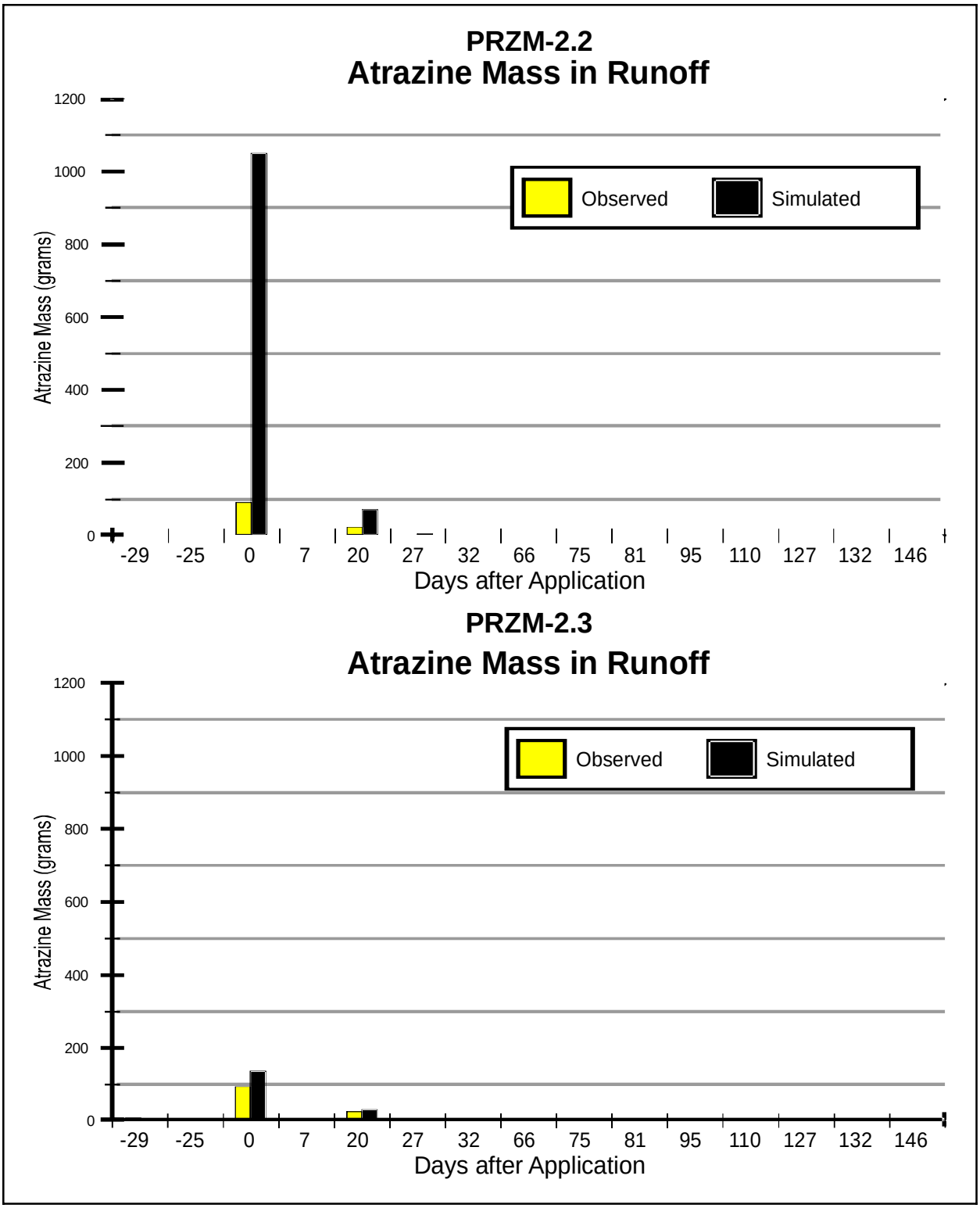


Figure 6.24 Comparison of PRZM-2.2 and PRZM-3 at Tennessee study site. (PRZM-3 results are the same as those generated by the experimental version 2.3)

6.6 Biodegradation Theory and Assumptions

The biodegradation model is based on Soulas (1982). The soil is divided into two phases: the solid phase, consisting of the dry soil including the organic matter, and the aqueous phase dispersed within it, consisting of the soil moisture, various organic substrates, and all the biomass. Some of the organic and inorganic components constituting the solid phase can adsorb the pesticide. This adsorption is represented as a linear isotherm, instantaneous and without hysteresis.

The microbial population is divided into four groups. The first two are responsible for the degradation of the pesticide. These are the metabolizing and co-metabolizing populations. The former corresponds to normal metabolic utilization, whereas the latter represents that fraction of the microflora which degrades without energy recovery.

The non-degrading population was divided into microorganisms that are sensitive to the lethal action of the chemical and those that are indifferent.

In the original development of the equations, all concentrations were expressed with respect to the soil solution. Soulas (Soulas 1982) reports that these concentrations are somewhat theoretical when considering the different biomasses and are not easy to evaluate by experiment. Thus, all concentrations were expressed with respect to the weight of the moist soil. For these biomasses, the simple proportionality

$$X_i = W^s X_i^e, \qquad i = m,c,s,r \tag{6.141}$$

was chosen where

X_i = concentration of the X_i population in the moist soil
X_i^e = concentration of the X_i population in the soil solution, and

$$W_s = \frac{H/P}{1 + H/P} \tag{6.142}$$

where

H = weight of the aqueous phase (soil solution)
P = weight of the solid phase (dry soil)

For the metabolizing population, growth is described by:

$$\frac{dX_m}{dt} = \mu_{sm} W_d S_t \frac{X_m}{K_{sm} + W_d S_t} + \mu_{cm} C_w \frac{X_m}{K_{cm}} - k_{dm} X_m \tag{6.143}$$

This represents growth at the expense of both the pesticide (S) and the carbon (C) in the soil solution. The population decreases as a result of a first-order death process with a death rate constant k_{dm}.

For the co-metabolizing population,

$$\frac{dX_c}{dt} = \mu_c C_w \frac{X_c}{K_c \left(1 + \frac{X_r + X_s}{K_{in}}\right)} - k_{dc} X_c \tag{6.144}$$

This reflects growth only at the expense of soil carbon. Allowance was also made for possible antagonistic effects by the non-degrading portion of the soil microflora. These antagonisms were assumed to result only in a reduction of the growth rate of the co-metabolizing population. Michaelis-Menten kinetics with non-competitive inhibition were used to simulate these conflicts.

For the sensitive population,

$$\frac{dX_s}{dt} = \mu_s C_w \frac{X_s}{K_s} - k_1 W_d S_t X_s - k_{ds} X_s \tag{6.145}$$

This equation assumes a death process that follows second-order kinetics. For the non-sensitive, non-degrading population X_r, the population is given by:

$$\frac{dX_r}{dt} = \mu_r C_w \frac{X_r}{K_r} - k_{dr} X_r \tag{6.146}$$

This is the basic relation of first-order growth and death terms.

The equation describing the pesticide concentration, S_t,

$$\frac{dS_t}{dt} = \frac{1}{Y_{sm}} W_s \mu_{sm} S_t \frac{X_m}{K_{sm} + W_d S_t} - k_2 E_e \frac{S_t}{K_m + W_d S_t} \tag{6.147}$$

has two parts. The first term describes the degradation due to the metabolizing population, while the second describes the action of the co-metabolizing population. The concentration of carbon in the moist soil, C_w is given by:

$$\frac{dC_w}{dt} = K_s \frac{C_m}{W_s} + \frac{Q(k_{dm}X_m + k_{dc}X_c + k_{ds}X_s + k_1 W_d S_t X_s + k_{dr}X_r)}{W_s} - C_w - \frac{1}{Y_{cm}} W_s \tag{6.148}$$

is derived on the basis that the concentration is determined by the difference between two reaction rates – the solubilization rate of carbon compounds from solid soil organic matter and the rate of microbial consumption. It is assumed that soluble carbon in the soil solution is, in first approximation, sufficiently low to be neglected when compared to the saturation constant.

Definitions:

X_i	=	Concentration of the X_i population in the moist soil ($i = m, c, s, r$)*
S_t	=	Pesticide concentration in the moist soil
C_w	=	Carbon concentration in the moist soil
μ_i	=	Maximum specific growth rate of the X_i population ($i = sm, cm, c, s, r$)*
K_i	=	Saturation constant of the X_i population ($i = sm, cm, c, s, r$)*
k_{di}	=	Death rate of the X_i population ($i = m, c, s, r$)*
Y_i	=	True growth yield of the X_i population ($i = sm, cm, c, s, r$)*
k_1	=	Second-order death rate of the X_s population
k_2	=	Dissociation constant of the enzyme-substrate complex
K_{in}	=	Inhibition constant

In addition,

$$W_d = \frac{1 + W}{K_d + W} \tag{6.149}$$

where

K_d = distribution coefficient

$$W = \frac{H}{P} \tag{6.150}$$

and

H = weight of soil solution (aqueous phase)
P = weight of dry soil (solid phase)

These equations are to be solved simultaneously, and the results used to determine the amount of pesticide in the soil

that is degraded biologically over the timestep interval.

These equations are solved in PRZM-3 using a fourth-order Runge-Kutta method. This subprogram uses the carbon concentration and the pesticide concentration in the moist soil of each compartment as input. Using the populations of organisms in each compartment, which is saved between calls, the subprogram solves the degradation algorithm to determine the new pesticide amount, and thus the amount degraded, over the PRZM-3 time step. Also, the changes to the organism populations are calculated and saved for use in the subsequent timestep.

SECTION 7
Vadose Zone Flow and Transport Model (VADOFT) Code and Theory

7.1 Introduction

VADOFT is a finite-element code for simulating moisture movement and solute transport in the vadose zone. It is the second part of the two-component PRZM-3 model for predicting the movement of pesticides within and below the plant root zone and assessing consequent groundwater contamination. The VADOFT code simulates one-dimensional, single-phase moisture movement in unconfined, variably saturated porous media. The code considers only single-porosity media and also ignores the effects of hysteresis. Transport of dissolved contaminants may also be simulated within the same domain. Transport processes accounted for include hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. VADOFT also simulates solute transformations in order to account for parent/daughter relationships.

7.2 Overview of VADOFT

7.2.1 Features

7.2.1.1 General Description

The VADOFT code can be used to perform one-dimensional modeling of water flow and transport of dissolved contaminants in variably or fully saturated soil/aquifer systems. VADOFT can be operated as a stand-alone code or operated in conjunction with the root zone model, PRZM. In the latter case, boundary conditions at the interfaces of the modeled domains are established via model linkage procedures.

7.2.1.2 Process and Geometry

VADOFT performs one-dimensional transient or steady-state simulations of water flow and solute transport in variably saturated porous media. The code employs the Galerkin finite-element technique to approximate the governing equations for flow and transport. It allows for a wide range of nonlinear flow conditions, and handles various transport processes, including hydrodynamic dispersion, advection, linear equilibrium sorption, and first-order decay. Steady-state transport can not be simulated when decay is considered. Boundary conditions of the variably saturated flow problems are specified in terms of prescribed pressure head or prescribed volumetric water flux per unit area. Boundary conditions of the solute transport problem are specified in terms of prescribed concentration or prescribed solute mass flux per unit area. All boundary conditions may be time dependent.

7.2.1.3 Assumptions

The VADOFT code contains both flow and solute transport models. Major assumptions of the flow model are:

- Flow of the fluid phase is one-dimensional and considered isothermal and governed by Darcy's law.
- The fluid considered is slightly compressible and homogeneous.
- Hysteresis effects in the constitutive relationships of relative permeability versus water saturation, and water saturation versus capillary pressure head, are assumed to be negligible.

Major assumptions of the solute transport model are:

- Advection and dispersion are one-dimensional.
- Fluid properties are independent of concentrations of contaminants.
- Diffusive/dispersive transport in the porous-medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion.

- Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first-order decay constant.
- Vapor transport can be neglected.

7.2.1.4 Data Requirements

Data required for the simulation of variably saturated flow include values of the saturated hydraulic conductivity and specific storage of the porous media, the geometry and configuration of the flow region, as well as initial and boundary conditions associated with the flow equation. Soil moisture relationships are also required. These include relative permeability versus water phase saturation and capillary head versus water phase saturation. These relationships may be supplied to the code using tabulated data or functional parameters.

Data required for the simulation of solute transport in variably saturated soil include dispersivity and porosity values, retardation and decay constants, Darcy velocity and water saturation values, as well as initial and boundary conditions associated with the transport equation.

7.2.2 Limitations

Major limitations of the VADOFT code are:

- In performing a variably saturated flow analysis, the code handles only single-phase flow (i.e., water) and ignores the flow of a second phase (i.e., air) which, in some instances, can be significant.
- The code ignores the effects of hysteresis on the soil moisture constitutive relations.
- The code does not take into account sorption nonlinearity or kinetic sorption effects which, in some instances, can be important.
- The code considers only single-porosity (granular) soil media. It cannot handle fractured porous media or structured soils.
- The code does not take into account transverse dispersion, which can be important for layered media.

7.3 Description of Flow Module

7.3.1 Flow Equation

VADOFT considers the problem of variably saturated flow in a soil column in the vadose zone of an unconfined aquifer. The code solves the Richards' equation, the governing equation for infiltration of water in the vadose zone:

$$\frac{\partial}{\partial z}\left[K k_{rw} \frac{\partial \psi}{\partial z}\right] = \eta \frac{\partial \psi}{\partial t} \qquad \textbf{(7.1)}$$

where

ψ	=	the pressure head (L)
K	=	the saturated hydraulic conductivity (LT^{-1})
k_{rw}	=	the relative permeability
z	=	the vertical coordinate pointing in the downward direction (L)
t	=	time (T)
η	=	an effective water storage capacity (L^{-1}) defined as:

$$\eta = S_w S_s + \phi \frac{dS_w}{d\psi} \qquad \textbf{(7.2)}$$

where

S_s	=	specific storage (L^{-1}),

S_w = water saturation
ϕ = the effective porosity.

Specific storage is defined by

$$S_s = \rho g[\phi c_f + (1-\phi) c_s] \tag{7.3}$$

where

c_f = the fluid compressibility (LT^2M^{-1})
c_s = the solid skeleton compressibility (LT^2M^{-1})
ρ = the fluid density (ML^{-3}), and
g = the gravitational acceleration (LT^{-2})

The initial and boundary conditions of the one-dimensional infiltration problem may be expressed as:

$$\psi(z,0) = \psi_i \tag{7.4}$$

either

$$V(0,t) = I \tag{7.5}$$

or

$$\psi(0,t) = \psi_0 \tag{7.6}$$

either

$$\psi(L,t) = \psi_L \tag{7.7}$$

or

$$V(L,t) = 0 \tag{7.8}$$

where

ψ_i = the initial pressure head value (L)
ψ_o = the pressure head at the upper boundary (L)
ψ_L = the pressure head at the lower boundary (L)
I = the rate of infiltration at the soil surface (LT^{-1})
L = the thickness of the vadose zone (L)
V = the vertical Darcy velocity (LT^{-1}) (defined by Equation 7.12).

The boundary condition in Equation 7.8 is valid because the bottom boundary of VADOFT allows fluid to exit.

To solve the variably saturated infiltration problem, it is also necessary to specify the relationships of relative permeability versus water saturation and pressure head versus water saturation. Two alternative function expressions are used to describe the relationship of relative permeability versus water saturation. These functions are given by Brooks and Corey (1966) and van Genuchten (1980):

$$k_{rw} = S_e^n \tag{7.9}$$

and

$$k_{rw} = S_e^{1/2}[1 - (1 - S_e^{1/\gamma})^\gamma]^2 \tag{7.10}$$

where

n and γ are empirical parameters
S_e = the effective water saturation defined as $S_e = (S_w - S_{wr})/(1 - S_{wr})$; S_{wr} denotes the residual water saturation.

The relationship of pressure head versus water saturation is described by the function (Mualem 1976, van Genuchten 1980):

$$\frac{S_w - S_{wr}}{1 - S_{wr}} = \begin{cases} \dfrac{1}{[1 + (a \cdot |\psi - \psi_a|)^{\beta}]^{\gamma}} & \psi < \psi_a \\ 1 & \psi \geq \psi_a \end{cases} \tag{7.11}$$

where

α, β, and γ	=	empirical parameters; $\gamma = 1 - 1/\beta$,
ψ_a	=	the air entry pressure head value (L)
S_{wr}	=	the residual water phase saturation.

Descriptive statistical values for α, β, and γ have been determined by Carsel and Parrish (Carsel and Parrish 1988) for 12 soil classifications (see Section 5). Using the mean parameter values, the relationships of effective saturation versus capillary head and relative permeability versus effective saturation are plotted. Logarithmic plots are shown in **Figure 7.1** through **Figure 7.3**. To show more vividly the high degree of nonlinearities, the relationships of relative permeability versus effective saturation are also plotted on arithmetic scales and presented in **Figure 7.4** through **Figure 7.6**. It is important that the finite element flow module be capable of handling such high nonlinearities to be successful in performing a Monte Carlo study of infiltration in the unsaturated zone.

Equation 7.1 is solved using the Galerkin finite element subject to the initial and boundary conditions given in Equations 7.4 through 7.7. After the distributions of ψ and S_w have been determined, the Darcy velocity is computed from:

$$V = -K k_{rw} \left(\frac{\partial \psi}{\partial z} - 1 \right) \tag{7.12}$$

7.3.2 Numerical Solution

7.3.2.1 Numerical Approximation of the Flow Equation

A numerical approximation of the one-dimensional flow equation in the vadose zone is obtained using a Galerkin finite-element formulation with spatial discretization performed using linear elements. Time integration is performed using a backward finite difference approximation. This leads to a system of nonlinear algebraic equations. For a typical node "*I*" in the finite-element grid (see **Figure 7.7**),

$$\alpha_i \psi_{i-1}^{k+1} + \beta_i \psi_i^{k+1} + \gamma_i \psi_{i+1}^{k+1} = d_i \tag{7.13}$$

where k+1 is the current time level, and α_i, β_i, γ_i, and d_i are given by

$$\alpha_i = \frac{-\{K k_{rw}\}_{i-1}}{\Delta z_{i-1}} \tag{7.14}$$

$$\beta_i = \frac{\{K k_{rw}\}_{i-1}}{\Delta z_{i-1}} + \frac{\{K k_{rw}\}_i}{\Delta z_i} + \frac{\eta_i}{\Delta t_k} \left(\frac{\Delta z_{i-1} + \Delta z_i}{2} \right) \tag{7.15}$$

$$\gamma_i = \frac{-\{K k_{rw}\}_i}{\Delta z_i} \tag{7.16}$$

$$d_i = \frac{\eta_i}{\Delta t_k}\left(\frac{\Delta z_{i-1} + \Delta z_i}{2}\right)\psi_i^k + \{Kk_{rw}\}_{i-1} - \{Kk_{rw}\}_i \tag{7.17}$$

and Δz_i and Δt_k are the spatial and time increments, respectively. Note that braces ({}) are used in the equationsabove (and below) to denote the value of the enclosed quantity at the element centroid. The nonlinear system of equations is solved for each time step. Three nonlinear schemes are provided in the VADOFT code. The first scheme is a Picard-type iteration scheme, the second scheme is a Newton-Raphson, and the third is a Newton-Raphson scheme modified by Huyakorn (1988, Personal Communication).

In the Picard scheme, the matrix coefficients, α_i, β_i, γ_i, and d_i, are first evaluated using an initial estimate of pressure head values, ψ_i^k. The resulting system of linearized equations is then solved for ψ_i^{k+1} using the Thomas algorithm. Updating of the matrix coefficient is performed by recomputing values of nonlinear soil parameters. Iterations are performed until the successive change in pressure head values is within a prescribed tolerance.

In the Newton-Raphson scheme, the nonlinear system of equations is treated by applying the Newton-Raphson technique (see Huyakorn and Pinder 1983) to Equation 7.13. This leads to the following system of linearized algebraic equations:

$$(\alpha_i + \alpha_i^*)^r \psi_{i-1}^{k+1} + (\beta_i + \beta_i^*)^r \psi_i^{k+1} + (\gamma_i + \gamma_i^*)^r \psi_{i+1}^{k+1} = (d_i + d_i^*)^r \tag{7.18}$$

where superscript r is used to denote the r-th iterate; α_i, β_i, γ_i, and d_i were defined previously; α_i^*, β_i^*, and γ_i^*, are given by

$$\alpha_i^* = -\frac{\{D\}_{i-1}}{\Delta z_{i-1}} - \frac{1-\omega}{2}\{V\}_{i-1} + \frac{\lambda\{\theta R\}_{i-1}\Delta z_{i-1}}{6} \tag{7.19}$$

$$\beta_i^* = \left(\frac{\{D\}_{i-1}}{\Delta z_{i-1}} + \frac{\{D\}_i}{\Delta z_i}\right) + \frac{\lambda}{3}(\{\theta R\}_{i-1}\Delta z_{i-1} + \{\theta R\}_i \Delta z_i) + \frac{1-\omega}{2}\{V\}_{i-1} - \frac{1+\omega}{2}\{V\}_i \tag{7.20}$$

$$\gamma_i^* = -\frac{\{D\}_i}{\Delta z_i} + \frac{1+\omega}{2}\{V\}_i + \frac{\lambda\{\theta R\}_i \Delta z_i}{6} \tag{7.21}$$

The initial solution and subsequent iterations of the Newton-Raphson scheme are performed in the same manner as that described for the Picard scheme.

7.3.2.2 General Guidance on Selection of Grid Spacings and Time Steps, and the Use of Solution Algorithms

In designing a finite-element grid for variably saturated flow simulations, one should select nodal spacings that will yield reasonable approximations to the expected moisture profiles.

In the analysis of the given variably saturated flow problem, small nodal spacings should be used in the zones where head gradients or moisture fronts are steep. The nodal spacings may be gradually increased in the zone where no abrupt changes in hydraulic conductivities occur and the head gradients are gradually sloping. The variably saturated flow simulation can be performed using either the Picard algorithm or one of the Newton-Raphson solution algorithms. For one-dimensional cases where convergence difficulties are not expected, the efficiencies of these algorithms have been found to be similar. For certain steady-state cases involving highly nonlinear soil moisture characteristics, the use of either of the Newton-Raphson algorithms is preferable, particularly when the Picard algorithm fails to converge within a reasonable number of iterations (say between 10 and 20).

7.4 Description of the Transport Module

7.4.1 Transport Equation

The governing equation for one-dimensional transport of a nonconservative solute species in a variably saturated soil takes the form

$$\frac{\partial}{\partial z}(D\frac{\partial c}{\partial z}) - V\frac{\partial c}{\partial z} = \theta R(\frac{\partial c}{\partial t} + \lambda c) \tag{7.22}$$

where D is the apparent dispersion coefficient (L^2T^{-1}), c is the solute concentration (ML^{-3}), θ is the volumetric water content ($\theta = \phi S_w$), R is the retardation coefficient, and λ is the first-order decay constant (T^{-1}). Note that the apparent dispersion coefficient is defined as $D = \alpha_L V + \phi D^*$, where α_L is the longitudinal dispersivity, and D^* is the effective molecular diffusion coefficient.

The initial and boundary conditions of the one-dimensional transport problem may be expressed as:

$$c(z,0) = c_i \tag{7.23}$$

either

$$-D\frac{\partial c}{\partial z}(0,t) = V(c_0 - c) \tag{7.24}$$

or

$$c(0,t) = c_0 \tag{7.25}$$

$$\frac{\partial c}{\partial z}(L,t) = 0 \tag{7.26}$$

where c_i is the initial concentration (ML^{-3}), and c_o is the leachate concentration at the source (ML^{-3}).

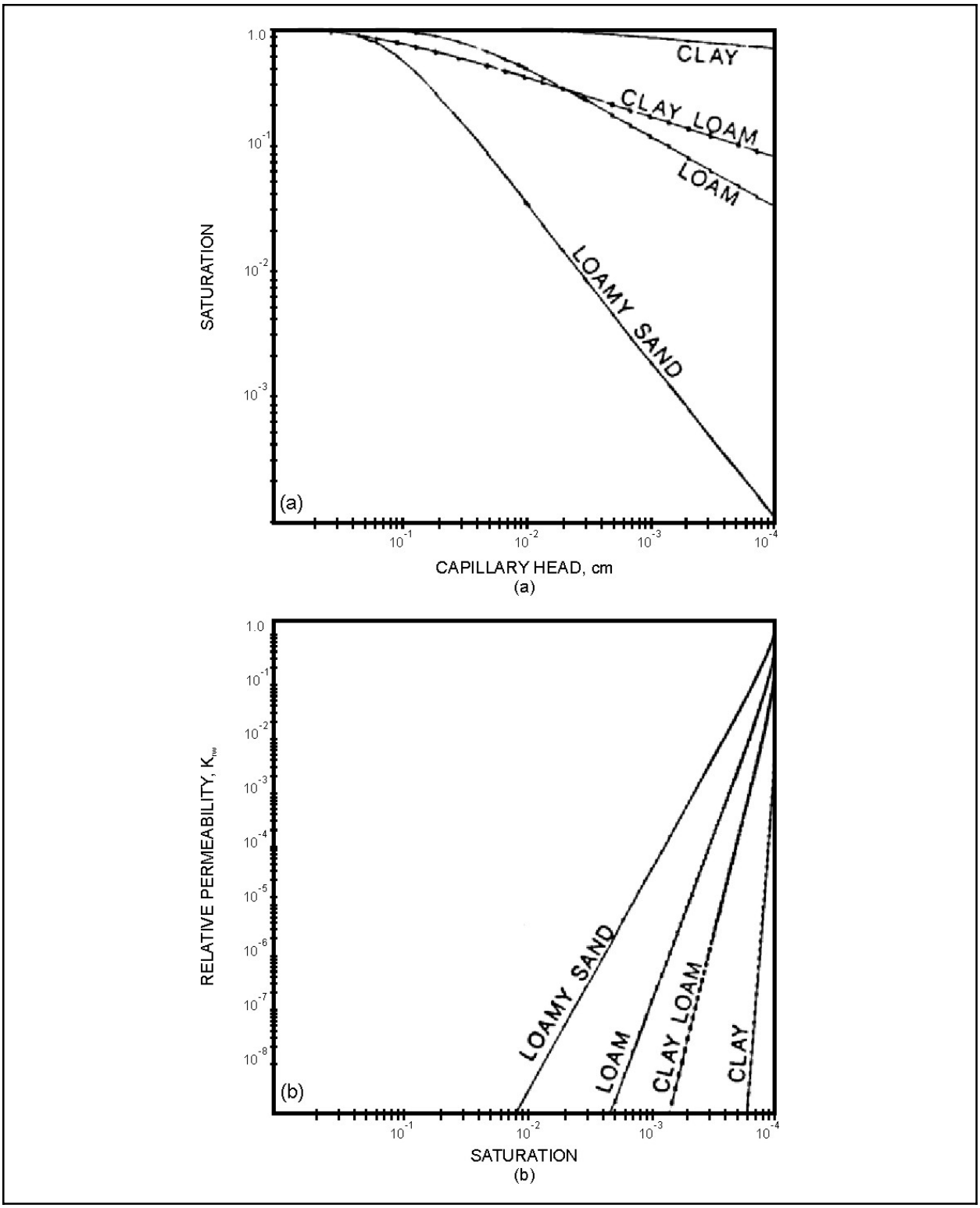


Figure 7.1 Logarithmic plot of constitutive relations for clay, clay loam, and loam sandy soils: (a) saturation vs. capillary head and (b) relative permeability vs. saturation.

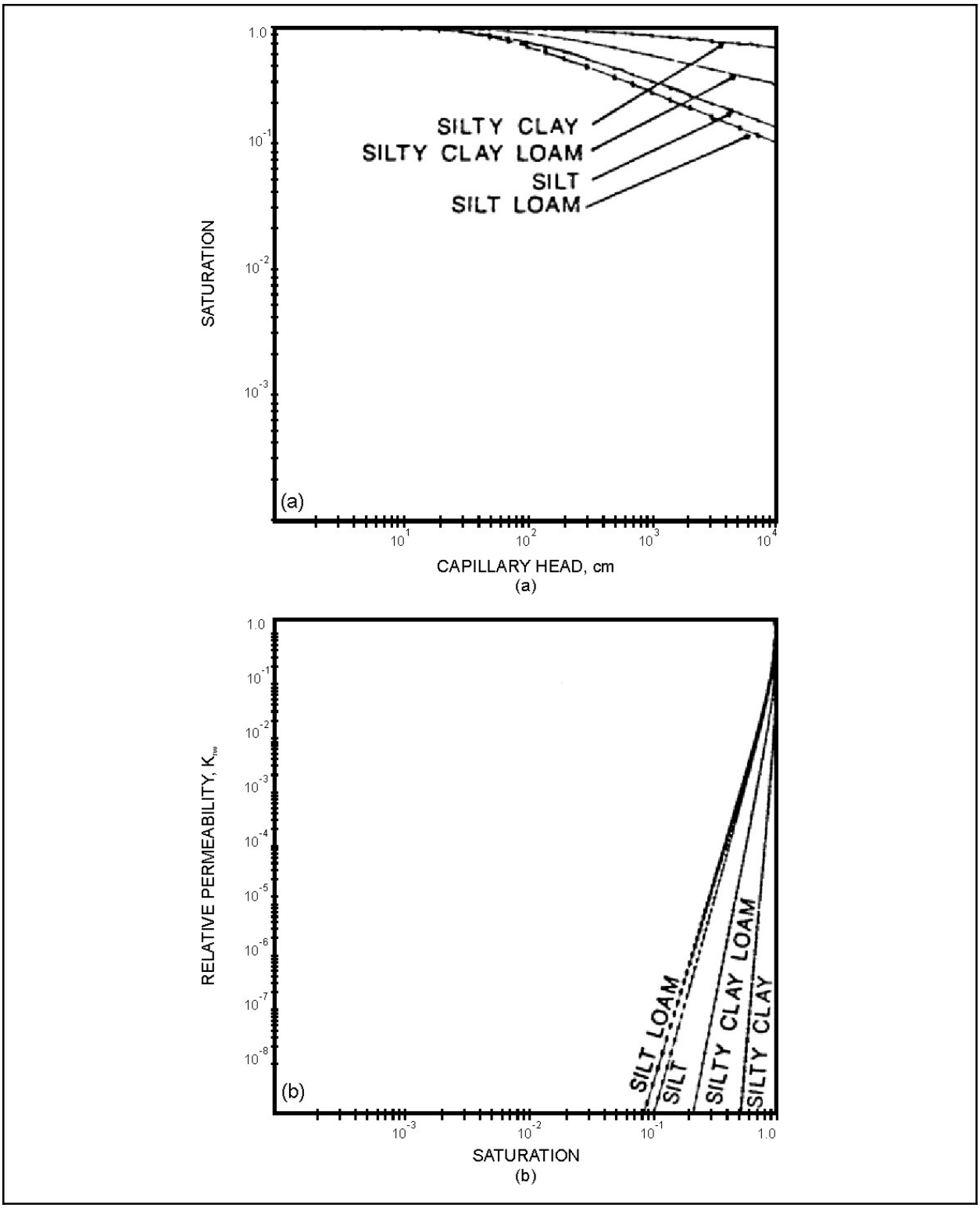


Figure 7.2 Logarithmic plot of constitutive relations for silt, silty clay loam, silty clay, and silty loam soils.

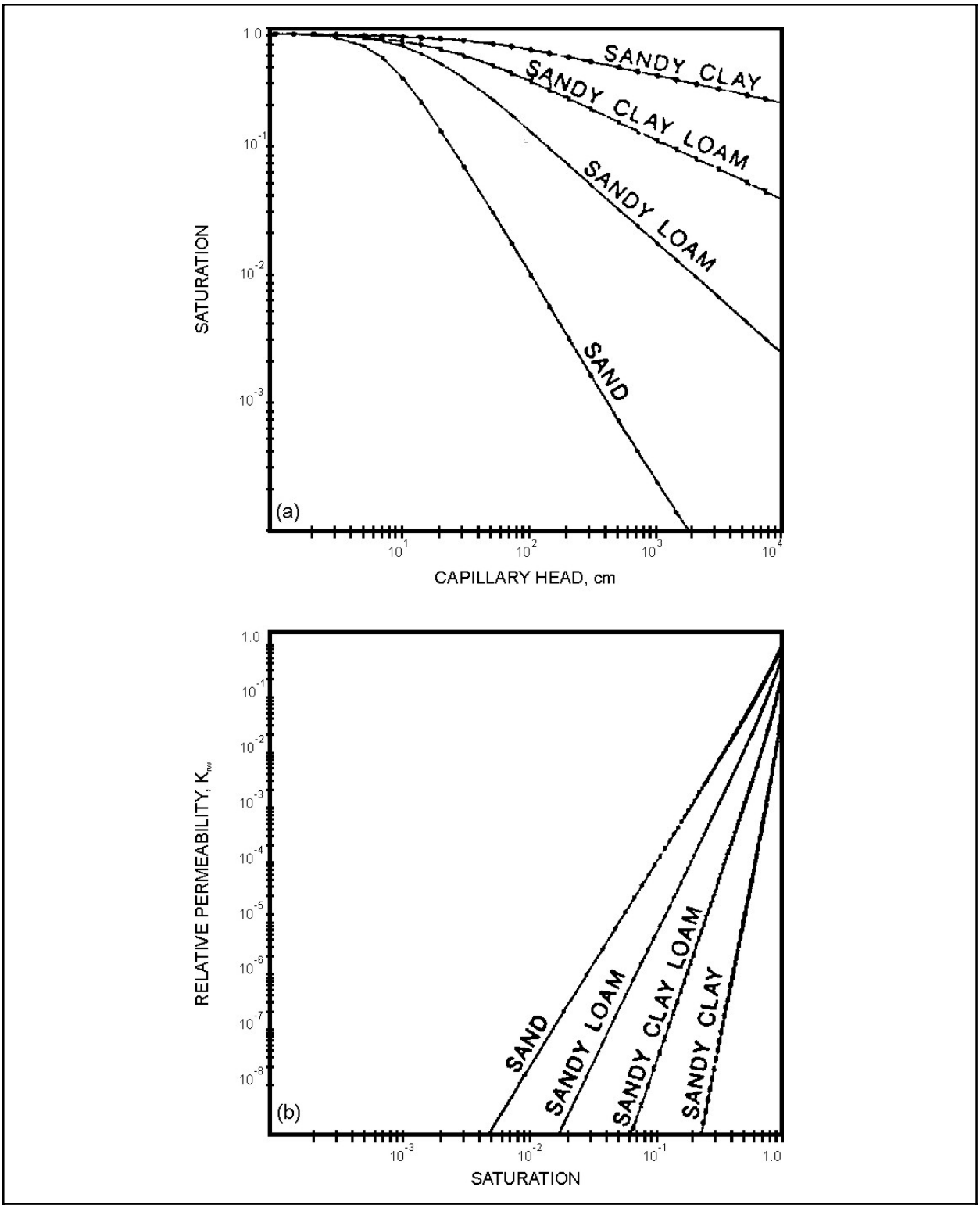


Figure 7.3 Logarithmic plot of constitutive relations for sandy clay, sandy clay loam, sandy loam, and sandy soils.

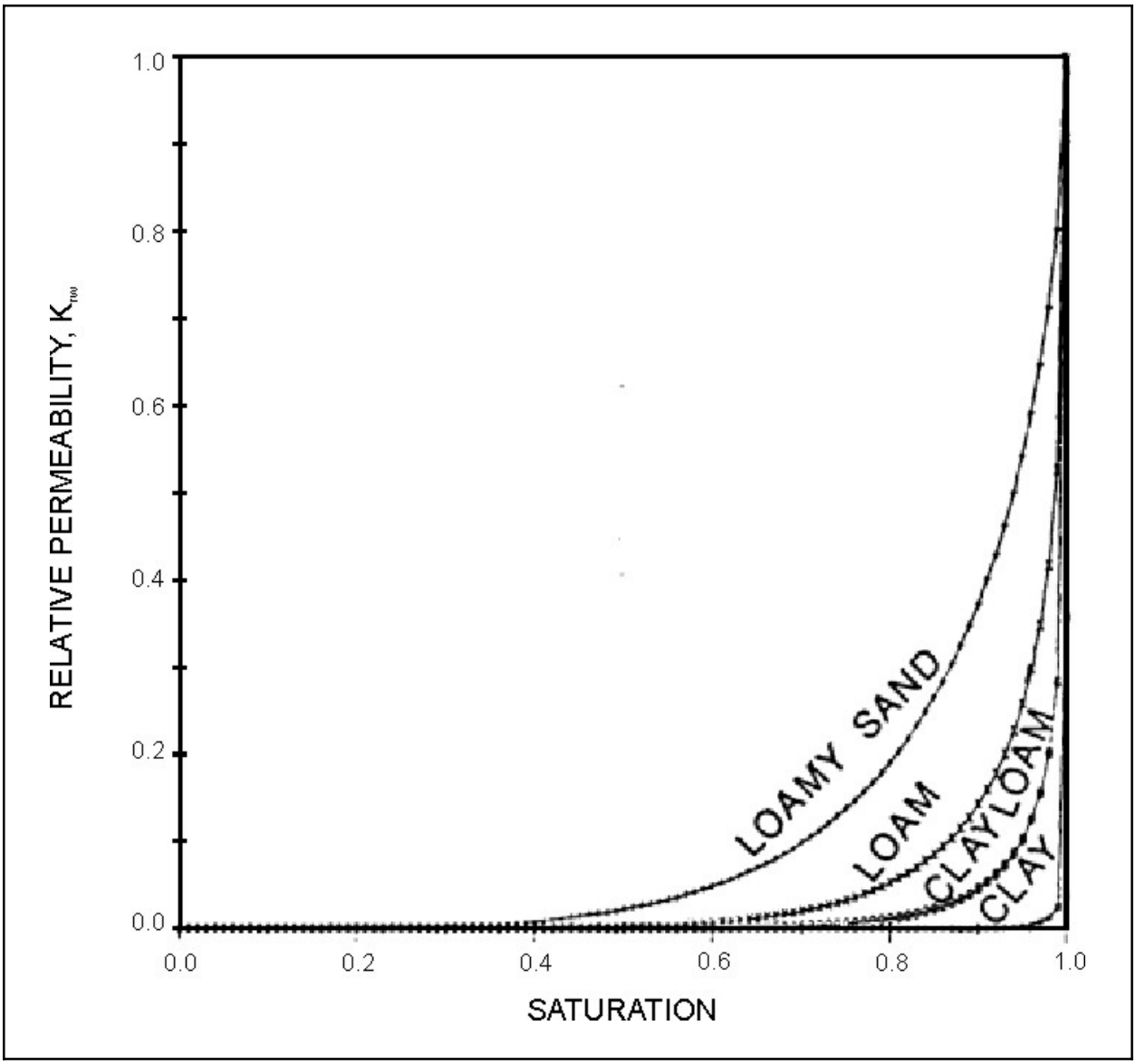


Figure 7.4 Standard plot of relative permeability vs. saturation for clay, clay loam, loam and loam sandy soils.

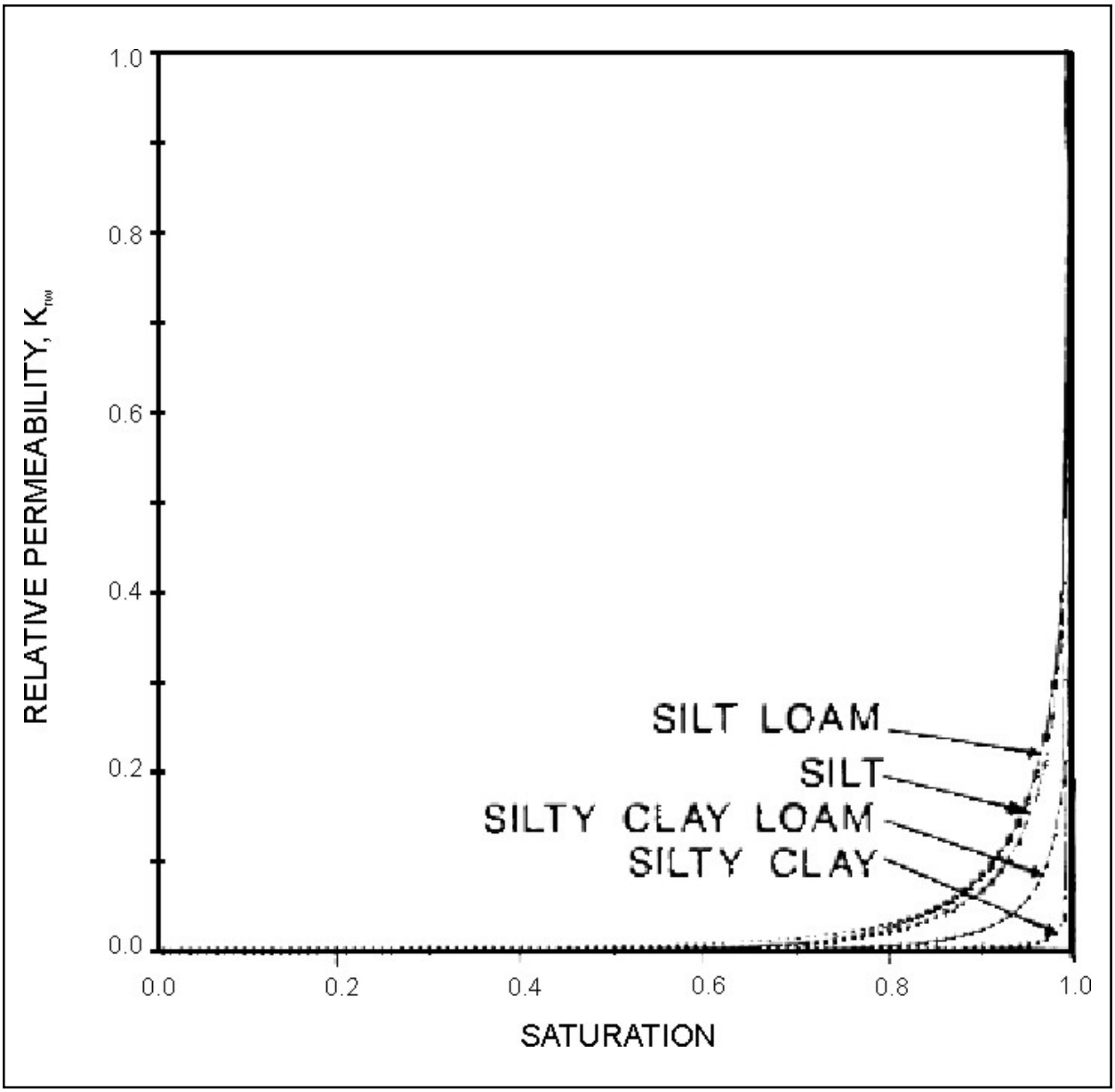


Figure 7.5 Standard plot of relative permeability vs. saturation for silt, silt clay loam, silty clay and silty loam soils.

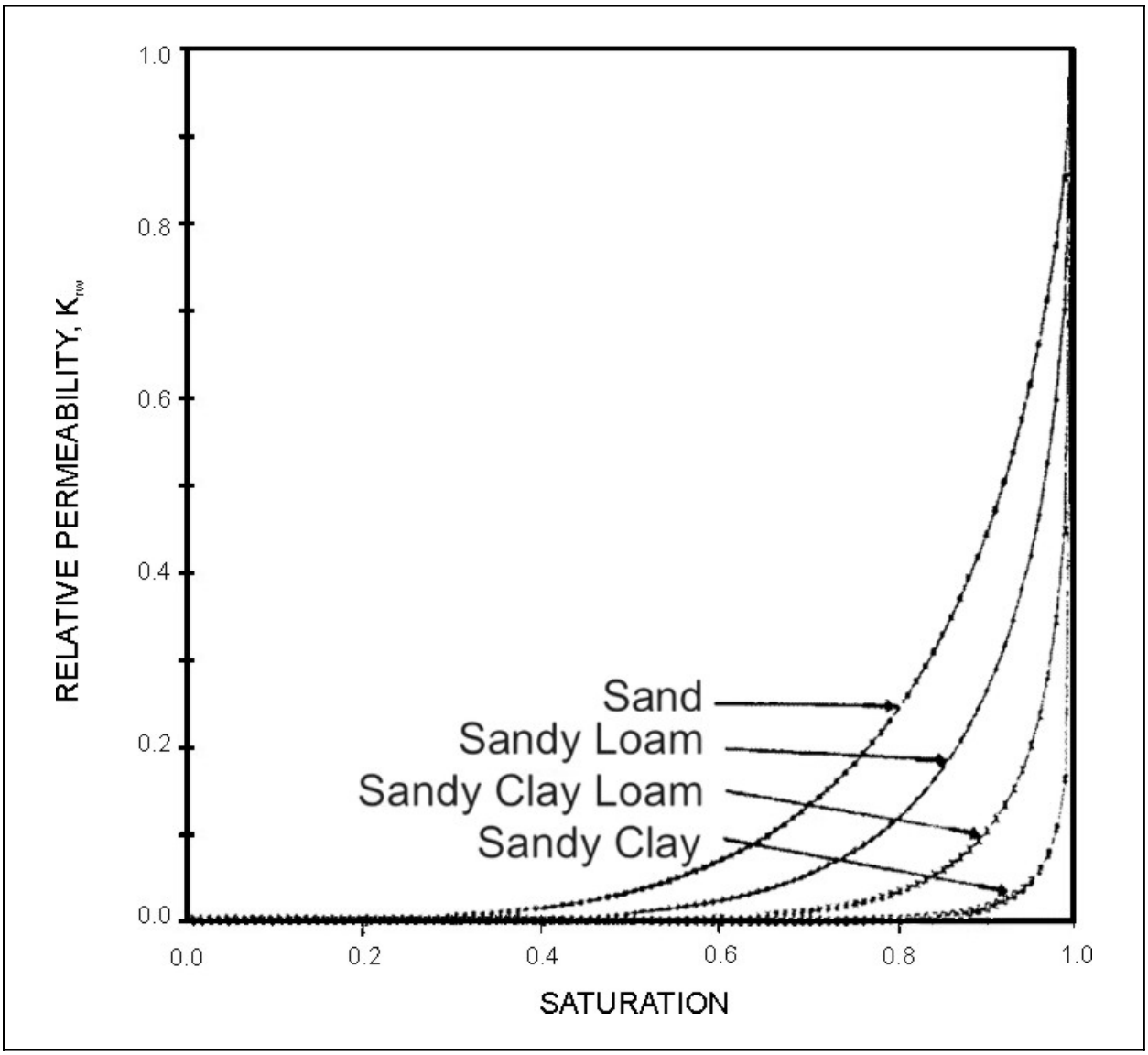


Figure 7.6 Standard plot of relative permeability vs. saturation for sandy clay, sandy clay loam, sandy loam and sandy soils.

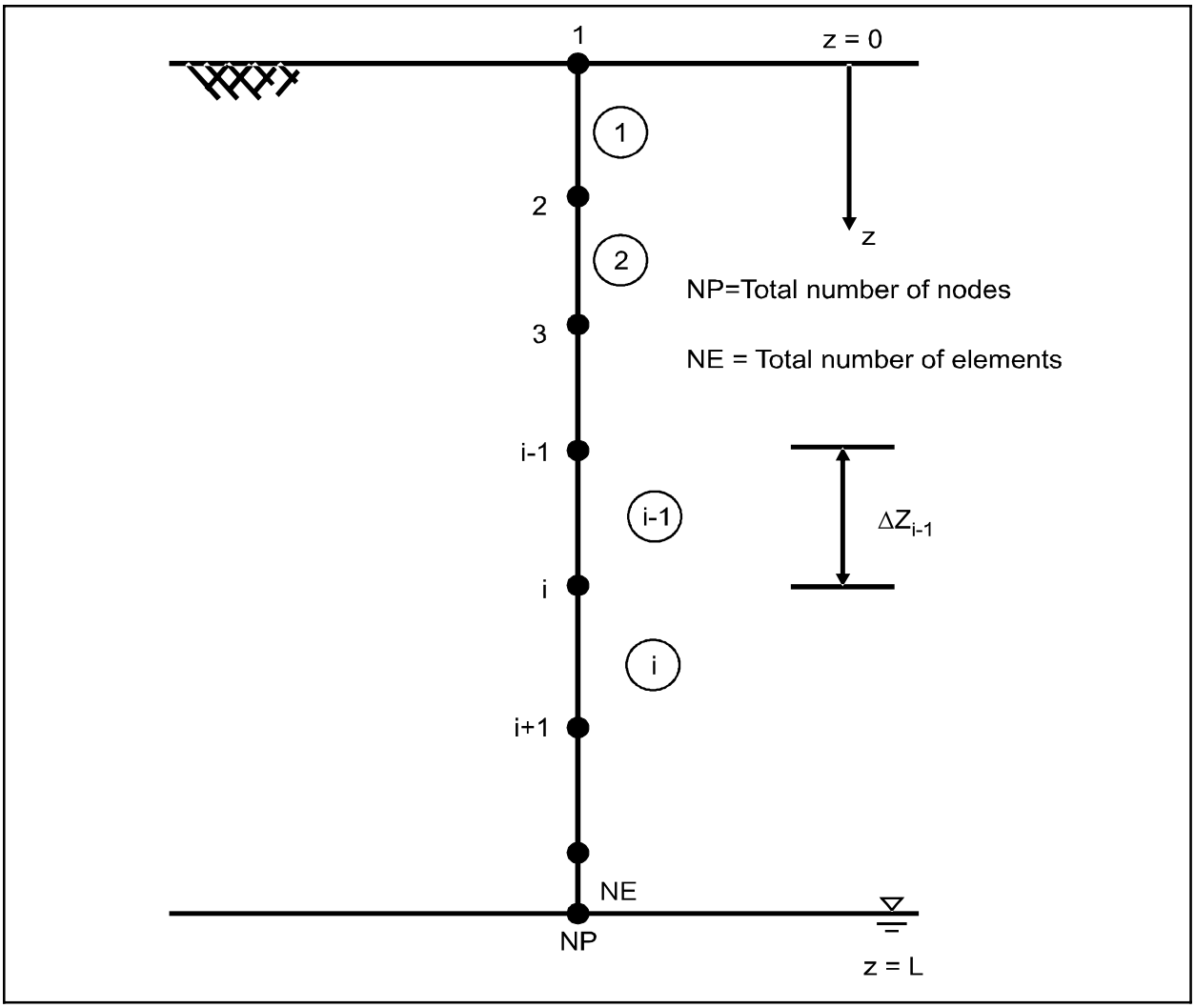


Figure 7.7 Finite element discretization of soil column showing node and element numbers.

7.4.2 Numerical Solution of the Transport Equation

7.4.2.1 Numerical Approximation of the Transport Equation

A numerical approximation of the one-dimensional transport equation is obtained using an upstream-weighted finite-element formulation with spatial discretization performed using linear elements. Time integration is performed using a central finite-difference approximation. This leads to a system of linear algebraic equations. The equation corresponding to node "*i*" takes the form:

$$\alpha_i c_{i-1}^{k+1} + \beta_i c_i^{k+1} + \gamma_i c_{i+1}^{k+1} = d_i \tag{7.27}$$

where

$$\begin{aligned}
\alpha_i &= \tau\alpha_i^* + \frac{\{\theta R\}_{i-1}\Delta z_{i-1}}{6\Delta t_k} \\
\beta_i &= \tau\beta_i^* + \frac{\{\theta R\}_i \Delta z_i + \{\theta R\}_{i-1}\Delta z_{i-1}}{3\Delta t_k} \\
\gamma_i &= \tau\gamma_i^* + \frac{\{\theta R\}_i \Delta z_i}{6\Delta t_k} \\
d_i &= (\tau - 1)\times(\alpha_i^* c_{i-1}^k + \beta_i^* c_i^k + \gamma_i^* c_{i+1}^k) + \frac{\{\theta R\}_{i-1}\Delta z_{i-1}}{6\Delta t_k}(c_{i-1}^k + 2c_i^k) + \frac{\{\theta R\}_i \Delta z_i}{6\Delta t_k}(c_{i+1}^k + 2c_i^k) \\
\alpha_i^* &= -\frac{\{D\}_{i-1}}{\Delta z_{i-1}} - \frac{1-\omega}{2}\{V\}_{i-1} + \frac{\lambda\{\theta R\}_{i-1}\Delta z_{i-1}}{6} \\
\beta_i^* &= \frac{\{D\}_{i-1}}{\Delta z_{i-1}} + \frac{\{D\}_i}{\Delta z_i} + \frac{\lambda}{3}(\{\theta R\}_{i-1}\Delta z_{i-1} + \{\theta R\}_i \Delta z_{i)} + \frac{1-\omega}{2}\{V\}_{i-1} - \frac{1+\omega}{2}\{V\}_i \\
\gamma_i^* &= -\frac{\{D\}_i}{\Delta z_i} + \frac{1+\omega}{2}\{V\}_i + \frac{\lambda\{\theta R\}_i \Delta z_i}{6}
\end{aligned} \tag{7.28}$$

with τ and ω denoting the time weighting factor and the upstream weighting factor, respectively.

To obtain a second-order temporal approximation, the value of τ is set equal to ½. This corresponds to using the Crank-Nicholson central difference time stepping scheme. The upstream weighting factor ω is introduced in the above numerical approximation to curb numerical oscillations that may occur when the selected finite-element grid is not sufficiently refined for a given value of longitudinal dispersivity. For each time step, the linear system of algebraic equations is solved using the Thomas algorithm.

Transport of a daughter species in a decay chain can also be handled by the VADOFT code. In this case, the right side of the governing equation for single species transport (Equation 7.22) is modified by adding a source term accounting for transformation of parent components. This source term is given by

$$m = -\sum_{j=1}^{n_p} \phi S_w \varepsilon_j \lambda_j R_j c_j \tag{7.29}$$

where

subscript j	=	the parent species
n_p	=	the number of parent species
ε_j	=	the mass fraction of parent component that is transformed into the daughter species under consideration

The numerical solution of the modified transport equation can be performed in the same manner as that described

previously for a single species. The source term from Equation 7.29 is incorporated into the finite element matrix equation by adding d_i^* to the right side,

$$d_i^* = \frac{1}{2}\left(\sum_{j=1}^{n_p} \varepsilon_j \lambda_j R_j c_{j_i}^{k+1}\right)(\Delta z_i + \Delta z_{i-1})(\phi S_w)_i \tag{7.30}$$

In performing the solute transport analysis, the selection of nodal spacing (Δz) and time step value (Δt) should follow the so-called Peclet number and Courant number criteria where possible. These two criteria are

$$\frac{\Delta z}{\alpha_L} \le 4 \tag{7.31}$$

$$\frac{V_{sol}\,\Delta t}{\Delta z} \le 1 \tag{7.32}$$

$$V_{sol} = \frac{V}{\theta R} \tag{7.33}$$

where

α_L	=	the longitudinal dispersivity
V_{sol}	=	the solute velocity
V	=	Darcy velocity
θ	=	water content
R	=	retardation coefficient

The VADOFT code also provides the user with the option of using upstream weighting to curb numerical oscillations that may occur in solving the advective-dispersive transport equation. The recommended value of ω, the weighing factor, is given by

$$\omega = \begin{cases} 1 - \dfrac{4\alpha_L}{\ell} & \ell > 4\alpha_L \\ 0 & \ell \le 4\alpha_L \end{cases} \tag{7.34}$$

where

α_L	=	the longitudinal dispersivity
ℓ	=	the length of the element.

7.5 Results of VADOFT Testing Simulations

Three sets of benchmark problems were used to test the VADOFT code. The first set consists of two steady and transient problems designed to test the variably saturated flow component of the code. The second set consists of four transient one-dimensional transport problems. The third set consists of two coupled flow-transport problems. Numerical results obtained from VADOFT are compared with analytical solutions and results obtained using two other finite-element codes, UNSAT2 and SATURN. These test problems were simulated using VADOFT before it was linked in PRZM-3.

7.5.1 Flow Module (Variably Saturated Flow Problems)

7.5.1.1 Transient Upward Flow in a Soil Column

This problem concerns transient, vertically upward moisture movement in a 20 cm long soil column. The soil column is subject to zero pressure head at the base and zero flux at the top. The initial distribution of pressure head

is hydrostatic: (t = 0) = -90 + z cm, where z is the depth below the top of the soil column. Soil properties and discretization data used in the simulation are presented in Table 7.1. The simulation was performed for 15 time steps with constant time step value of t = 0.01 d. Numerical results given by the Picard and the Newton-Raphson schemes are virtually identical. Both schemes require between 2 and 3 iterations per time step to converge to a head tolerance of 0.01 cm. The simulation results obtained from VADOFT are compared with those obtained from UNSAT2 and SATURN (the two-dimensional finite-element codes described by Davis and Neuman (1983), and Huyakorn et al. (1984)) respectively. Shown in **Figure 7.8** and **Figure 7.9** are plots of distributions of pressure head and water saturation, respectively. As can be seen, the results of VADOFT are in good agreement with the results of the other two codes.

7.5.1.2 Steady Infiltration in a Soil Column

This problem concerns steady-state infiltration in a soil column. The column is 550 cm in length and is subject to an infiltration rate of 4.07 cm day^{-1} at the top and zero pressure head at the bottom. Soil properties used in the simulation are presented in Table 7.2. Five cases of varying degree of nonlinearity of relative permeability function ($k_{rw} = S_e^n$) were simulated. Both the Picard and the Newton-Raphson schemes were used in conjunction with a finite-element grid having constant nodal spacing, z = 10 cm. The performance of the two iterative schemes are illustrated in Table 7.3. Note that the Newton-Raphson scheme converges for all cases, whereas the Picard scheme fails to converge when the nonlinear exponent n exceeds 4. Simulated distributions of pressure head and water saturation are shown in **Figure 7.10** and **Figure 7.11**, respectively. These results of the VADOFT code are virtually identical to corresponding results obtained using the SATURN code.

7.5.2 Transport Module

7.5.2.1 Transport in a Semi-Infinite Soil Column

This problem concerns one-dimensional transport of a conservative solute species in a saturated soil column of infinite length. The solute is introduced into the column at the inlet section where z = 0. The initial concentration is assumed to be zero, and the dimensionless constant inlet concentration is prescribed as 1. Values of physical parameters and discretization data used in the numerical simulation are given in Table 7.4. The finite-element grid representing the soil column was 400 cm in length. The simulation was performed for 20 time steps. Thus the duration of the simulation time of transport in the soil column was 50 hours. For this duration, the selected grid length is sufficient to avoid the end boundary effect. The numerical solution obtained from the VADOFT code was checked against the analytical solution of Ogata and Banks (1961). Shown in **Figure 7.12** and Table 7.5 are concentration values at t = 25 hours and t = 50 hours. As can be seen, the numerical and analytical solutions are in excellent agreement.

7.5.2.2 Transport in a Finite Soil Column

In this problem, downward vertical transport of dissolved contaminants in a soil column above the water table of an unconfined aquifer is considered. The length of the soil column is 20 m and the Darcy velocity and water content are assumed to be constant and equal to 0.25 m day^{-1} and 0.25, respectively. The initial concentration is zero, and water with dimensionless solute concentration of 1 enters the soil surface at a rate of 0.25 m day^{-1}. At the water table, a zero dispersive-flux boundary condition is assumed. A list of physical parameter values and discretization data used in the simulation is provided in Table 7.6. Two cases involving conservative and nonconservative species were simulated. Results obtained from the VADOFT code are compared in **Figure 7.13** and Table 7.7 with the analytical solution given by van Genuchten and Alves (1982). There is excellent agreement between the numerical and analytical solutions for both cases.

7.5.2.3 Transport in a Layered Soil Column

This problem concerns one-dimensional transport of a conservative solute species in a soil column consisting of three layers. The initial concentration in the soil column is assumed to be zero, and the two boundary conditions prescribed are a unit concentration at the top and a zero dispersive flux boundary condition at the bottom. A list of

physical parameter values and discretization data used in the simulation is provided in Table 7.8. Two cases corresponding to those considered by Shamir and Harleman (1967) were simulated. Both cases have contrasting longitudinal dispersivity values among the three layers. The dispersivity values of the second case are ten times those of the first case for the same layers. The intention here is to test the numerical scheme used in the VADOFT code, as well as to check the validity of an approximate analytical solution presented by Shamir and Harleman (1967) and Hadermann (1980). It should be noted here that the approximate solutions are valid only for relatively small values of dispersivity. Therefore, for a small dispersivity value, the solutions can be employed to verify the VADOFT code. Then with appropriate discretization, the VADOFT code could be used to determine the validity of the analytical solutions at large dispersivity values.

Table 7.1 Soil Properties and Discretization Data Used in Simulating Transient Flow in a Soil Column

Parameter	**Value**
Length of soil column, L	20 cm
Saturated hydraulic conductivity, K	10 cm d^{-1}
Porosity, ϕ	0.45
Residual water phase saturation, S_{wr}	0.333
Air entry value, ψ_a	0.0 cm
Constitutive relations: $k_{rw} = (S_w - S_{wr})/(1 - S_{wr})$ $(\psi - \psi_a)/(\psi_r - \psi_a) = (1 - S_w)/(1 - S_{wr})$ where $\psi_r = -100$ cm. $\Delta z = 0.5$ cm $\Delta t = 0.01$ d	

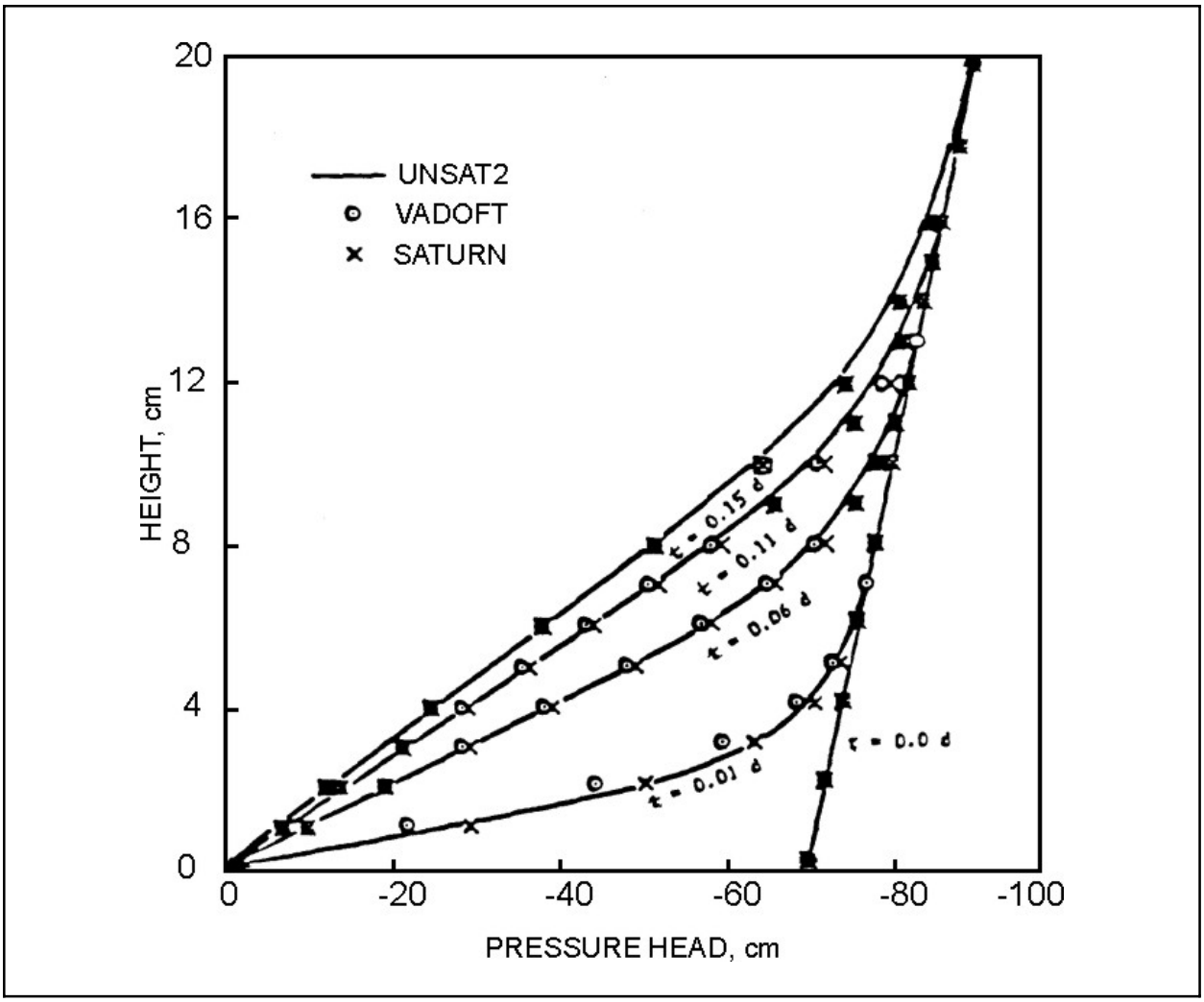


Figure 7.8 Simulated pressure head profiles for the problem of transient upward flow in a soil column. (Adapted from Battelle and GeoTrans, 1988).

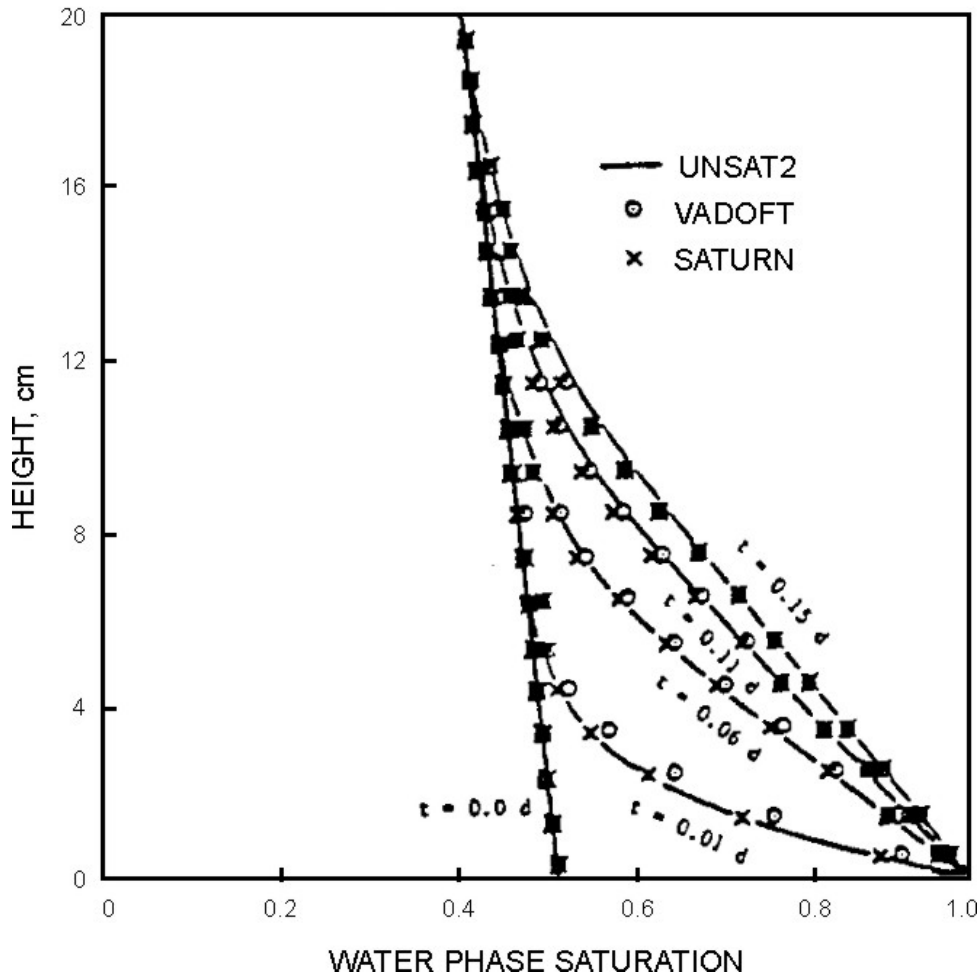


Figure 7.9 Simulated profile of water saturation for the problem of transient upward flow in a soil column.

Table 7.2 Soil Properties Used in Simulating Steady-state Infiltration

Parameter	**Value**
Length of soil column, L	550 cm
Saturated hydraulic conductivity, K	25 cm d^{-1}
Porosity, ϕ	0.331
Residual water saturation, S_{wr}	0.0
Air entry value, ψ_a	0.0 cm

Constitutive relations:

$$k_{rw} = S_e^n \ , n = 3,4,6,8,10$$

$$S_e = \frac{1}{[1 + (\alpha \cdot |\psi - \psi_a|)^{\beta}]^{\gamma}}$$

where $S_e = (S_w - S_{wr})/(1 - S_{wr})$, $\alpha = 0.014\ cm^{-1}$, $\psi_a = 0$ cm, $\beta = 1.51$, $\gamma = 0.338$

Table 7.3 Iterative Procedure Performance Comparison

Case	Number of Nonlinear Iterations	
	Newton-Raphson	**Picard**
n = 3	12	33
n = 4	13	56
n = 6	19	n.c.*
n = 8	27	n.c.
n = 10	31	n.c.

* No convergence. Head tolerance = 0.0001 cm. Grid spacing z = 10 cm.

Table 7.4 Values of Physical Parameters and Discretization Data Used in Simulating One-dimensional Transport in a Semi-infinite Soil Column

Parameter	Value
Darcy velocity, V	1 cm hr^{-1}
Porosity, ϕ	0.25
Longitudinal dispersivity, α_L	5 cm
Concentration at the source, c_o	1

$\Delta z = 10$ cm
$\Delta t = 2.5$ hr

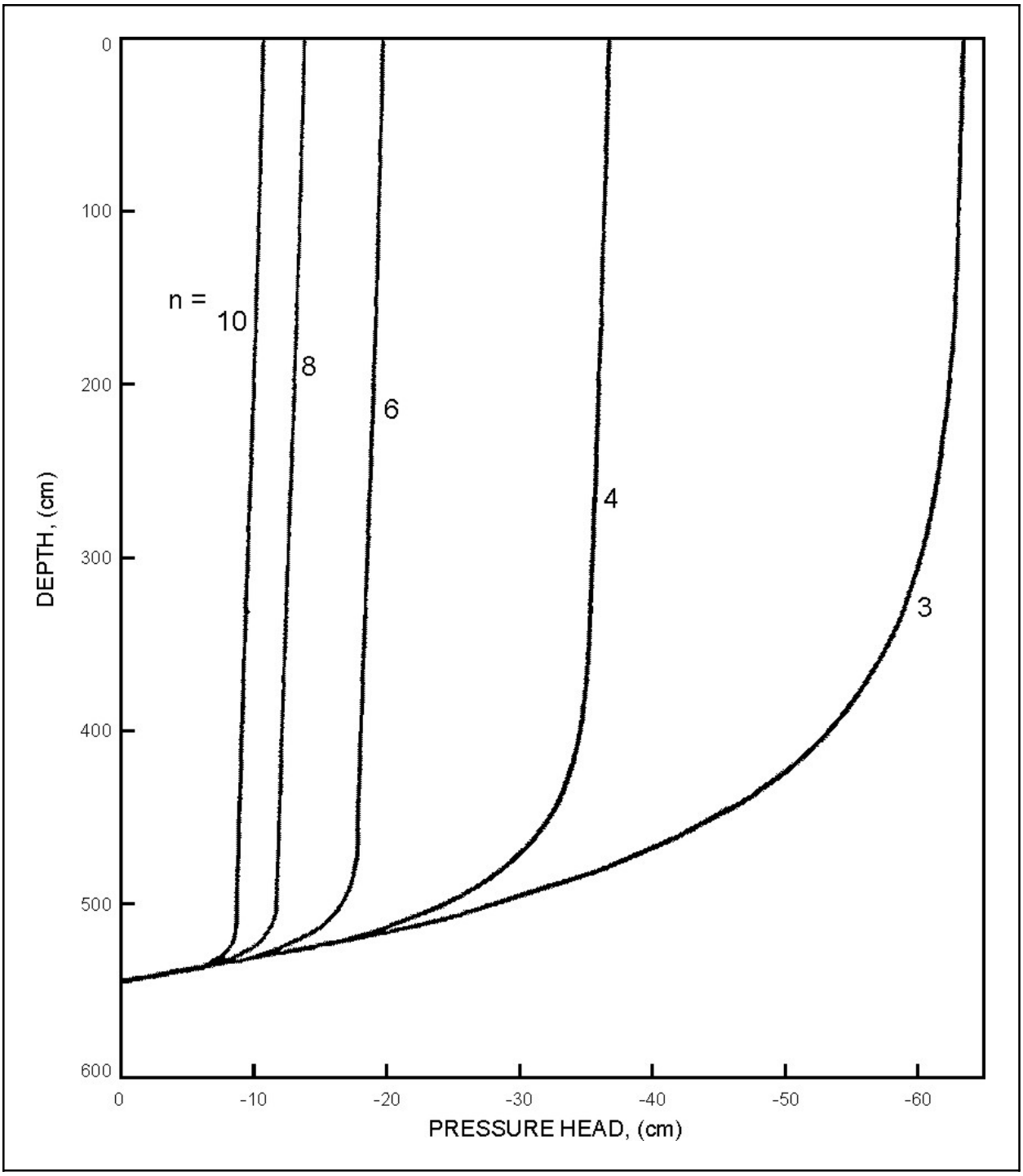


Figure 7.10 Simulated pressure head profiles for five cases of the problem of steady infiltration in a soil column. (Adapted from Springer and Fuentes, 1987).

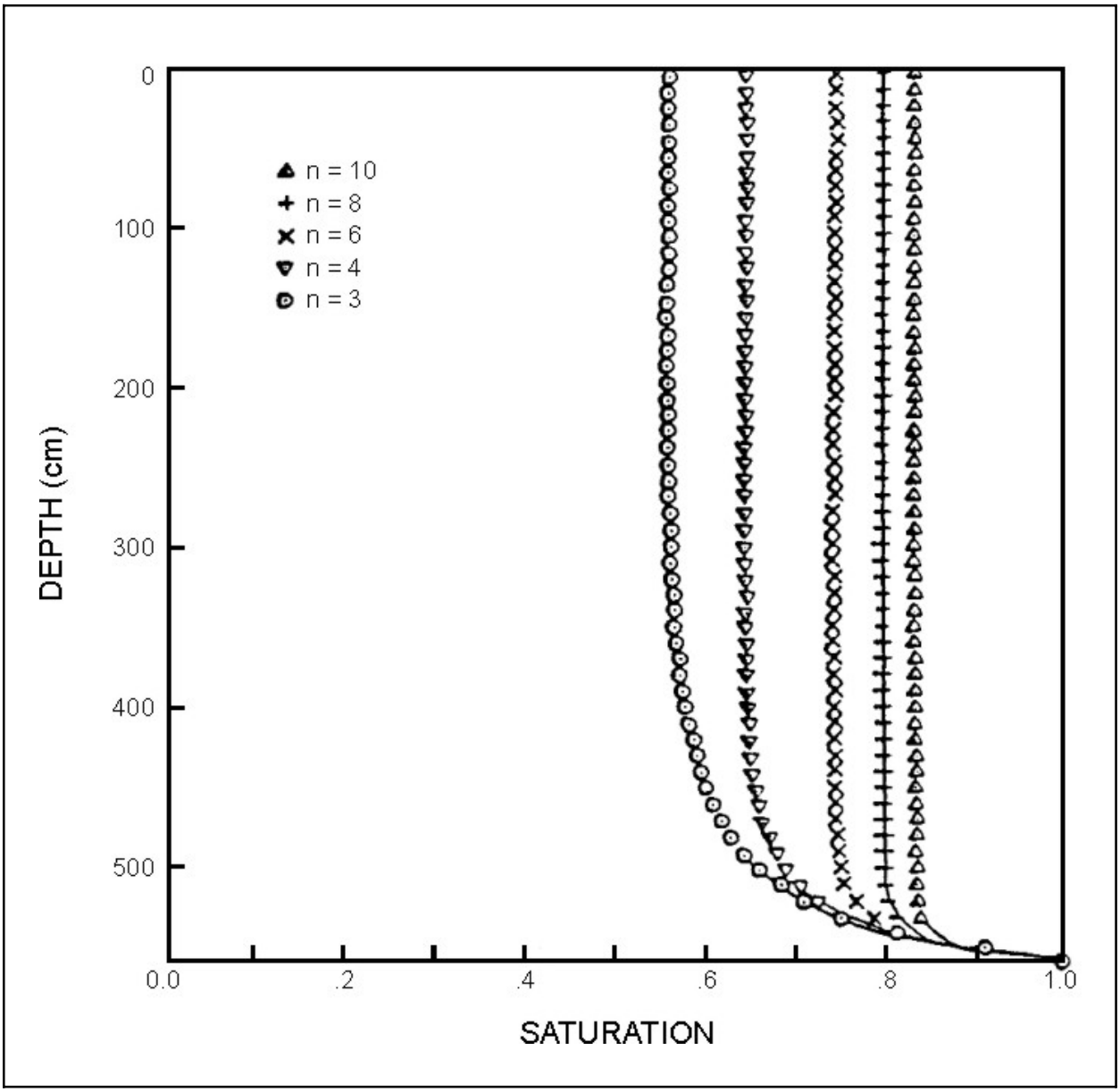


Figure 7.11 Simulated profiles of water saturation for five cases of the problem of steady infiltration in a soil column. (Adapted from Springer and Fuentes, 1987).

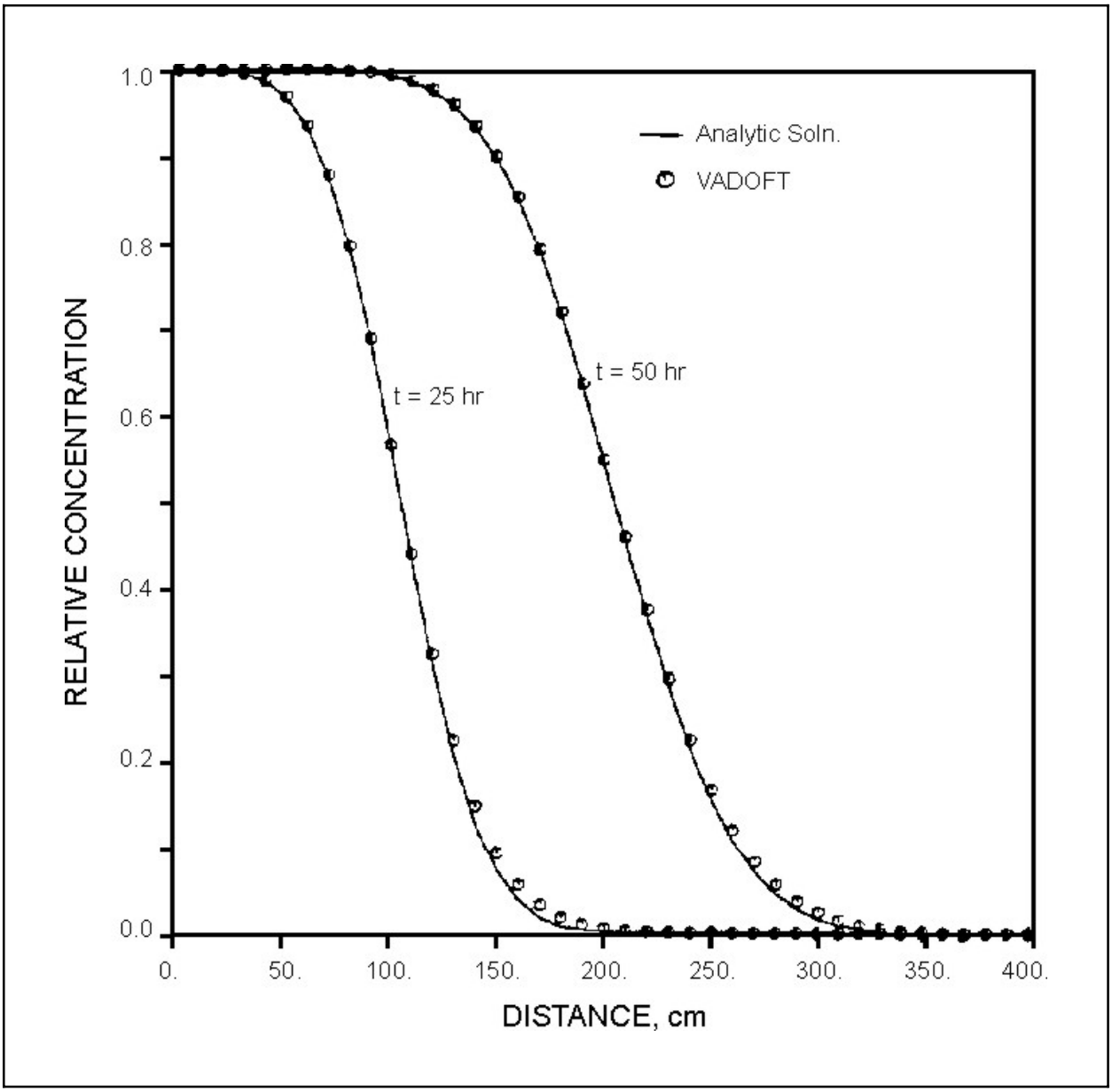


Figure 7.12 Simulated concentration profiles for the problem of solute transport in a semi-infinite soil column.

Table 7.5 Concentration Profile Curves at *t* = 25 hr and *t* = 50 hr Showing Comparison of the Analytical Solution and Results from VADOFT

	Concentration Values			
	t = 25 hr		t = 50 hr	
z Distance (cm)	Analytical	VADOFT	Analytical	VADOFT
00.0	1.0000	1.0000	1.0000	1.0000
10.0	0.9997	0.9998	1.0000	1.0000
20.0	0.9983	0.9987	1.0000	1.0000
30.0	0.9945	0.9954	1.0000	1.0000
40.0	0.9854	0.9870	0.9999	1.0000
50.0	0.9662	0.9688	0.9999	0.9999
60.0	0.9313	0.9346	0.9996	0.9997
70.0	0.8745	0.8781	0.9991	0.9994
80.0	0.7924	0.7956	0.9981	0.9985
90.0	0.6858	0.6889	0.9960	0.9967
100.0	0.5619	0.5660	0.9921	0.9933
110.0	0.4321	0.4394	0.9854	0.9871
120.0	0.3099	0.3222	0.9743	0.9767
130.0	0.2060	0.2235	0.9570	0.9599
140.0	0.1264	0.1474	0.9313	0.9348
150.0	0.0713	0.0928	0.8953	0.8991
160.0	0.0369	0.0560	0.8475	0.8513
170.0	0.0175	0.0327	0.7872	0.7908
180.0	0.0075	0.0184	0.7151	0.7186
190.0	0.0030	0.0101	0.6331	0.6368
200.0	0.0011	0.0054	0.5447	0.5491
210.0	0.0003	0.0029	0.4541	0.4598
220.0	0.0000	0.0015	0.3660	0.3736
230.0			0.2845	0.2942
240.0			0.2129	0.2246
250.0			0.1532	0.1662

Table 7.5 Concentration Profile Curves at *t* = 25 hr and *t* = 50 hr Showing Comparison of the Analytical Solution and Results from VADOFT

	Concentration Values			
	t = 25 hr		t = 50 hr	
z Distance (cm)	**Analytical**	**VADOFT**	**Analytical**	**VADOFT**
260.0			0.1058	0.1193
270.0			0.0701	0.0831
280.0			0.0444	0.0563
290.0			0.0270	0.0371
300.0			0.0157	0.0239
310.0			0.0087	0.0150
320.0			0.0046	0.0092
330.0			0.0000	0.0055

Table 7.6 Values of Physical Parameters and Discretization Data Used in Simulating One-dimensional Transport in a Finite Soil Column

Parameter	**Value**
Thickness of soil column, L	20 m
Darcy velocity, V	0.25 m d^{-1}
Water content, θ	0.25
Retardation coefficient, R	1
Longitudinal dispersivity, α_L	4 m
Source leachate concentration, c_o	1
Case 1:	
Decay constant, λ	0 d^{-1}
Case 2:	
Decay constant, λ	0.25 d^{-1}

Δz = 1.0 m
Δt = 0.5 d

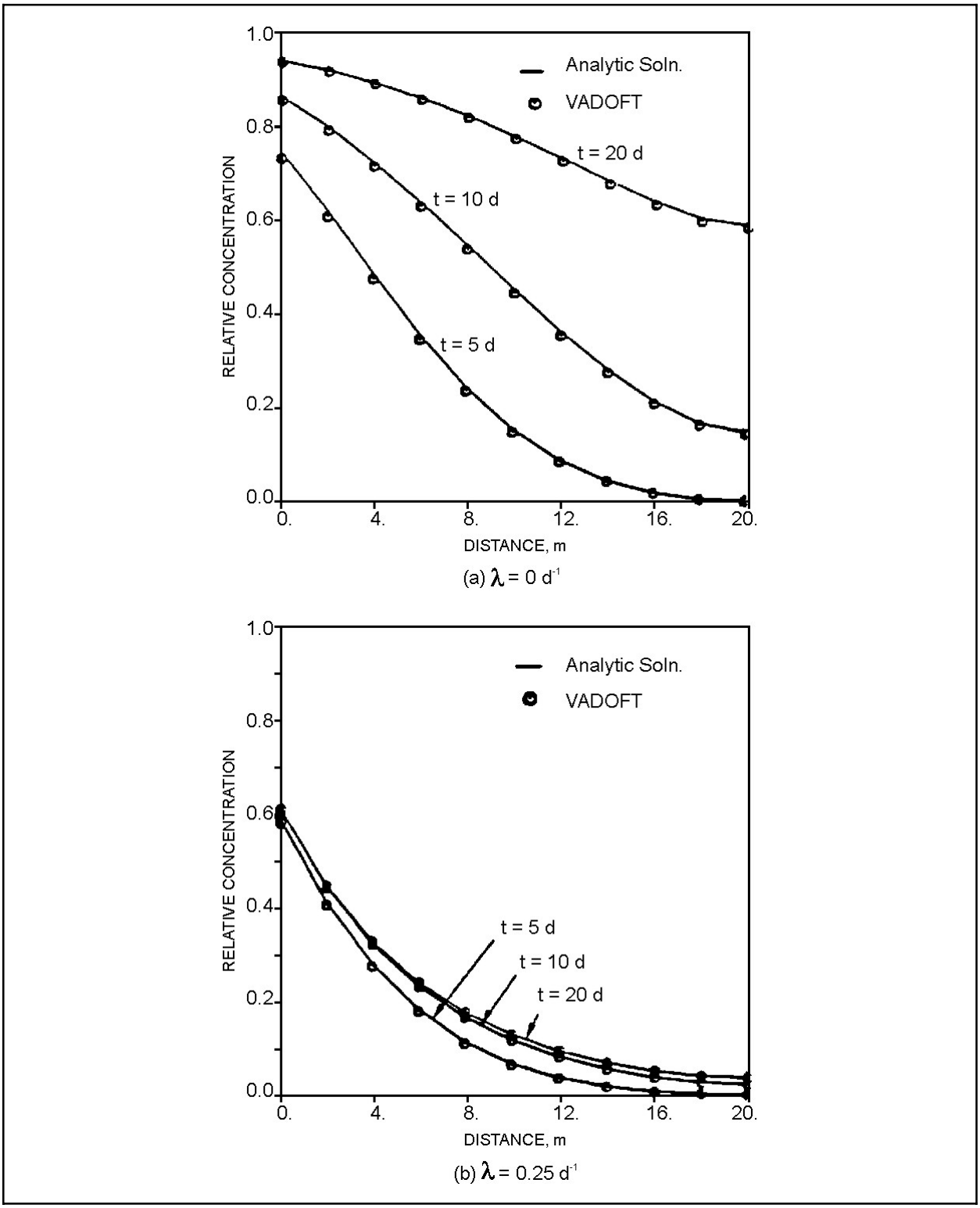


Figure 7.13 Simulated concentration profiles for two cases of the problem of solute transport in a soil column of finite length, (a) $\lambda = 0\ d^{-1}$, and (b) $\lambda = 0.25\ d^{-1}$.

Table 7.7 Concentration Profile Curves Showing Comparison of the Analytical Solution and VADOFT

	Case 1: $\lambda = 0\ d^{-1}$					
	***t* = 5 d**		***t* = 10 d**		***t* = 20 d**	
Distance z, (m)	**Analytical**	**VADOFT**	**Analytical**	**VADOFT**	**Analytical**	**VADOFT**
0.0	0.764	0.751	0.884	0.878	0.963	0.961
2.0	0.638	0.624	0.820	0.812	0.942	0.939
4.0	0.502	0.489	0.742	0.733	0.914	0.911
6.0	0.371	0.360	0.655	0.645	0.881	0.877
8.0	0.256	0.247	0.561	0.552	0.841	0.837
10.0	0.164	0.158	0.466	0.457	0.796	0.791
12.0	0.097	0.094	0.375	0.367	0.748	0.742
14.0	0 053	0.052	0.293	0.286	0.698	0.692
16.0	0.027	0.027	0.224	0.219	0.652	0.646
18.0	0.013	0.014	0.176	0.171	0.617	0.610
20.0	0.009	0.009	0.157	0.152	0.602	0.595

	Case 1: $\lambda = 0\ d^{-1}$					
	***t* = 5 d**		***t* = 10 d**		***t* = 20 d**	
Distance z, (m)	**Analytical**	**VADOFT**	**Analytical**	**VADOFT**	**Analytical**	**VADOFT**
0.0	0.593	0.588	0.615	0.613	0.618	0.617
2.0	0.416	0.411	0.449	0.447	0.453	0.452
4.0	0.283	0.279	0.326	0.325	0.333	0.332
6.0	0.186	0.182	0.236	0.234	0.244	0.243
8.0	0.116	0.113	0.169	0.167	0.179	0.178
10.0	0.069	0.067	0.119	0.118	0.131	0.131
12.0	0.038	0.037	0.083	0.083	0.096	0.096
14.0	0.020	0.019	0.057	0.057	0.071	0.071
16.0	0.009	0.009	0.039	0.039	0.053	0.053
18.0	0.004	0.004	0.028	0.028	0.042	0.042
20.0	0.002	0.002	0.024	0.024	0.038	0.038

Using the discretization data given in Table 7.8, the VADOFT code was run for 180 time steps. Simulated breakthrough curves at the bottom end of the column (z = 86.1 cm) are presented in **Figure 7.14** and **Figure 7.15** and in Tables 7.9 and 7.10. As can be seen, the numerical solution of the VADOFT code compares very well with the analytical solution for case 1: The small dispersivity case, where the analytical assumption of infinite ratio of layer thickness to layer dispersivity–i.e., each layer extends to infinity–is fairly accurate. There is a slight discrepancy of the analytical solution from the numerical solution for case 2, where the analytical assumption is less accurate.

7.5.3 Combined Nonlinear Flow and Transport Modules

7.5.3.1 Transport During Absorption of Water in a Soil Tube

This problem is selected to provide simultaneous testing of the flow and the transport modules of VADOFT. The problem is depicted schematically in **Figure 7.16**. A conservative solute species has a uniform initial concentration and moisture content. The initial concentration is assumed to be zero, and the inlet concentration c_o is assumed to be 1 p.m. The solute is transported by dispersion and advection. Note that the solute front and the wetting front advance at different rates. The solute velocity, V_{sol}, was previously defined as Equation 7.33. The velocity of the wetting front is dependent upon the rate of water sorption into the soil, which is dependent on moisture diffusivity; thus, calculation of the wetting front velocity requires integration of the mass balance equation. For the sake of convenience, all physical data pertaining to the geometry of the soil tube and the physical parameter values are kept the same as those used in the paper by Huyakorn et al. (1985). The complete set of data is listed in Table 7.11. The simulation was performed in two stages. In the first stage, the transient water flow problem was analyzed to determine the distributions of Darcy velocity and water saturation for each time level. These results are written on an output file. In the second stage, the transient solute transport problem was analyzed to determine concentration distributions using the velocity and water saturation data file obtained from the flow simulation.

The spatial and temporal discretization data used in running the VADOFT code are also given in Table 7.11. Both the flow and the transport analyses were performed for 50 time steps. Results of the flow analysis are plotted in **Figure 7.17**. The water saturation profiles given by VADOFT compare well with those obtained using the semi-analytical solution of Phillip (1955) and the UNSAT2 finite-element flow code. Results of the transport analysis are plotted in **Figure 7.18**. The concentration distributions given by VADOFT also compare well with those obtained using the semi-analytical solution of Smiles et al. (1978) and the FEMWASTE finite-element transport code documented by Yeh and Ward (1981).

7.5.3.2 Transient Infiltration and Contaminant Transport in the Vadose Zone

This problem, schematically depicted in **Figure 7.19**, involves variable infiltration and contaminant transport in a layered system in which layer permeabilities differ by more than two orders of magnitude. The problem was chosen to demonstrate the capability of VADOFT to handle a higher nonlinear situation involving soil materials with sharp contrast in drainage properties. Shown in Table 7.12 are values of physical parameters and discretization data used in the flow and transport simulations. For the unsaturated flow simulation, the transient infiltration rates illustrated in **Figure 7.20** were used. It was assumed that the initial condition corresponded to a hydrostatic pressure head distribution in the soil with pressure head values at the water table and the top of the soil equal to 0 and -420 cm, respectively. The simulation was performed for 20 time steps using $\Delta t = 1\ d$. Shown in **Figure 7.21** through **Figure 7.23** are simulated profiles of water saturation, pressure head, and vertical Darcy velocity, respectively. As expected, the two sand layers exhibit fast drainage response, whereas the intervening clay-loam layer exhibits slow drainage response. This behavior is seen in **Figure 7.21**. The pressure head and velocity profiles depicted in **Figure 7.22** and **Figure 7.23** directly reflect the effect of temporal change in the infiltration rate. Note that the values of Darcy velocity at the soil surface (**Figure 7.23**) are equal to the values of infiltration rate for the same time values. Following the unsaturated flow simulation, the transport simulation was performed using the Darcy velocity file from the flow computation as an input file for the transport computation. Concentration profiles determined by the code are plotted in **Figure 7.24**. As illustrated, the contaminant front exhibits slow movement through the clay loam layer.

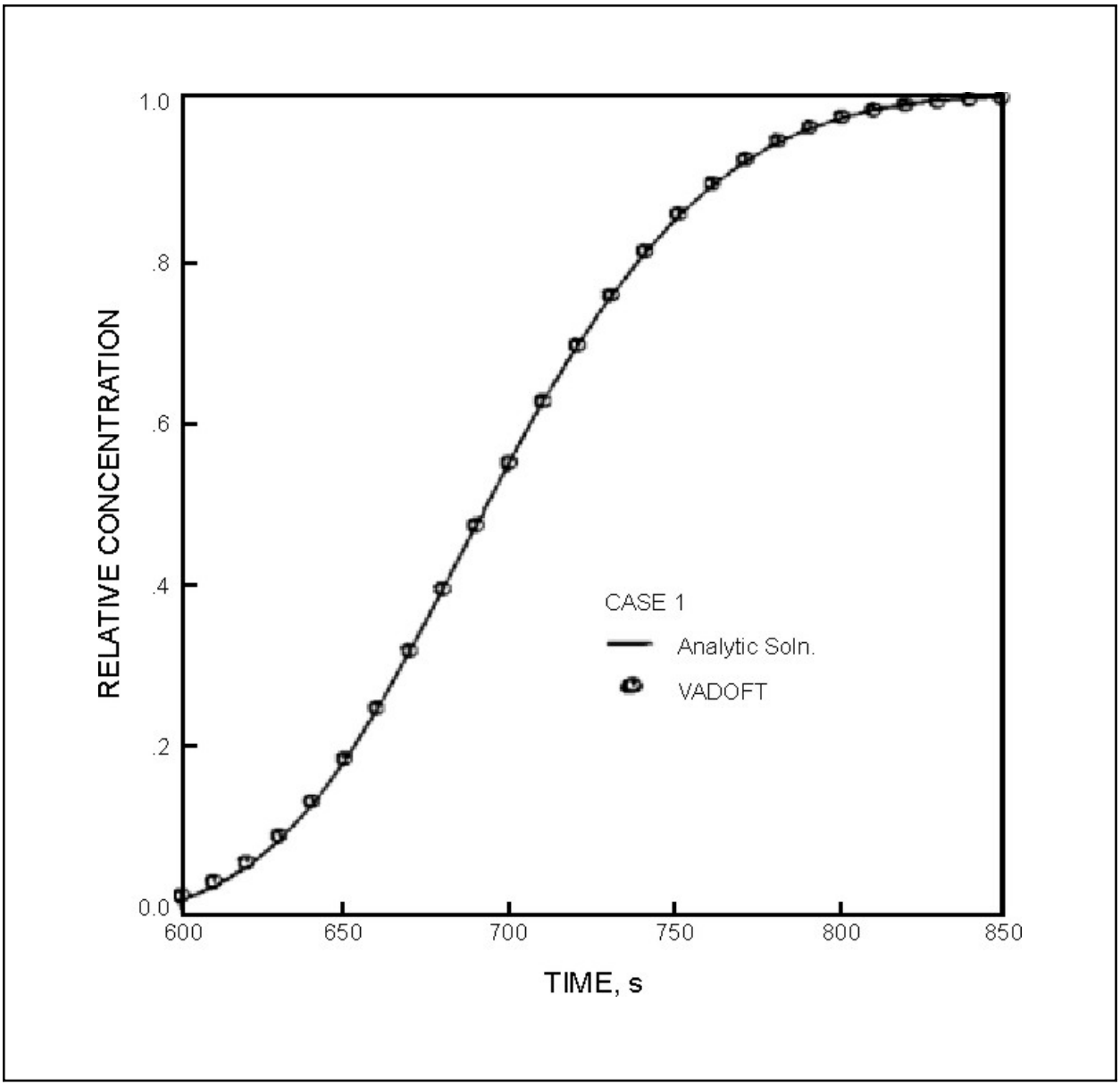


Figure 7.14 Simulated outflow breakthrough curve for case 1 of the problem of solute transport in a layered soil column.

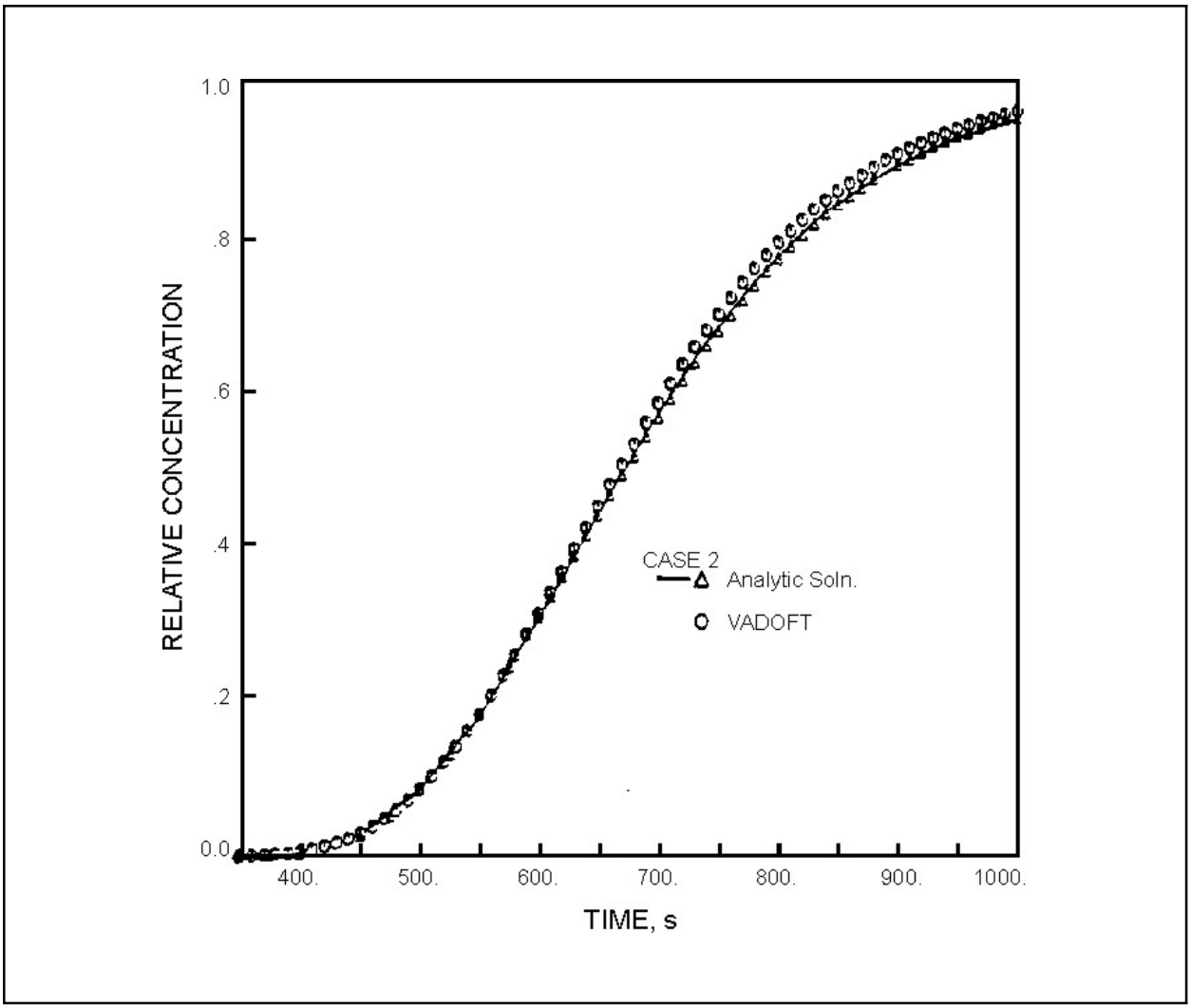


Figure 7.15 Simulated outflow breakthrough curve for case 2 of the problem of solute transport in a layered soil column.

Table 7.8	Values of Physical Parameters Used in the Simulation of Transport in a Layered Soil Column		
	Value for Layer I		
Parameter	**Layer 1**	**Layer 2**	**Layer 3**
Layer thickness, ℓ_i	25.48	30.31	30.31 cm
Seepage velocity, u_i	0.127	0.123	0.121 cm s^{-1}
Retardation coeff., R_i	1.0	1.0	1.0
Decay constant, λ_i	0	0	0 s^{-1}
Source concentration, c_o	1.0		
<u>Case 1</u>:			
Dispersivity, α_{Li}	0.076	0.174	0.436 cm
<u>Case 2</u>:			
Dispersivity, α_{Li}	0.76	1.74	4.36 cm
Δz = 0.6888 cm Δt = 5 s			

Table 7.9	Breakthrough Curves (at z = 86.1 Cm) Computed Using the Analytical Solution and VADOFT (Case 1)	
	Concentration Values for Case 1	
Time, *t* (s)	**Analytical Solution**	**Numerical VADOFT**
600	0.0204	0.0262
610	0.0361	0.0427
620	0.0596	0.0665
630	0.0923	0.0989
640	0.1354	0.1410
650	0.1887	0.1930
660	0.2514	0.2543
670	0.3217	0.3234
680	0.3971	0.3981
690	0.4748	0.4755
700	0.5518	0.5526
710	0.6255	0.6266

Table 7.9 Breakthrough Curves (at z = 86.1 Cm) Computed Using the Analytical Solution and VADOFT (Case 1)

	Concentration Values for Case 1	
Time, *t* (s)	**Analytical Solution**	**Numerical VADOFT**
720	0.6935	0.6951
730	0.7544	0.7564
740	0.8072	0.8096
750	0.8517	0.8542
760	0.8881	0.8907
770	0.9172	0.9197
780	0.9400	0.9421
790	0.9573	0.9590
800	0.9704	0.9715
810	0.9800	0.9805
820	0.9870	0.9869
830	0.9919	0.9913
840	0.9950	0.9943
850	0.9970	0.9964

Table 7.10 Breakthrough Curves (at z = 86.1 cm) Computed Using the Analytical Solution and VADOFT (Case 2)

	Concentration Values for Case 2	
Time, *t* (s)	**Analytical Solution**	**Numerical VADOFT**
600	0.303	0.310
610	0.330	0.337
620	0.357	0.365
630	0.384	0.394
640	0.412	0.422
650	0.439	0.450
660	0.466	0.478
670	0.493	0.505

Table 7.10 Breakthrough Curves (at z = 86.1 cm) Computed Using the Analytical Solution and VADOFT (Case 2)

	Concentration Values for Case 2	
Time, *t* (s)	**Analytical Solution**	**Numerical VADOFT**
680	0.519	0.532
690	0.544	0.558
700	0.569	0.584
710	0.593	0.608
720	0.617	0.632
730	0.639	0.655
740	0.661	0.677
750	0.681	0.698
760	0.701	0.718
770	0.720	0.737
780	0.738	0.755
790	0.755	0.772
800	0.771	0.788
810	0.787	0.804
820	0.801	0.818
830	0.815	0.831
840	0.828	0.844
850	0.840	0.856
900	0.889	0.904

Table 7.11	Values of Physical Parameters and Discretization Data Used in Simulating Transport in a Variably Saturated Soil Tube
Parameter	Value
Length of soil column, L	20 cm
Saturated hydraulic conductivity, K	1 cm d^{-1}
Initial pressure head, ψ_i	-83.33 cm
Remaining flow parameters	See Table 7.2
Initial concentration, c_i	0 ppm
Longitudinal dispersivity, α_L	0 cm
Molecular diffusion, D^*	1 cm^2 d^{-1}
Decay constant, λ	0 d^{-1}
Retardation coefficient, R	1
Δz = 0.25 cm Δt = 0.0025 d	

Table 7.12	Values of Physical Parameters and Discretization Data Used in Simulating Transient Infiltration and Contaminant Transport in the Vadose Zone	
Property	**Material 1(Sand)**	**Material 2 (clay loam)**
Saturated conductivity, K	713	6.24 cm d^{-1}
Porosity, ϕ	0.43	0.41
Residual Water Saturation, S_{wr}	0.105	0.232
Air entry value, ψ_a	0.0	0.0 cm
Soil moisture parameter, α	0.145	0.019cm^{-1}
Soil moisture parameter, β	2.68	1.31
Soil moisture parameter, γ	0.63	0.24
Longitudinal dispersivity, α_L	1.0	1.0 cm
Retardation coefficient, R	1.1	1.5
Decay coefficient, λ	0.00274	0.00274 d^{-1}
Δz = 4 cm Δt = 1 d		

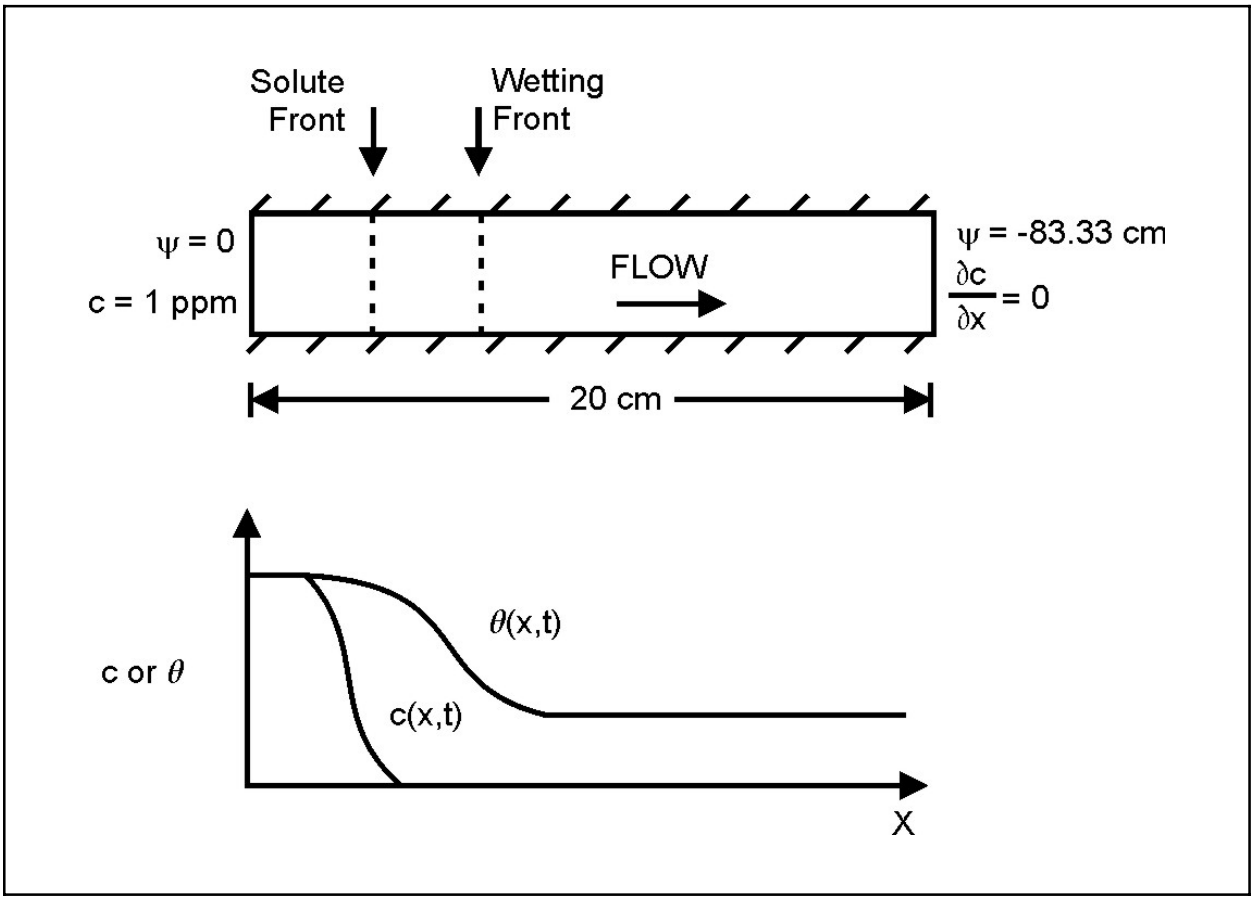


Figure 7.16 One-dimensional solute transport during absorption of water in a soil tube. (Adapted from Huyakorn et al., 1985).

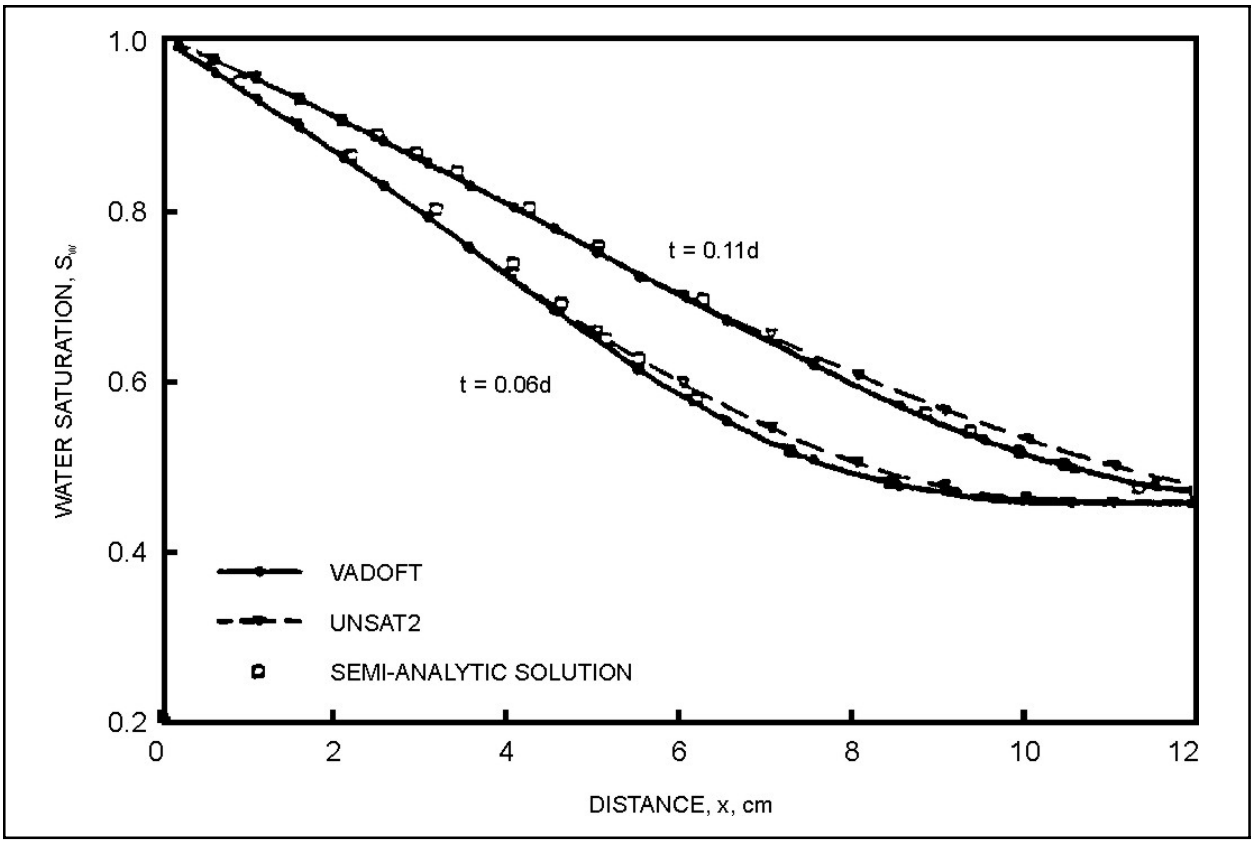


Figure 7.17 Simulated profiles of water saturation during absorption of water in a soil tube. (Adapted from Huyakorn et al., 1984a).

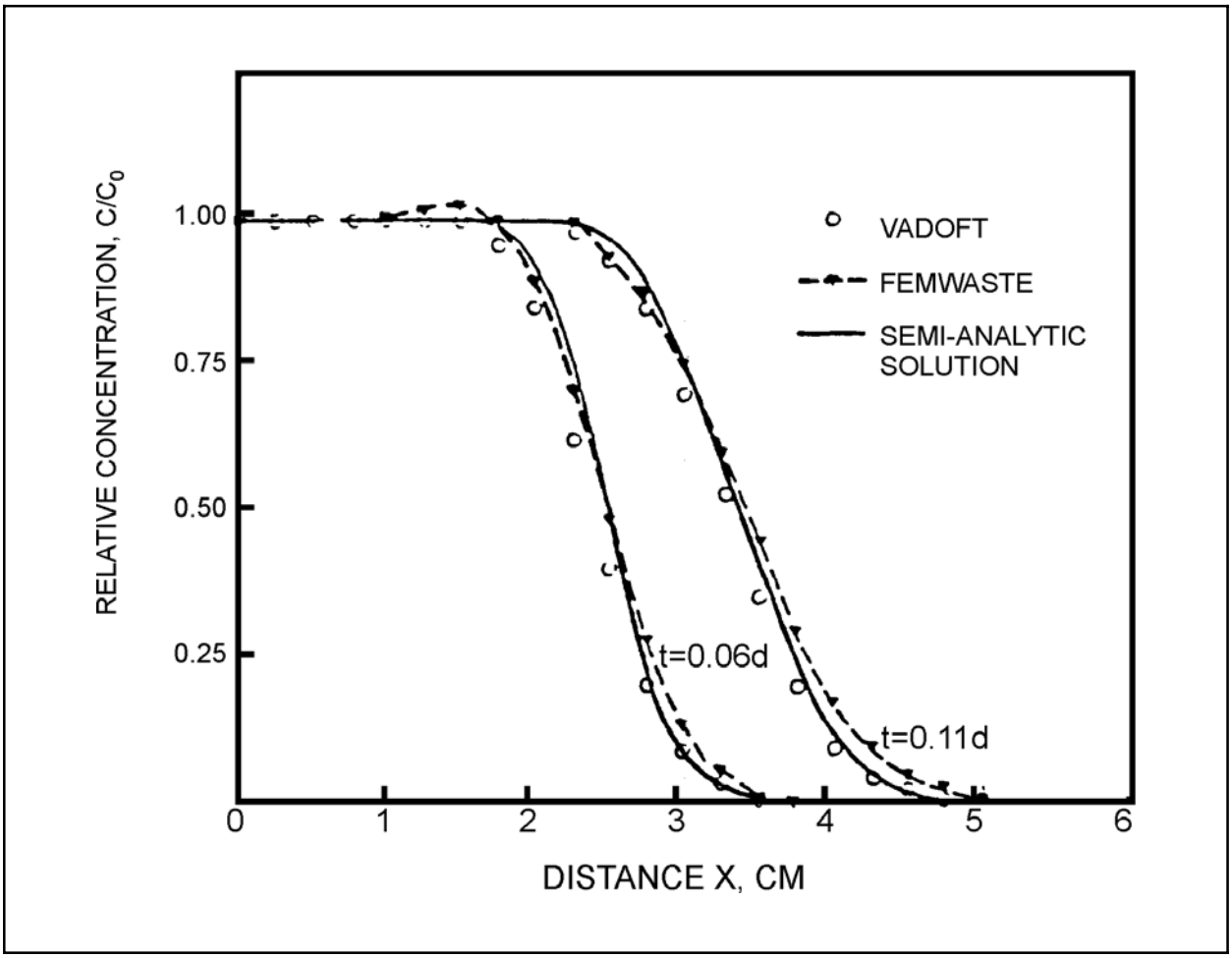


Figure 7.18 Simulated concentration profiles for the problem of one-dimensional solute transport during adsorption of water in a soil tube. (Adapted from Huyakorn, et al., 1985).

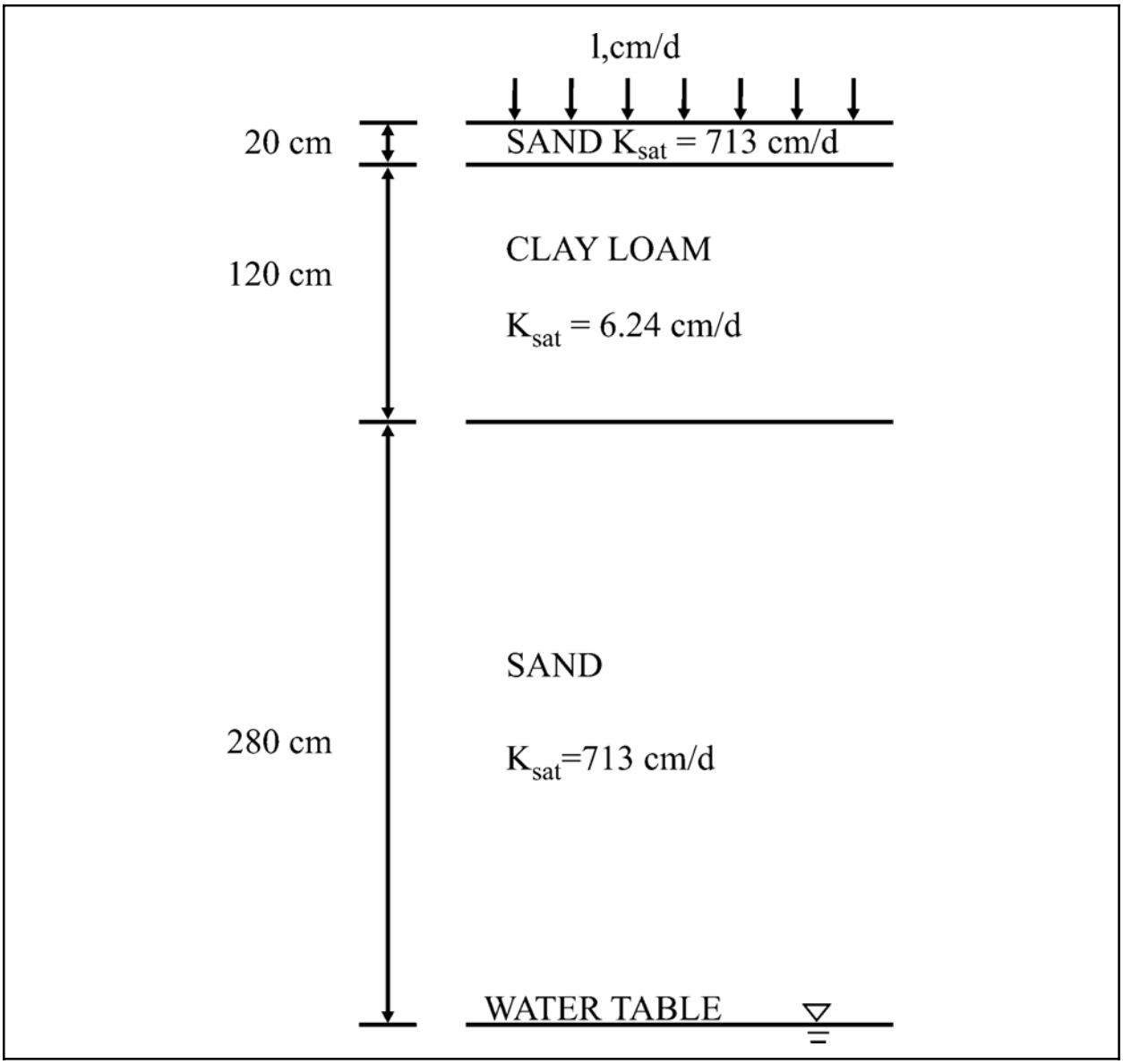


Figure 7.19 Problem description for transient water infiltration and contaminant transport in the vadose zone.

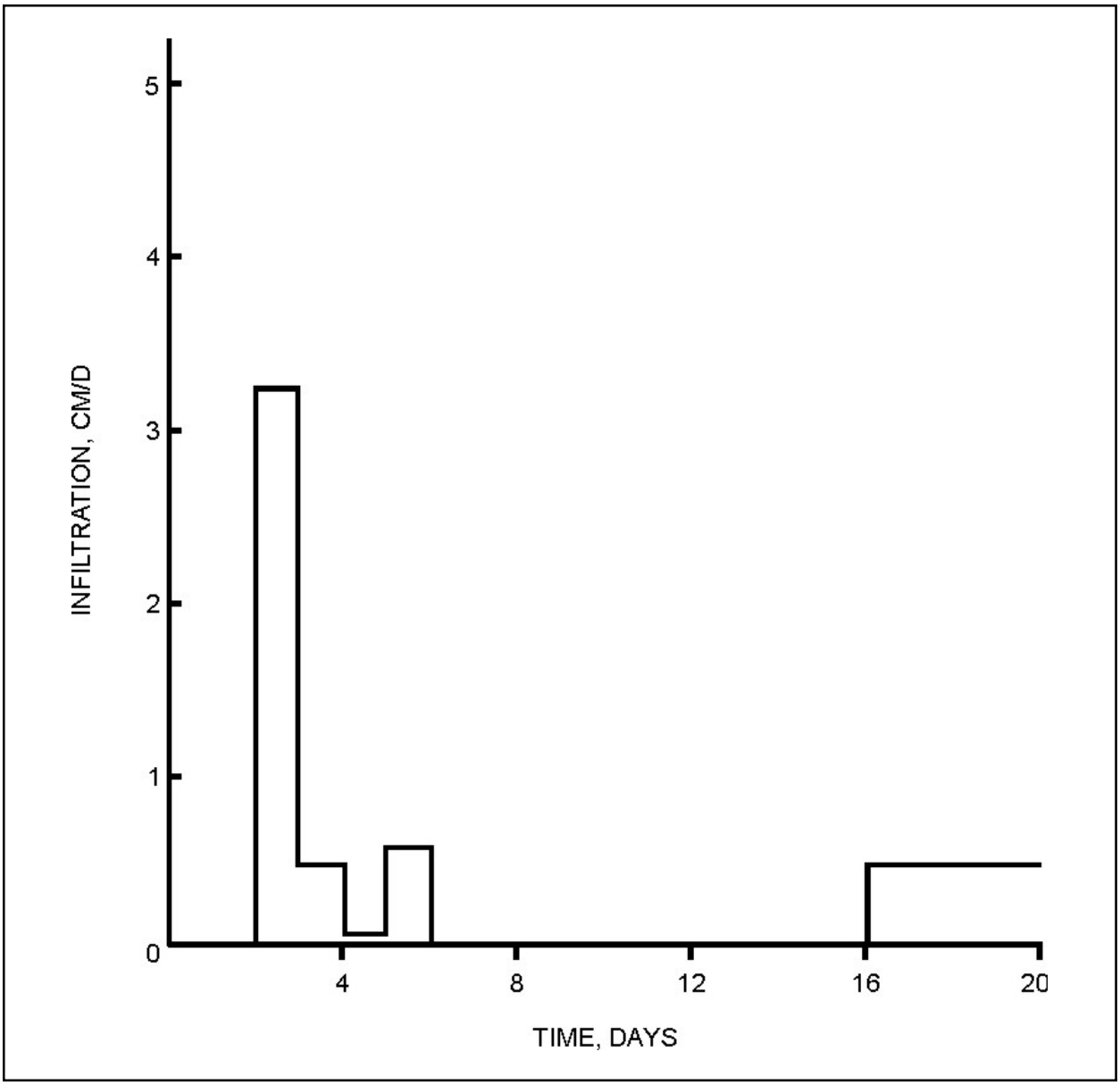


Figure 7.20 Water Infiltration rate vs. time relationship used in numerical simulation.

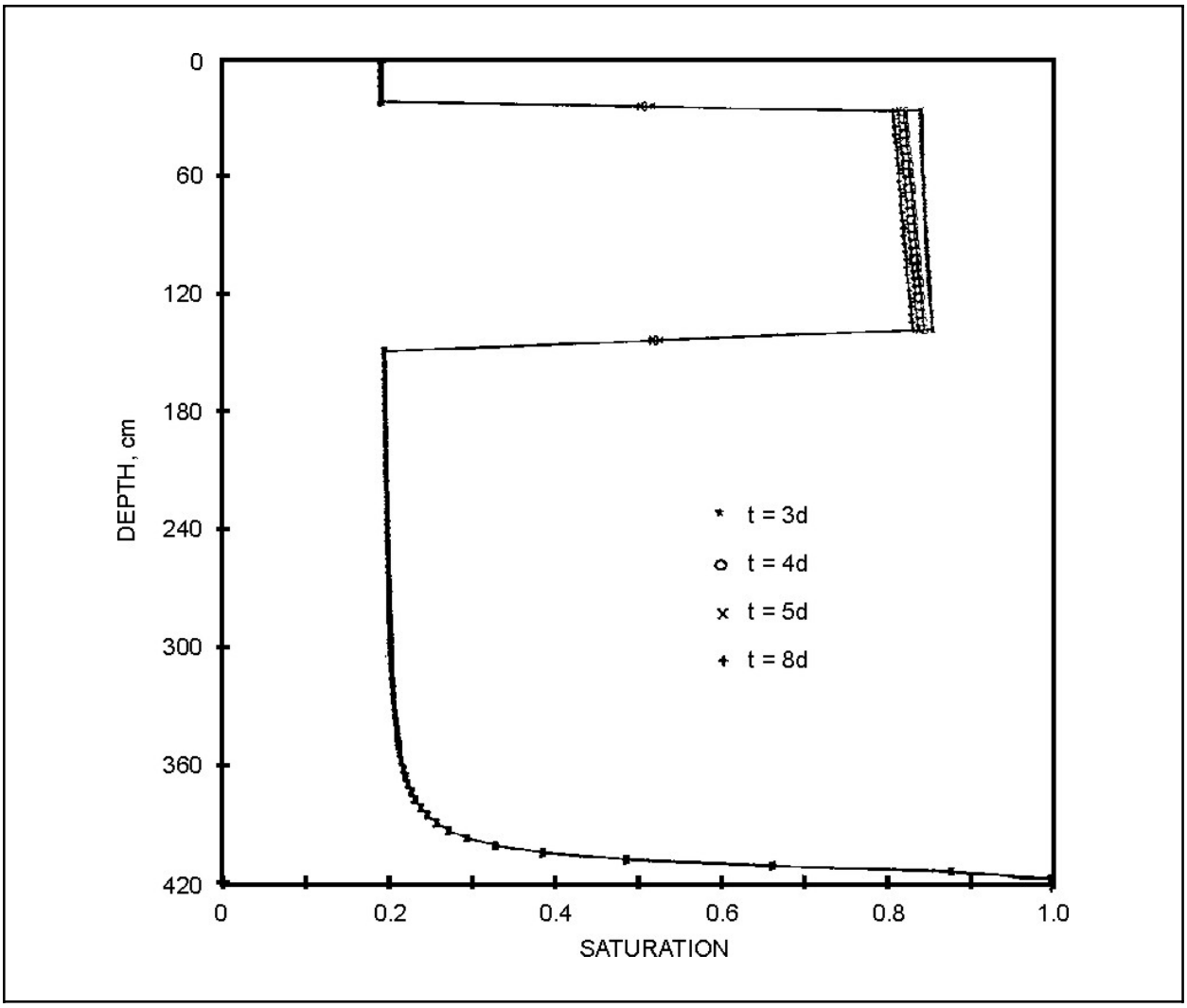


Figure 7.21 Simulated water saturation profiles.

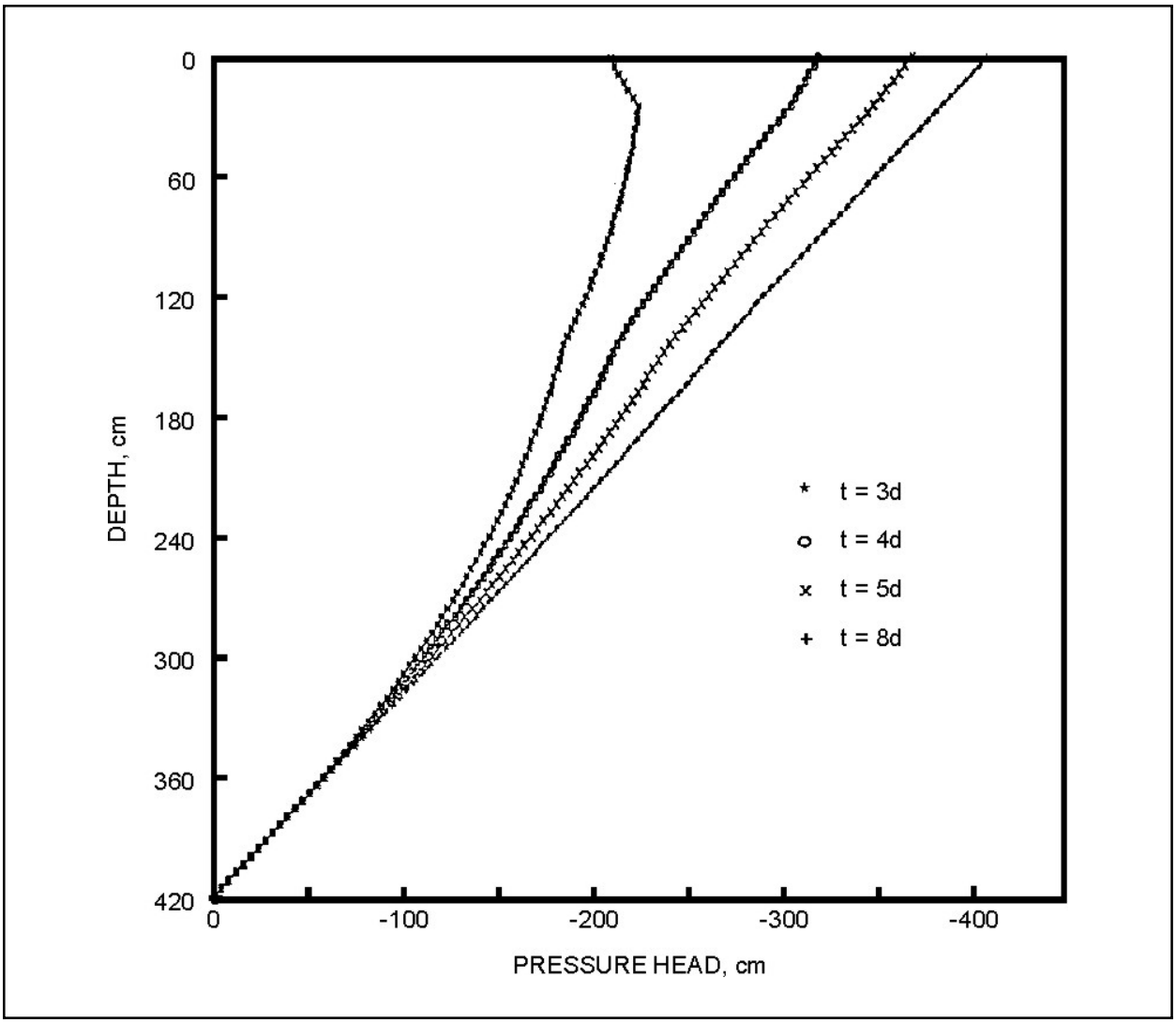


Figure 7.22 Simulated pressure head profiles.

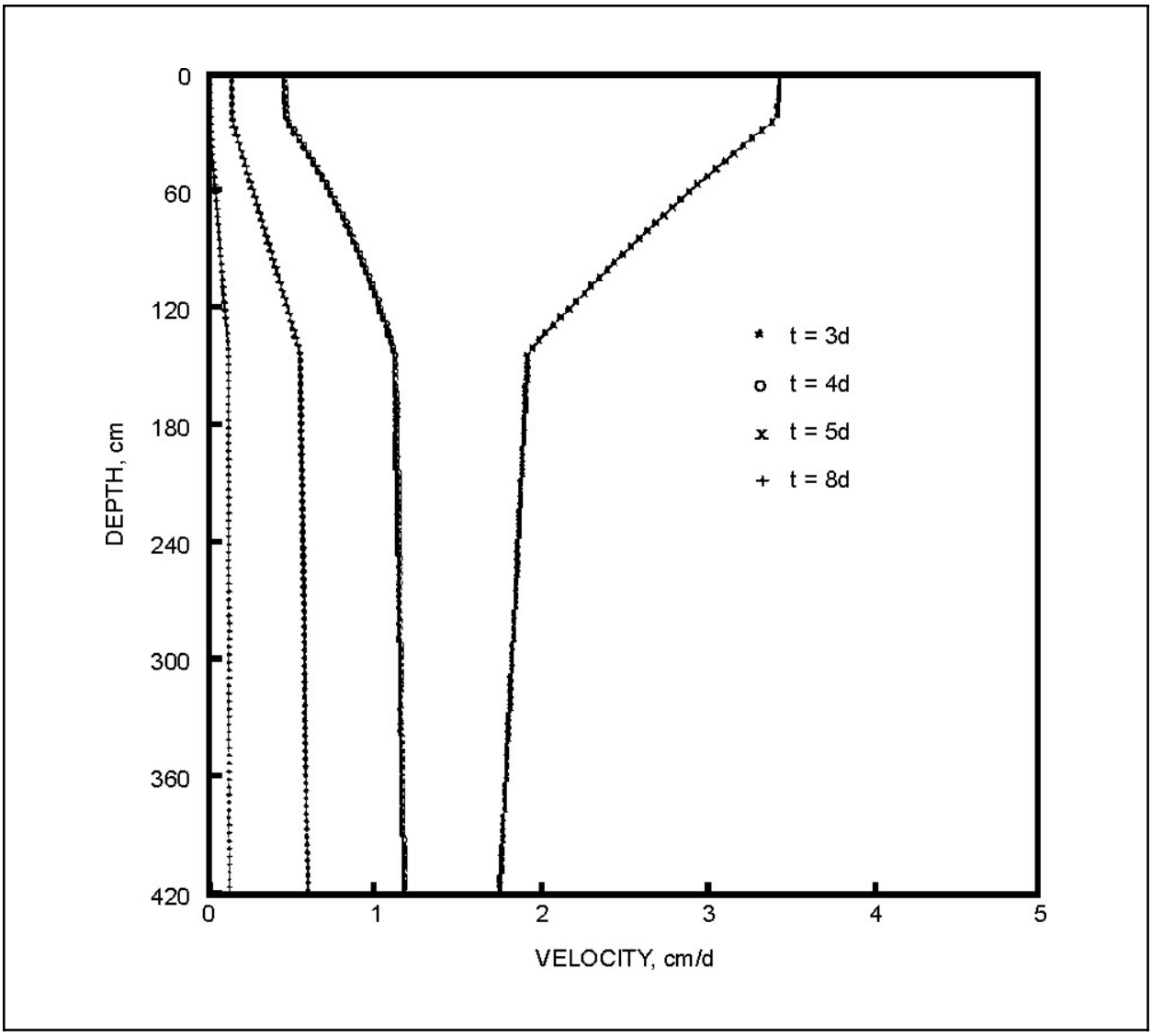


Figure 7.23 Simulated vertical Darcy velocity profiles.

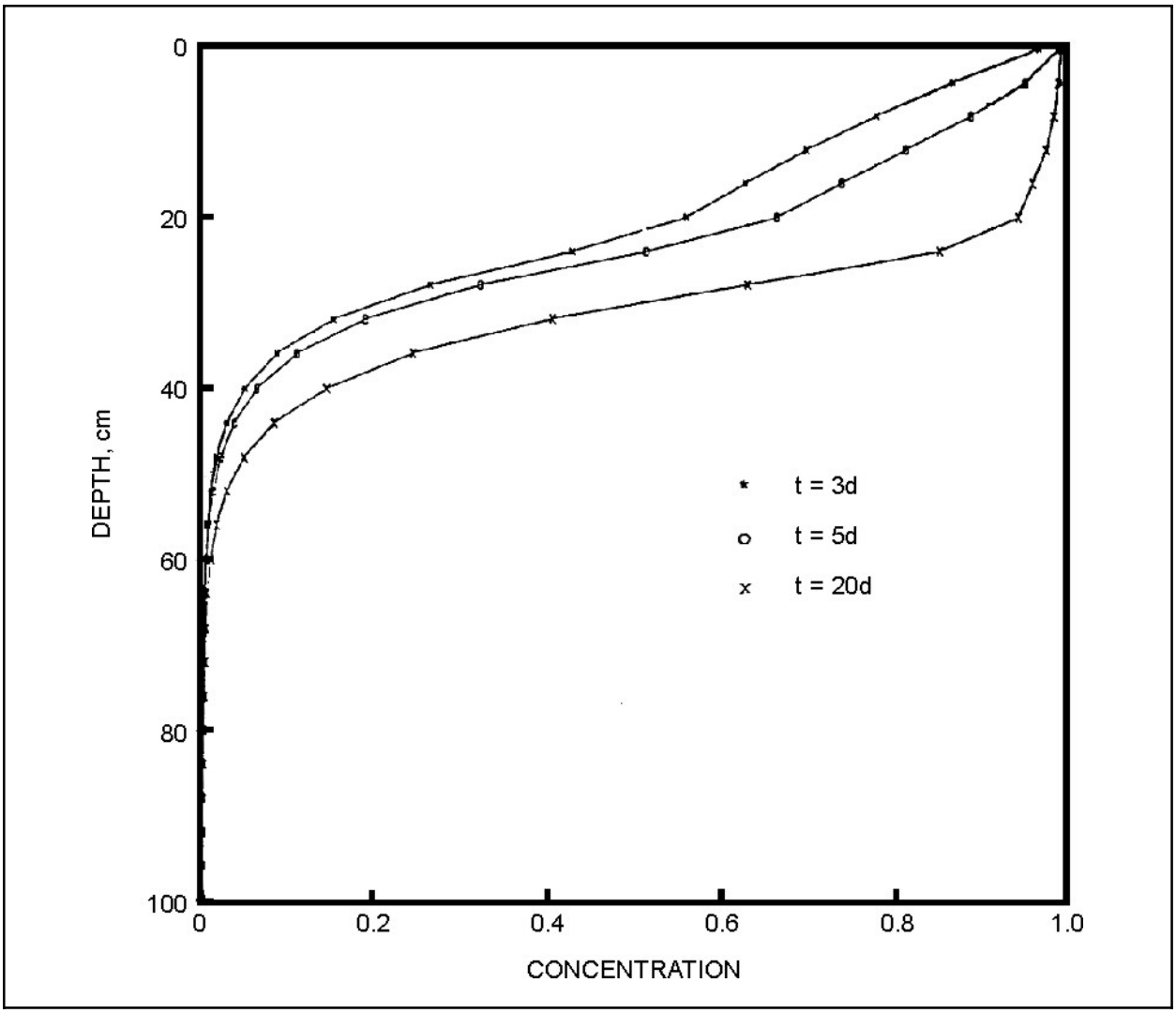


Figure 7.24 Simulated solute concentration profiles.

SECTION 8
Uncertainty Preprocessor

8.1 Introduction

In recent years, the use of quantitative models to assess the transport and transformation of contaminants in the environment has increased significantly. Typically these models include a set of algorithms that simulate the fate of a contaminant within a medium (e.g., unsaturated zone, saturated porous media, air or a surface water body) based on a number of user-specified parameters. These parameters describe the properties of the chemical, the transport medium, and the effects that man has on the system.

Unfortunately, the values of these parameters are not known exactly due to measurement errors and/or inherent spatial and temporal variability. Therefore, it is often more appropriate to express their value in terms of a probability distribution rather than a single deterministic value and to use an uncertainty propagation model to assess the effect of this variability on the transport and transformation of the contaminant.

This section describes the Monte Carlo method of uncertainty propagation and a Monte Carlo shell that is coupled with the PRZM-3 model (subsequently referred to as the deterministic code in this report). The composite code (i.e., the uncertainty shell coupled with the deterministic code) can be used for the quantitative estimate of the uncertainty in the concentrations at the monitoring point due to uncertainty in the (fate) model input parameters.

8.2 Overview of the Preprocessor

The objective of the uncertainty analysis/propagation method is to estimate the uncertainty in model output (e.g., the concentration at a monitoring point) given the uncertainty in the input parameters and the transport and transformation model. Alternatively stated, the objective is to estimate the cumulative probability distribution of the concentration at a receptor location given the probability distribution of the input parameters. If C_w represents the concentration at the receptor, then

$$C_w = g(\underline{X}) \tag{8.1}$$

where the function g represents the fate model and $\underline{X}$ represents the vector of all model inputs. Note that some or all of the components of $\underline{X}$ may vary in an uncertain way, i.e. they are random variables defined by cumulative probability distribution functions. Thus the goal of an uncertainty propagation method is to calculate the cumulative distribution function $F_{C_w}(C_w^*)$ given a probabilistic characterization of $\underline{X}$. Note that $F_{C_w}(C_w^*)$ is defined as:

$$F_{C_w}(C_w^*) = \text{Probability}(C_w \le C_w^*) \tag{8.2}$$

where C_w^* is a given output concentration.

8.2.1 Description of the Method

Given a set of deterministic values for each of the input parameters, $X_1, X_2, \ldots X_n$, the composite model computes the output variable (e.g., a downgradient receptor well concentration C_w) as:

$$C_w = g(X_1, X_2, \cdots, X_n) \tag{8.3}$$

Application of the Monte Carlo simulation procedure requires that at least one of the input variables, $X_1 \ldots X_n$, be uncertain and the uncertainty represented by a cumulative probability distribution. The method involves the repeated generation of pseudo-random number values of the uncertain input variable(s) (drawn from the known distribution and within the range of any imposed bounds) and the application of the model using these values to generate a series of model responses i.e. values of C_w. These responses are then analyzed statistically to yield the cumulative probability distribution of the model response. Thus, the various steps involved in the application of the Monte Carlo

simulation technique involve:

1. Selection of representative cumulative probability distribution functions for describing uncertainty in the relevant input variables.

2. Generation of pseudo-random numbers from the distributions selected in (1). These values represent a possible set of values for the input variables.

3. Application of the model to compute the derived inputs and output(s).

4. Repeated application of steps (2) and (3).

5. Presentation of the series of output (random) values generated in step (3) as a cumulative probability distribution function (CDF).

6. Analysis and application of the cumulative probability distribution of the output as a tool for decision making.

8.2.2 Uncertainty in the Input Variables

The parameters required by a transport and transformation model can be broadly classified into four different sets that exhibit different uncertainty characteristics. These are:

- Chemical parameters. Examples of pesticide parameters include the octanol-water partition coefficient, acid, neutral, and base catalyzed hydrolysis rate, soil-adsorption coefficient, Henry's Law Constant, etc. Examples of parameters for nitrogen species include rates for plant uptake and return, ammonia adsorption/desorption, nitrate immobilization, organic N ammonification, denitrification, nitrification, ammonia immobilization, and ammonia volatilization.

- Media parameters. Examples of these variables include the groundwater velocity, soil porosity, organic carbon content, dispersivity values, etc

- Meteorological parameters. Examples include precipitation, evaporation, solar radiation.

- Management parameters. Examples include irrigation timing, pesticide application timing, well pumping rates, etc.

Uncertainty in chemical parameters primarily arises due to laboratory measurement errors or theoretical methods used to estimate the numerical values. In addition to experimental precision and accuracy, errors may arise due to extrapolations from controlled (laboratory) measurement conditions to uncontrolled environmental (field) conditions. Further, for some variables, semi-empirical methods are used to estimate the values. In this case, errors in using the empirical relationships also contribute to errors/uncertainty in the model outputs.

Uncertainty in the second and third sets of parameters, identified above, may include both measurement and extrapolation errors. However, the dominant source of uncertainty in these is the inherent natural (spatial and temporal) variability. This variability can be interpreted as site-specific or within-site variation in the event that the fate model is used to analyze exposure due to the use and/or the disposal of a contaminant at a particular site. Alternatively it can represent a larger scale (regional/national) uncertainty if the model is used to conduct exposure analysis for a specific chemical or specific disposal technology on a generic, nation-wide or regional basis. Note that the distributional properties of the variables may change significantly depending upon the nature of the application. Uncertainty in the fourth set of parameters may arise from a complex variety of factors including climate, sociology, economics, and human error.

Whatever the source of uncertainty, the uncertainty preprocessor developed here requires that the uncertainty be

quantified by the user. This implies that for each input parameter deemed to be uncertain, the user select a distribution and specifies the parameters that describe the distribution.

The current version of the preprocessor allows the user to select one of the following distributions.

- Uniform
- Normal
- Log-normal
- Exponential
- Johnson SB distribution
- Johnson SU distribution
- Empirical
- Triangular

Depending on the distribution selected, the user is required to input relevant parameters of the distribution. The first requires minimum and maximum values. The second and third distributions require the user to specify the mean and the variance. The fourth distribution requires only one parameter – the mean of the distribution. For the empirical distribution, the user is required to input the coordinates of the cumulative probability distribution function (minimum 2 pairs, maximum 20 pairs) which is subsequently treated as a piecewise linear curve. For the triangular distribution the user is required to input the minimum, maximum and the most likely value. Finally, the Johnson SB and SU distribution requires four parameters – mean, variance, and the lower and upper bounds.

In addition to the parameters of the distribution, the user is required to input the bounds of each model parameter. These bounds may be based on available data or simply physical considerations, e.g., to avoid the generation of negative values. Values generated outside these bounds are rejected.

Of the above eight distributions, the characteristics of the majority are easily available in the literature (Benjamin and Cornell 1970). The triangular distribution has been discussed in Megill (1977). Details of the Johnson system of distributions are presented in McGrath and Irving (1973) and Johnson and Kotz (1970). Additional details for each of these distributions are presented in the following discussion.

In some cases, it may be desirable to include correlations among the variables. For example, there may be a correlation between hydraulic conductivity and particle size or between adsorption and degradation coefficients. The uncertainty processor allows the generation of (linearly) correlated variables for cases where the underlying distribution of the variables is either normal and/or lognormal.

8.3 Description of Available Parameter Distributions

The Monte Carlo shell has the ability to generate data from a number of probability distributions listed above. A description of each of these distributions is provided in the following paragraphs, including parameters of the distributions, equations for the probability and cumulative density functions, and a brief discussion of the properties of each distribution.

8.3.1 Uniform Distribution

A uniform distribution is a symmetrical probability distribution in which all values within a given range have an equal chance of occurrence. A uniform distribution is completely described by two parameters: 1) the minimum value (lower bound) A, and 2) the maximum value (upper bound) B. The equation for the uniform probability density distribution of the variable x is given by:

$$f_u(x) = \frac{1}{B - A} \qquad \textbf{(8.4)}$$

where

$f_u(x)$ = the value of the probability density function at x

The cumulative distribution *F(x)* is obtained by integrating Equation 8.4. This yields the probability distribution:

$$F_u(x) = \frac{x - A}{B - A} \tag{8.5}$$

where

$F_u(x)$ = the probability that a value less than or equal to x will occur

8.3.2 Normal Distribution

The term "normal distribution" refers to the well known bell-shaped probability distribution. Normal distributions are symmetrical about the mean value and are unbounded, although values further from the mean occur less frequently. The spread of the distribution is generally described by the standard deviation. The normal distribution has only two parameters) – the mean and the standard deviation. The probability density function of x is given by:

$$f_n(x) = \frac{1}{S_x \sqrt{2\pi}} \exp\left[- \frac{1}{2} \left(\frac{x - m_x}{S_x} \right)^2 \right] \tag{8.6}$$

where

S_x = the standard deviation of x

m_x = the mean of x

The cumulative distribution is the integral of the probability density function:

$$F_n(x) = \int_{-\infty}^{x} f_u(x)\,dx \tag{8.7}$$

Tables of values of $F_n(x)$ are widely available in the statistical literature.

8.3.3 Log-Normal Distribution

The log-normal distribution is a skewed distribution in which the natural log of variable x is normally distributed. Thus, if y is the natural log of x, then the probability distribution of y is normal with mean m_y, and standard deviation S_y and a probability density function similar to Equation 8.9. The mean and standard deviation of x (m_x and S_x) are related to the log-normal parameters m_y and S_y as follows:

$$\begin{aligned} m_x &= \exp[m_y + \frac{S_y^2}{2}] \\ S_x^2 &= m_x^2[\exp(S_y^2) - 1] \end{aligned} \tag{8.8}$$

To preserve the observed mean and standard deviation of x, the parameters of the log-normal distribution (m_y and S_y) are selected such that the above relationships are satisfied. Note that m_y and S_y do not equal the natural log of m_x and S_x, respectively. Log-normal distributions have a lower bound of 0.0 and no upper bound, and are often used to describe positive data with skewed observed probability distributions.

8.3.4 Exponential Distribution

The probability density function for an exponential distribution is given by:

$$f_e(x) = \frac{1}{m_x} \exp[- \frac{x}{m_x}] \tag{8.9}$$

where m_x is the mean of x. The cumulative distribution is given by:

$$F_e(x) = 1 - \exp[-\frac{x}{m_x}] \tag{8.10}$$

The probability density function has its maximum at $x = 0$ and decreases exponentially as x increases in magnitude.

8.3.5 The Johnson System of Distributions

The Johnson system involves two main distribution types – S_B (log-ratio or bounded) and S_U (unbounded or hyperbolic arcsine). These two distribution types represent two different transformations applied to a random variable such that the transformed variable is normally distributed. The specific transformations are:

$$S_B\text{:}\ Y = \ln\left(\frac{x - A}{B - x}\right) \tag{8.11}$$

$$\begin{aligned} S_U\text{:}\ Y &= \sinh^{-1}\left(\frac{x - A}{B - x}\right) \\ &= \ln\left[\frac{x - A}{B - x} + \sqrt{1 + \left(\frac{x - A}{B - x}\right)^2}\right] \end{aligned} \tag{8.12}$$

where

x	=	untransformed variable, $A < x < B$
Y	=	the transformed variable with a normal distribution.

Selection of a particular Johnson distribution for sample data set is accomplished by plotting the skewness and kurtosis of the sample data. The location of the sample point indicates the distribution for the sample data.

For additional details of the Johnson system of distributions, the reader is referred to McGrath and Irving (1973) and Johnson and Kotz (1970).

8.3.6 Triangular Distribution

A triangular distribution is a relatively simple probability distribution defined by the minimum value, the maximum value, and the mode (the most frequent value). **Figure 8.1** shows an example triangular probability density function. The cumulative distribution is given by:

$$F(x) = \begin{cases} \dfrac{(x - x_1)^2}{(x_2 - x_1)(x_m - x_1)} & x_1 \le x \le x_m \\ 1 - \dfrac{(x_2 - x)^2}{(x_2 - x_1)(x_2 - x_m)} & x_m \le x \le x_2 \end{cases} \tag{8.13}$$

where

x_1	=	the minimum value
x_2	=	the maximum value
x_m	=	the mode of the distribution.

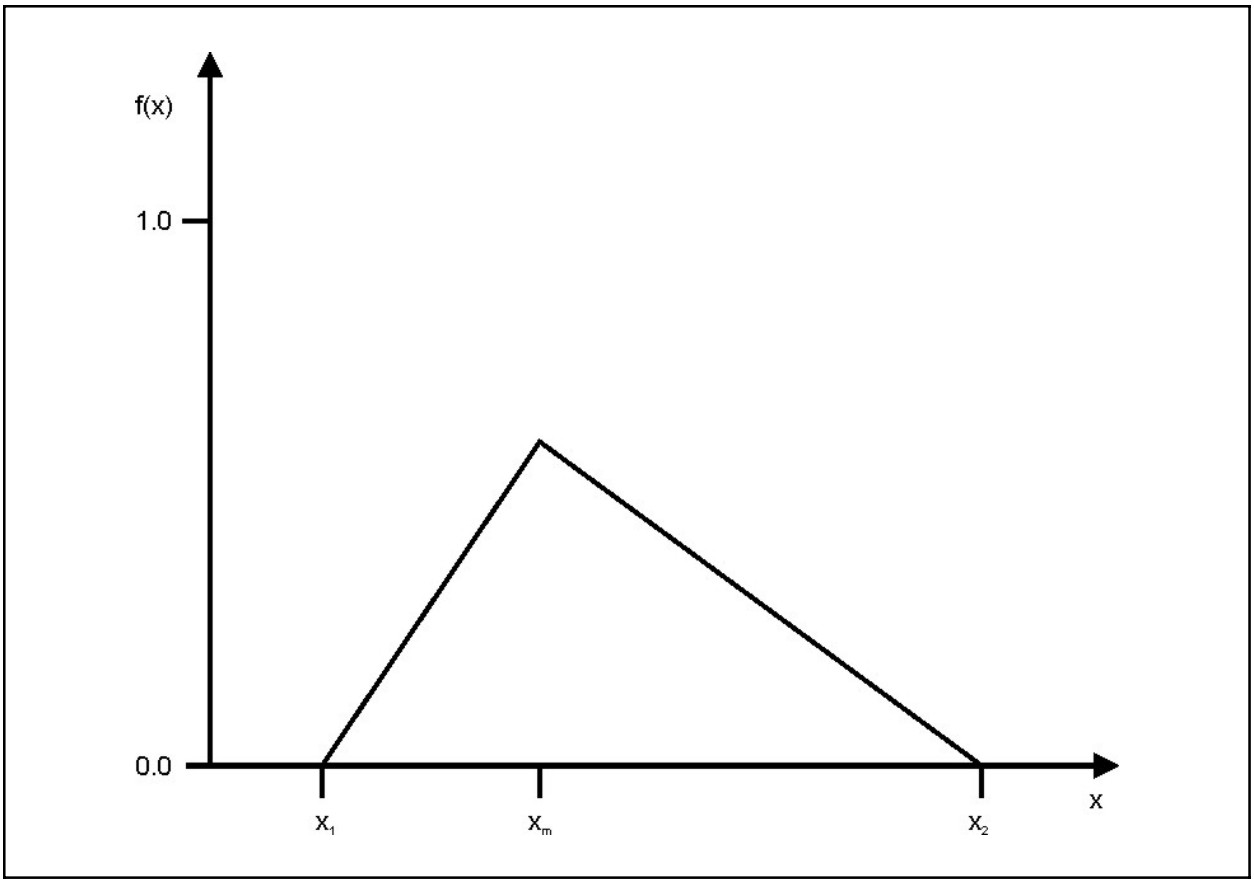


Figure 8.1 Triangular probability distribution.

8.3.7 Empirical Distribution

At times it may be difficult to fit a standard statistical distribution to observed data. In these cases, it is more appropriate to use an empirical piecewise-linear description of the observed cumulative distribution for the variable of interest.

Cumulative probabilities can be estimated from observed data by ranking the data from lowest (rank = 1) to highest (rank = number of samples) value. The cumulative probability associated with a value of *x* is then calculated as a function of the rank of *x* and the total number of samples. The cumulative probabilities of values between observed data can be estimated by linear interpolation.

8.3.8 Uncertainty in Correlated Variables

In many cases model input variables are correlated due to various physical mechanisms. Monte Carlo simulation of such variables requires not only that parameters be generated from the appropriate univariate distributions, but also that the appropriate correlations be preserved in the generated input sequences. The Monte Carlo module currently has the ability to generate correlated normal, log-normal, Johnson SB, and Johnson SU numbers; the procedures used are described in the following paragraphs.

The correlation coefficient is a measure of the linear dependence between two random variables and is defined as:

$$\rho_{x,y} = \frac{\mathrm{cov}(x,y)}{\rho_x \rho_y} \tag{8.14}$$

where

$\rho_{x,y}$	=	the correlation coefficient between the random variables x and y
$\mathrm{cov}(x,y)$	=	the covariance of x and y as defined below
ρ_x, ρ_y	=	the standard deviation of x and y.

The covariance of x and y is defined as:

$$\begin{aligned} \mathrm{cov}(x,y) &= \mathrm{E}[(x - m_x)(y - m_y)] \\ &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (x - m_x)(y - m_y) f_{x,y}(x,y)\,dx\,dy \end{aligned} \tag{8.15}$$

where

E	=	the expected value
m_x, m_y	=	the mean of the random variables x and y
$f_{x,y}(x,y)$	=	the joint probability distribution of x and y.

Note that the linear correlation coefficient between x and y can be computed using

$$\rho_{x,y} = \frac{\left(\sum_{i=1}^{n} x_i y_i\right) - n\bar{x}\bar{y}}{\sqrt{\left[\sum_{i=1}^{n}(x_i^2) - n\bar{x}^2\right]\left[\sum_{i=1}^{n}(y_i^2) - n\bar{y}^2\right]}} \tag{8.16}$$

To generate correlated random variables, three steps are required. First uncorrelated, normally distributed random numbers are generated. This vector is then transformed to a vector of normally distributed numbers with the desired correlation. Finally, the normally distributed numbers are transformed to numbers with the desired distribution.

The transformation of uncorrelated to correlated normal numbers consists of multiplying the uncorrelated vector of numbers with a matrix B:

$$Y' = Be \tag{8.17}$$

where

e	=	the vector of uncorrelated, normally distributed random numbers.
B	=	an N by N matrix
Y'	=	a vector of standard normal deviates of mean zero and standard deviation of unity.

The matrix B is related to the variance-covariance matrix S as follows:

$$S = BB^T \tag{8.18}$$

where B^T is the transpose of the B matrix. Since the normal variables Y' have means of zero and unit variances, the variance-covariance matrix is equivalent to the correlation matrix.

Thus, if the correlation matrix S is known, B can be found from Equation 8.18 by using a Choleski decomposition algorithm. This algorithm will decompose a symmetric positive definite matrix, such as S, into a triangular matrix such as B (de Marsily 1986).

Having generated a vector of correlated normally distributed random numbers, the user can convert vector Y', through appropriate transformations, to the distribution of choice. Thus for parameters X_i that have a normal

distribution, the Y' numbers are transformed as follows.

$$X_i = m_x + \sigma_x Y_i' \tag{8.19}$$

For parameters that follow the lognormal distribution, the following transformation applies.

$$X_i = \exp[Y_i' \sigma_{\ln,i} + \mu_{\ln,i}] \tag{8.20}$$

where

$\mu_{ln,i}$	=	the log mean of the ith parameter
$\sigma_{ln,i}$	=	the log standard deviation of the ith parameter

For parameters with Johnson SB and SU distributions, the Y' are first transformed to normally distributed variables Y with mean M_y and standard deviation σ_y:

$$Y_i = M_y + \sigma_y Y_i' \tag{8.21}$$

Johnson SB numbers are then computed from Y_i as follows.

$$X_i = \frac{B\exp(Y_i) - A}{\exp(Y_i) + 1} \tag{8.22}$$

Johnson SU numbers are computed by:

$$\begin{aligned} x_i &= A + (B - A)\sinh(Y_i) \\ &= A + (B - A)\frac{\exp(Y_i) - \exp(-Y_i)}{2} \end{aligned} \tag{8.23}$$

Other distributions can be easily incorporated into the analyses at a later time when suitable transformations from the normal distribution can be found. It is important to note that, in using this technique, the correlations are maintained in normal space, so if these correlations are estimated using actual data, the data should be transformed to a normal distribution before correlation coefficients are estimated.

For two correlated variables, one with a normal distribution (x_2) and the other with a log normal distribution (x_1), the following equation is used to transform correlations to normal space (Meija and Rodriguez-Iturbe 1974).

$$\sigma_{y_1,y_2} = \frac{\sigma_{x_1,x_2}}{\sigma_{y_1}}\sqrt{\exp(\sigma_{y_1}^2) - 1} \tag{8.24}$$

where

σ_{y_1,y_2}	=	the correlation coefficient between the two variables in the normal space
σ_{x_1,x_2}	=	the correlation coefficient between the two variables in the arithmetic space
σ_{y_1}	=	the variance of y_1 derived from Equation 8.8

If both x_1 and x_2 are log-normally distributed then the correlation coefficient is transformed using Meija and Rodriguez-Iturbe (1974):

$$\sigma_{y_1,y_2} = \frac{1}{S_{y_1}S_{y_2}}\ln\left[1 + \sigma_{x_1,x_2}\left|\frac{S_{x_1}S_{x_2}}{m_{x_1}m_{x_2}}\right|\right] \tag{8.25}$$

where the relationship between S_{x_i} and S_{y_i} are given by Equation 8.8.

Thus, for log-normal variables, the user enters the values of the correlation coefficients in log-normal space; Equations 8.24 and 8.25 are then used to transform the correlation coefficients into normal space.

No direct transformation of Johnson SB or SU correlations to normal correlations is currently known. For these distributions, the user must supply the correlation coefficients between normal-transformed numbers. This may be accomplished by first transforming Johnson SB and SU data to normal data using Equations 8.11 and 8.12. The covariance matrix *S* is then derived using only normal, log-normal, and normal-transformed SB and SU data.

8.3.9 Generation of Random Numbers

Having selected the distribution for the various input parameters, the next step is the generation of random values of these parameters. This requires the use of pseudo-random-number generating algorithms for Normal and Uniform numbers. Numerous proprietary as well as non-proprietary subroutines can be used to generate random numbers. Many of these are comparable in terms of their computational efficiency, accuracy, and precision. The performance of the algorithms included in this preprocessor has been checked to ensure that they accurately reproduce the parameters of the distributions that are being sampled (Woodward-Clyde Consultants 1988a, b).

8.4 Analysis of Output and Estimation of Distribution Quantiles

Model output generally will consist of a volume of data that represents a sample of outcomes. Given the natural variability and the uncertainty of various model components, there will be variability in the output. All of the factors that were allowed to vary within the model contribute to variability in model predictions. Taken as a whole, the model output depicts possible events in terms of their relative frequency of occurrence. Values produced by the model generally are treated as if they were observations of real field events. In interpreting these values, it is important to maintain the perspective dictated by the design and scope of the study.

Model output can be analyzed in various ways depending upon current objectives. Many features of the distribution may be characterized. Quite often, for example, it is of interest to estimate certain quantiles or percentiles of the distribution. Since the model output is treated as a sample from an unknown parent population, the methods of statistical inference normally are used to estimate distribution parameters and to associate measures of uncertainty with these parameters.

One of the most frequently asked questions concerns the number of samples required for some given purpose. In modeling, this translates into the number of model runs needed. For the most part, since methods of basic inference are being applied in a Monte Carlo framework, resulting model output values are treated as observations forming a random sample. The sample size required to estimate a given parameter depends on a number of factors. These include the nature of the parameter that is being estimated, the form of the underlying distribution, the variability in the observations, the degree of precision and/or accuracy desired, the level of confidence to be associated with the estimate, and the actual statistical estimator used to provide the estimate.

Generally, if the output distribution is to be accurately characterized with respect to its many features, the number of model runs needed will be higher than if only a few parameters are to be estimated. The simulation strategy should be determined by the issues addressed by the modeling effort. It may be important, for example, to estimate the extreme upper percentiles of the output distribution. In this case, the choice of simulation design should account for the relative difficulty of obtaining such estimates. If it is not known exactly how the data will be utilized, then the problem becomes one of establishing a distributional representation that is as good as possible under the most extreme usage or estimation scenario. For example, if only a distribution mean were to be estimated, the sample size required could be determined without concern for estimating, say, the 99th percentile.

8.4.1 Estimating Distribution Quantiles

In the following section, a summary is given for statistical techniques used to estimate distribution quantiles. Many such methods are available to estimate a given percentile of an unknown distribution on the basis of sample data. In the PRZM-3 code, four such methods can be used. Among these are distribution-free or nonparametric techniques as

described below. Others include methods specific to certain distributions that assume a knowledge of the distributional form. First, the point estimators are given, then the method for constructing a confidence interval is briefly described.

The order statistics of a sample are merely the ordered values denoted by $x_{(1)}, x_{(2)}, \ldots, x_{(n)}$, where n represents the sample size. The empirical cdf can be defined simply as

$$g(x) = \begin{cases} 0 & x < x_{(1)} \\ \dfrac{1}{n} & x_{(i)} \le x < x_{(i+1)},\ i = 1, \cdots, n-1 \\ 1 & x \ge x_{(n)} \end{cases} \tag{8.26}$$

Mathematically, $g(x)$ is a step function discontinuous at each value $x_{(I)}$.

By definition, the 100p-th percentile (i.e., the p-level quantile) is given by u_p where

$$p = \Pr\{X < u_p\} \tag{8.27}$$

If $F(x)$ denotes the cumulative distribution function,

$$p = F(u_p) \text{ and } u_p = F^{-1}(p) \tag{8.28}$$

When only sample information is available, u_p is unknown, but it can be estimated by forming an appropriate function of the observations.

Nonparametric point estimates of u_p can be constructed as linear combinations of the order statistics. In particular, each of Y_1 through Y_3 below is an estimator of u_p. Let $[z]$ denote the largest integer less than or equal to z. Define

$$\begin{aligned} j &= [n{\cdot}p], & g &= n{\cdot}p - j \\ i &= [n{\cdot}p + 0.5], & r &= (n{\cdot}p + 0.5) - i \\ k &= [(n+1){\cdot}p], & h &= (n+1){\cdot}p - k \end{aligned} \tag{8.29}$$

Then

$$\begin{aligned} Y_1 &= (1-h)X_{(k)} + hX_{(k+1)} \\ Y_2 &= \begin{cases} \dfrac{X_{(j)} + X_{(j+1)}}{2} & g = 0 \\ X_{(j+1)} & g > 0 \end{cases} \\ Y_3 &= (1-r)X_{(i)} + rX_{(i+1)} \\ &= (0.5 + i - n{\cdot}p)X_{(i)} + (0.5 - i + n{\cdot}p)X_{(i+1)} \end{aligned} \tag{8.30}$$

In each of these definitions, only the values of n and p determine which order statistics are used in forming an estimate of u_p. Thus, the estimators do not depend on the underlying distributions. However, the relative performance of these estimators is dependent upon several criteria involving the level p, the sample size n, the type of parent distribution from which samples are drawn, estimator bias, and the mean squared error. If the sample size is very large, the differences among the estimates are not very great. Of the estimators available, the three shown above exhibit the best performance in relatively small samples ($n \le 50$) from normal and lognormal distributions.

Another simple estimator used in the model is calculated by constructing the cdf of the output

$$F(x) = \frac{i}{n} \tag{8.31}$$

in which I is the rank of the outcome in the sample. The specific quantile of interest is then determined by interpolation.

8.4.2 Confidence of u_p

Approximate confidence statements can be placed on u_p by selecting appropriate order statistics to serve as the upper and lower confidence bounds. For a given distribution, the value u_p is such that exactly 100p% of all values of this distribution are less than u_p, and 100(1-p)% exceed this value. An individual value selected randomly from the distribution has probability p of being less than u_p. In a random sample of size n from this distribution, the probability of not exceeding u_p remains constant for each individual element of the sample. Thus, the number of values in the sample that are less than or equal to u_p is distributed binomially. The probability that the random interval ($X_{(j)}$, $X_{(j+1)}$) will contain u_p is equivalent to the probability that exactly I of the n elements of the sample will be less than u_p. Hence, this probability is

$$\binom{n}{i} p^{i}(1-p)^{n-i} \tag{8.32}$$

which is a simple binomial probability.

This expression can be calculated for each pair of consecutive order statistics $X_{(I)}$, $X_{(i+1)}$, for i =1, ..., n-1. However, it is more convenient to deal with these several intervals by calculating cumulative probabilities of the form

$$\Pr\{u_p \le X_{(i+1)}\} = \sum_{j=0}^{i} \binom{n}{j} p^{j}(1-p)^{n-j} \tag{8.33}$$

For practical convenience, the normal approximation

$$F\left\{\frac{(i+0.5)-n{\cdot}p}{\sqrt{n{\cdot}p(1-p)}}\right\} \tag{8.34}$$

can be used, where F represents the cdf of the standard normal distribution.

All of this is utilized for determining two order statistics, denoted below with subscripts i and j, with the property

$$\Pr\{X_{(i)} < u_p \le X_{(j)}\} = 1 - \alpha \tag{8.35}$$

where 1-α is a predetermined confidence coefficient; typically, 1-α = 0.95. i and j can be determined by solving the equations:

$$\begin{aligned} \frac{\alpha}{2} &= F\left\{\frac{(i+0.5)-n{\cdot}p}{\sqrt{n{\cdot}p(1-p)}}\right\} \\ 1-\frac{\alpha}{2} &= F\left\{\frac{(j+0.5)-n{\cdot}p}{\sqrt{n{\cdot}p(1-p)}}\right\} \end{aligned} \tag{8.36}$$

The solution is

$$\begin{aligned} i &= (n{\cdot}p-0.5) + \sqrt{n{\cdot}p(1-p)}\; F^{-1}(\alpha/2) \\ j &= (n{\cdot}p-0.5) + \sqrt{n{\cdot}p(1-p)}\; F^{-1}(1-\alpha/2) \end{aligned} \tag{8.37}$$

where F^{-1} denotes the inverse cdf of the standard normal distribution (e.g., for 1-α = 0.90, F^{-1}(1-α/2) = 1.645). For example, with n=100, p=0.95, and 1-α=0.90, i=90 and j=98, so that ($X_{(90)}$, $X_{(98)}$) forms the approximate 90%

confidence interval for u_p.

Although the expressions for the confidence interval do not depend in any way on the underlying distribution, the expected width of the interval does. In particular, it depends on the expected values of the order statistics involved. In the example above, if the sample is from a standard normal distribution, $u_p = 1.645$ and the expected half-width of the interval is 0.349. If the sample is from a lognormal distribution based on a standard normal, $u_p = 5.180$ and the expected half-width is 1.858. Also, note that, in normal sampling, the expected confidence interval half-width for n=500 is 0.192 for the same estimate.

SECTION 9
Linking PRZM-3 with Other Environmental Models

The popularity of the PRZM-3 model has led to a number of applications that were not originally envisioned. Among these are the model's use (1) as a means of estimating chemical and sediment loadings to watershed-scale modeling systems and (2) for evaluating wellhead protection strategies for nitrates. In order to support these applications, supplemental software has been developed that offers expanded modeling opportunities for PRZM-3 model users. Three linkage opportunities are described below. In accordance with the format used for presenting pertinent equations in the source documents for this section, the equations in Section 9 are not numbered.

9.1 HSPF

9.1.1 PZ2HSPF Bridge Program

The PZ2HSPF bridge program was developed to provide a linkage between the PRZM-2 (now PRZM-3) and HSPF models; the bridge program represents pesticide flow and transport processes between the field and stream. The program provides a simple means for the user to adjust field-generated pesticide fluxes for calibration of in-stream pesticide concentrations, but does not simulate these processes from the first principles represented in governing differential equations. In a sense, the bridge program is a lumped parameter model which simulates the total effects of travel time and losses due to processes such as volatilization, decay and adsorption, as well as resettlement of eroded sediment and water losses to deep groundwater, on the final pesticide load entering the stream. The bridge program accepts four pesticide concentration fluxes generated by the PRZM-3 model and outputs a total surface and subsurface runoff pesticide loading and a sediment associated pesticide loading for introduction into the RCHRES portion of the HSPF model (Bicknell et al. 1993) which simulates in-stream processes. The degree of sophistication of transport processes represented in the bridge program is dependent on the choice of the user and the amount and quality of field data which may be used for calibration.

To generate the four pesticide fluxes which are lagged and attenuated in the bridge program, PRZM-3 was modified to account for lateral drainage and associated lateral flux of pesticide (see Section 9.1.4). The other three pesticide fluxes generated by PRZM-3 are erosion flux, surface runoff flux and groundwater flux, which is generated from the bottom of the PRZM-3 soil column. The fluxes entered into the bridge program from PRZM-3 remain within their "compartment". For example, infiltration of surface runoff along the flow path from field to stream is not represented in the bridge program. As discussed above, the lack of representation of field-to-stream infiltration of the surface runoff and interflow fluxes will result in conservative estimates of these edge-of-stream loadings, since infiltration of these fluxes would increase lag in arrival times, thus also increasing magnitudes of mass losses due to decay and sorption processes. In the bridge program, sorption processes are considered only as part of the permanent loss processes and can be included in the fractional loss parameters for interflow and groundwater. Therefore, it is important to keep in mind that this means of representing "inter-scale" transport may not be appropriate for simulation of a highly sorbing chemical over long periods of time, where sorption/desorption processes play a large role in determining edge-of-stream pesticide loads.

The bridge program reads in the four pesticide fluxes generated by PRZM-3 and then calculates the following modifications of each flux:

<u>Erosion flux</u> - This flux may be lagged by an amount of time representative of the travel time between the field and stream. The loadings may decay during this lag time, with a first-order rate similar to the sorbed decay rate in PRZM-3. The flux may also be multiplied by a sediment delivery ratio (SEDRAT), such that the flux reaching the stream would be SEDRAT*flux.

<u>Surface runoff flux</u> - This flux may be lagged to represent travel time to the stream. It may also decay during this lag, with a first-order decay rate, similar to the PRZM-3 DWRATE for pesticide in water. This rate may differ from the PRZM-3 water decay rate if the user wants to consider additional processes, such as volatilization along the flow path from field to stream.

Lateral flux - This flux may be lagged and may decay with a first-order decay rate for pesticide in water. Other loss processes which may be better represented by a fractional loss equation (for example sorption processes) may be taken into account by using a fractional loss term (LATRAT) which is implemented in the same manner as the sediment delivery ratio, such that LATRAT*lateral flux = lateral flux delivered to the reach.

Groundwater flux - This flux can lag and decay, again with a first-order decay rate. In addition, there is a multiplicative factor similar to the sediment delivery ratio for the "groundwater delivery" (GWRAT), such that GWRAT*groundwater flux = groundwater flux delivered to the reach. The delivery ratio term may also be considered to represent losses due to adsorption. The remaining groundwater flux enters the deep groundwater sink.

The three pesticide fluxes associated with water runoff (surface, lateral and groundwater runoff) are summed within the bridge program to create a total daily edge-of-stream pesticide runoff mass flux. The transformed erosion pesticide flux is accounted for separately, and is input to HSPF as a daily edge-of-stream sorbed pesticide flux. These two daily flux time series generated by the bridge program are divided into 24 components (if the HSPF time step is hourly) to produce the total hourly flux load to be input to HSPF RCHRES.

The four pesticide fluxes which are generated by PRZM-3 are in the form of WDM data sets (Lumb et al. 1990). The bridge program then reads these input data sets and outputs the four transformed fluxes and the total runoff flux as WDM data sets. The total pesticide runoff flux and pesticide erosion flux are used as input into HSPF, where the daily fluxes are uniformly divided into the time step being used by the HSPF simulation. The bridge program also creates an ASCII output file that echoes input data and summarizes total pesticide mass in each storage flux, pesticide mass losses for each flux, and a pesticide mass balance. Note that the mass balance computations are restricted to considering the processes (lag and loss) and configuration (connectivity and areal extent) specified by the user as taking place in transition between the edge-of-field fluxes PRZM-3 computes and the edge-of-stream watershed-scale receiving water inputs HSPF RCHRES requires.

Users of the bridge code should be mindful that the nature of a 'bridge' from a model that computes unit area fluxes to a second model that requires information on both connectivity and areal extent of these fluxes does not allow a true mass balance computation for the entire system that is evaluated by the combined models.

The bridge program consists of a single main program, PZ2HSPF, and two parameter files, PZ2HSPF.INC and MASSBAL.INC. To run the bridge program requires an input parameter file and a WDM file containing the input pesticide flux data sets and output data sets. To invoke the program, type PZ2HSPF <input filename>. A detailed description of the input variables is provided in Table 9.1. A full list of definitions for all variables used in PZ2HSPF is included in the Appendices contained in Section 11.

9.1.2 Application Procedure

PZ2HSPF is a small, stand-alone program, which can be copied (using the DOS copy command) from the program disk to the directory where it will be used. The only requirements are a 386/486 computer and extended memory. The program has been structured to consider most scenarios that can take place in terms of connections between PRZM-3 and HSPF models. Before the user can run the bridge program, a careful layout of the HSPF simulation scenario is necessary to prepare the input parameter file. Most of the information for this file is extracted from the PRZM-3 simulation runs; hence it is imperative that the PRZM-3 runs be entirely consistent with the PRZM-3/HSPF scenario.

To execute the bridge program, an input parameter file is required. The input file contains information on the modeling start and end dates, number of pesticides, pesticide names, crop area treated with each pesticide, WDM dataset identification, and decay rates, 'delivery ratios', and lag times associated with the alternate flow paths of pesticides (i.e., erosion, surface runoff, interflow, groundwater). An example of a bridge program input file is provided in Table 9.2. A full list of definitions for all variables used in PZ2HSPF is included in the Appendices contained in Section 11.

The PRZM-3 program disk contains the executable code for PZ2HSPF, an example test run input parameter file and

the resulting output. The program disk also contains the PRZM-3 output files used in the example input file. To invoke the program, type PZ2HSPF at the command prompt. The user will be prompted to enter the input parameter filename and the names of the output nonpoint source and runoff files. All of the PRZM-3 generated files should be present in the same directory, or else the path must be specified. A detailed description of the example input parameter file and test run is given in the following section.

9.1.3 Example Input and Test Run

The ultimate function of the PZ2HSPF bridge program is to transform PRZM-3 generated, field-scale pesticide flux timeseries contained in WDM files into watershed-scale pesticide flux timeseries, again contained in WDM files, that are suitable for use as input to the receiving water module (RCHRES) of HSPF. The transformation includes consideration of areal and temporal issues, as well as potential losses prior to arriving at the edge of the stream.

The linked models have been used to simulate pesticide transport in the Potomac River Basin for the years 1984 through 1987 (Christian et al. 1993). PRZM-3 simulations were completed for three pesticides (atrazine, metolachlor and alachlor) to generate field-scale loadings, and the HSPF Chesapeake Bay Watershed Model (Donigian et al. 1991) was used to simulate in-stream transport. Three variations of the model applications were presented to demonstrate model sensitivity to single and multiple PRZM-3 pesticide application scenarios, and the effects of changing lag and loss parameters in the bridge program.

Table 9.1 Input Guide for the PZ2HSPF Bridge Program

RECORD 1	**FORMAT**	**A8**
col: 1-80	DESCRP:	description of run
RECORD 2	**FORMAT**	**I5,5X,A15,5X,6I5**
col: 1-5	SEGNUM:	model segment id number
col: 11-25	CRPNAM:	crop name
col: 31-45	STDATE:	simulation starting date: year, month, day
col: 46-60	ENDATE:	simulation ending date: year, month, day
RECORD 3	**FORMAT**	**I5**
col: 1-5	NUMPST	number of pesticides
RECORD 4	**FORMAT**	**A20,5X,F10.2**
Repeat this record up to NUMPST		
col: 1-20	PSTNAM:	pesticide name
col: 26-35	CRPAREA:	crop area treated with pesticide (ha)
RECORD 5	**FORMAT**	**I5**

col: 1-5	OPTFLG:	option flag for writing to WDM file; write if > 1

RECORD 6 FORMAT 9I5
Repeat this record up to NUMPST

col: 1-20	INPDSN:	input data set numbers for erosion, surface runoff, interflow and groundwater pesticide fluxes
col: 21-45	OUTDSN:	output data set numbers for transformed erosion, surface runoff, interflow, groundwater and total aqueous runoff pesticide fluxes

RECORD 7 FORMAT 2A20

col: 1-20	WDFLNM:	WDM file name
col: 21-40	OUFLNM:	output file name

RECORD 8 FORMAT 4F10.4
Repeat this record up to NUMPST

col: 1-10	DSRATE:	sediment associated pesticide decay rate (1/day)
col: 11-20	DRRATE:	surface runoff associated pesticide decay rate (1/day)
col: 21-30	DLRATE:	interflow associated pesticide decay rate (1/day)
col: 31-40	DGRATE:	groundwater associated pesticide decay rate (1/day)

RECORD 9 FORMAT 3F10.4
Repeat this record up to NUMPST

col: 1-10	SEDRAT:	sediment delivery ratio
col: 11-20	LATRAT:	interflow "delivery ratio" (allows for loss of interflow component)
col: 21-30	GWRAT:	groundwater "delivery ratio" (allows for fractional loss to deep groundwater)

RECORD 10 FORMAT 4F10.4
Repeat this record up to NUMPST

col: 1-10	TERO:	sediment associated pesticide time lag from field to stream (days or fraction of a day)
col: 11-20	TSUR:	surface runoff associated pesticide time lag from field to stream (days or fraction of a day)
col: 21-30	TLAT:	interflow associated pesticide time lag from field to stream (days or fraction of a day)

col: 31-40	TGW:	groundwater associated pesticide time lag from field to stream (days or fraction of a day)

Table 9.2 Example Input File for PZ2HSPF

```
BRIDGE PROGRAM INPUT FOR 160CG.CNT
  160     CORN GRAIN CNT       1984   01   01 1987   12   31
    3
ATRAZINE                     1461.38
METOLACHLOR                   673.22
ALACHLOR                      443.34
    2
   11   14   17   20 1011 1014 1017 1020 2001
   12   15   18   21 1012 1015 1018 1021 2002
   13   16   19   22 1013 1016 1019 1022 2003
..\POT.WDM           CGCNT.OUT
     .0231     .0231     .0231     .0116
     .0231     .0231     .0231     .0116
     .0462     .0462     .0462     .0231
       .15      1.00      1.00
       .15      1.00      1.00
       .15      1.00      1.00
       0.0       0.0       0.0       5.0
```

The example input sequence provided in Table 9.2 is one of the many developed for the study cited above. Given the nature of the bridge program functions (i.e., accessing timeseries files, manipulating the data, writing the transformed data to new files), output results for the example are not provided.

9.1.4 Lateral Drainage Modifications to PRZM-3

PRZM-3 has been modified to account for lateral outflow of pesticide from the soil column. A lateral water drainage option was previously implemented in the PRZM model in a study of the fate and transport of aldicarb in Florida (Dean and Atwood 1985b). The lateral drainage option is a part of the restricted vertical drainage option, which is presently included and documented in PRZM-3. The lateral drainage portion is not documented in the users manual, so it is briefly described here.

PRZM-3 simulates water and pesticide movement through a one-dimensional soil column, which is divided into a number of soil compartments for numerical calculation. Drainage within the soil column is calculated for each soil compartment, sequentially calculating water movement, starting with the top soil compartment and moving downward through the soil column. If there is surface infiltration on the current simulation day, water is moved into the soil column unrestrictedly, sequentially filling each soil compartment to saturation water content until the total volume of surface infiltration is accounted for. If there is no surface infiltration event on the current simulation day, the restricted drainage model is invoked. According to the restricted drainage rules, if the water content of a soil compartment is initially below saturation, water drains vertically only, into the compartment below, the flow rate controlled by the vertical drainage parameter of the exponential drainage model. Thus, during the drainage calculations for the current time step, compartments receiving water infiltrating from above may become oversaturated. If the compartment currently being considered has a water content above saturation content, then the exponential drainage model computes vertical and lateral drainage until the compartment water content reaches saturation. Once water content is below saturation, water continues to drain only vertically for the rest of the simulation day.

To understand the restricted lateral and vertical drainage model, it is revealing to consider a conceptual model of each soil compartment as a bucket with two holes of different sizes. One hole is near the bottom of the bucket, and another is at some height along the wall of the bucket. The volume of the bucket below the elevation of the second hole represents the quantity of water above field capacity required to fill the soil compartment to saturation. The volume of water below the lower hole represents the quantity of water stored at field capacity. If the water level rises above saturation due to infiltration from above, water will drain from both the side and the bottom hole at rates

determined by the size of the holes. Once the water level falls below the upper drainage hole, water will continue to drain only from the bottom of the bucket until it reaches the level of the lower hole. The quantity of water flowing out depends only on the depth of water in the bucket and the sizes of the holes.

The following equations describe how the water content in the soil compartment is calculated when the initial water content is above saturation (i.e., when the water level in the bucket is above the uppermost side wall hole). The governing differential equation is:

$$\frac{\partial(\Theta - \Theta_{FC})}{\partial t} = -(AD + ADL)(\Theta - \Theta_{FC}) \qquad \textbf{(9.1)}$$

subject to the initial condition:

$$\Theta|_{t=0} = \Theta_{FC} + (\Theta^{n-1} - \Theta_{FC}) \qquad \textbf{(9.2)}$$

The solution to this equation is:

$$\Theta^{n} = \Theta_{FC} + (\Theta^{n-1} - \Theta_{FC})\exp[-(AD + ADL)t] \qquad \textbf{(9.3)}$$

where

Θ^{n}	=	Water content of the compartment at time step *n*
Θ^{n-1}	=	Water content at end of previous time step
Θ_{FC}	=	Field capacity
AD	=	Vertical drainage parameter
ADL	=	Lateral drainage parameter
t	=	Time
n	=	Time step index
Δx	=	Compartment thickness

In terms of the conceptual model of the bucket, (Θ - Θ_{FC}) represents the amount of water in the bucket above the lower hole, and *AD* and *ADL* represent the size characteristics of the two holes.

If it takes less than one day to drain the compartment to saturation, then *t* equals that fraction of the day. Otherwise, *t* equals one day and the compartment remains oversaturated during the time step, while drainage is calculated for the remaining compartments. Then, oversaturation is dealt with, after applying these equations to every compartment, by redistributing water sequentially back up the soil column, from the oversaturated compartment upward, filling the overlying soil compartments to saturation until all excess water is accounted for.

The amount of water moving out of the compartment is described by the following equations:

$$\text{Lateral outflow} = \frac{ADL}{AD + ADL}(\Theta^{n-1} - \Theta_{FC})(1 - \exp[-(AD + ADL)t])\Delta x$$

$$\text{Vertical outflow} = \frac{AD}{AD + ADL}(\Theta^{n-1} - \Theta_{FC})(1 - \exp[-(AD + ADL)t])\Delta x$$

If the initial water content in the compartment is less than saturation, then water is moved only vertically. The water content of the soil compartment is calculated according to the following governing equation:

$$\Theta^{n} = \Theta_{FC} + (\Theta^{n-1} - \Theta_{FC})\exp[-(AD)t]$$

where water flowing vertically out of the compartment is given by:

$$\text{Vertical outflow} = (\Theta^{n-1} - \Theta_{FC})(1 - \exp[-(AD)t])\Delta x$$

where all parameters are as explained above. Time, *t*, is equal to either one day, if the compartment was below saturation at the start of the time step, or *t* equals (1-t_A), where t_A is *t* from the previous equation for water content

above saturation, to account for continued drainage during the same daily time step after water in excess of saturation has already been drained. Thus, lateral flow only occurs when the soil compartment has a water content above saturation.

The Dean and Atwood implementation of lateral drainage did not allow for associated lateral mass removal of pesticide. We have modified PRZM-3 to account for lateral pesticide movement based on the pesticide concentration within the soil compartment from which the lateral flow originates. Thus, the mass of pesticide which is removed laterally from each compartment is simply the product of the pesticide concentration of the water in the soil compartment and the volume of water which moves laterally from that soil compartment.

9.2 WASP

9.2.1 PRZWASP Bridge Program

The PRZWASP bridge program (Varshney et al. 1993) was developed to facilitate the use of PRZM-2 to generate nonpoint loads for direct input to the WASP model (Ambrose et al. 1993). The bridge code is now operational with PRZM-3, and it creates input nonpoint source and runoff files for the WASP model from the PRZM-3 generated output file for EXAMS (Burns 2000). The program enables the user to read in multiple PRZM-3 output files for several years of simulation runs and generates a single file with daily pesticide loads entering each WASP segment. The program reads an input parameter file which contains information on the WASP segments, systems, and PRZM-3 generated EXAMS input files. The PRZM-3 generated files contain information on the chemical application rate, the time of application, number of applications, surface runoff depth, and runoff fluxes for each chemical. If erosion is being simulated, then PRZM-3 output also contains the pesticide erosion fluxes as well as the soil loss in tonnes per ha. The array size of some of the parameters in the bridge program is governed by the PRZM-3 and WASP model dimensions, i.e., the maximum number of chemicals and applications that can be simulated during one simulation run, and the total number of systems that can be considered. The bridge program is structured to consider all scenarios and sequences that can possibly take place.

The input parameter file contains information on the starting date of the WASP simulation, the number of WASP segments, and systems. The surface area of each WASP segment, as well as the tributary area associated with a corresponding PRZM-3 segment, is required. Several flags, to check whether or not sediment is simulated, or how many and which chemicals are being considered, are included. If sediment is simulated in PRZM-3 and WASP, an option is available to distribute the total erosion load into three fractions, sand, silt, and clay for input to WASP. Also included in the program is the capability to accommodate spray drift deposition on the surface area of the WASP segments. If the flag is on, the user provides information on the mass loading rate of the chemical to be accounted for in spray drift. After reading the input, the program checks whether chemicals and/or sediment are simulated, proceeds with the calculation and generates the nonpoint source file. Next, the program writes the surface runoff and precipitation in volume of water per day reaching each WASP segment to a separate runoff file.

The bridge program is written in FORTRAN 77 and compiled using the LAHEY 32-bit compiler. It consists of a single main program, PRZWASP, which calls two functions, JULIAN and LENSTR, and a subroutine LPYEAR. Function JULIAN converts calendar date to julian date for any given year, and LENSTR gives the actual length of the character array. Subroutine LPYEAR checks whether the year in simulation is a leap year or a calendar year and accordingly sets up a flag which is then read in by JULIAN to calculate the day in consideration. The program can detect and report a number of errors in the input files, and contains more than twenty error messages, to help the user execute the model successfully.

The bridge program reads in the pesticide surface runoff and erosion fluxes and sediment loss generated by PRZM-3 and then calculates the following modifications of each flux:

> <u>Surface runoff and erosion flux</u> - The surface runoff and erosion flux for each chemical are output by PRZM-3 in $kg/cm^2/day$. In the bridge program, they are multiplied by the tributary areas associated with each PRZM-3 run, one for all PRZM-3 segments tributary to each WASP segment and converted into kg to get the total nonpoint source load for each chemical on a daily basis (i.e. kg/day).

Soil loss - The soil loss on a daily basis is multiplied by the tributary area associated with each PRZM-3 run for all corresponding WASP segments, and converted to kg/day.

Spray drift - Mass loading rate (kg/ha) of the chemical assumed to be deposited by spray drift is multiplied by the surface area of the WASP segment on the day of application, for each chemical simulated.

The bridge program creates two ASCII output files: a nonpoint source file and a runoff file. The nonpoint source file contains information directly echoed from the input parameter file as well as the chemical loads as a function of system (chemical and/or sediment), segment, and day. The program sums the chemical loads from surface runoff, erosion, and spray drift, and outputs the loads to the nonpoint source file in kg/day. The runoff file contains daily totals of surface runoff volume and precipitation volume, both expressed in m^3/day. If multiple PRZM-3 segments contribute to a WASP segment, the depth of precipitation falling on the WASP segment is assumed to be the area-weighted average of the precipitation falling on the tributary PRZM-3 areas.

Since PRZM-3 generates separate EXAMS files for each year, all the yearly output files have to be specified in the PRZWASP input parameter file; these files are processed one year at a time by the bridge program.

A detailed description of the input variables is provided in Table 9.3. A full list of definitions for all variables used in PRZWASP is included in the Appendices contained in Section 11.

Table 9.3 Input Guide for the PRZWASP Bridge Program

RECORD 1	**FORMAT**	**I4,2I3**
col: 1-10	WSDATE	start date of WASP simulation - year, month, date
RECORD 2	**FORMAT**	**3I5**
col: 1-5	NUMSEG	number of segments receiving nonpoint source loads
col: 6-10	INTOPT	interpolation option; 1=step function (only one in code now)
col: 11-15	NUMSYS	number of WASP systems (chemicals, sediments) receiving nonpoint source loads
RECORD 3	**FORMAT**	**I5,F10.0**
Repeat this record NUMSEG times		
col: 1-5	NPSSEG	segment number receiving loads
col: 6-15	SEGAREA	area of the WASP segment receiving loads (ha)
RECORD 4	**FORMAT**	**6I5**
col: 1-30	NPSSYS	WASP system number receiving loads
RECORD 5	**FORMAT**	**A15**
Repeat this record NUMSYS times		

Table 9.3	Input Guide for the PRZWASP Bridge Program	
col: 1-15	NPSNAME	name or description of the WASP system receiving loads
RECORD 6	**FORMAT**	**6I5**
col: 1-5	NUMPRZ	number of PRZM-3 segments
col: 6-10	NUMPYR	number of calendar years for which PRZM-3 has been simulated; PRZM-3 generated EXAMS output files must be present for each year
RECORD 7	**FORMAT**	
col: 1-75	HEADER	this record is not read, the program skips this line
RECORD 8	**FORMAT**	**A8,2X,I2,6(5X,I1),3(4X,F4.0)**
Repeat this record NUMPRZ times		
col: 1-8	PRZMFILE	name of the PRZM-3 file
col: 11-12	NTRIB	number of tributary areas associated with this PRZM-3 file
col: 18-18	TNAPP	total number of chemical applications
col: 24-24	ISED	flag to ensure if erosion has been simulated (0=no,1=yes)
col: 30-42	ICHEM	three flags indicating which chemicals are simulated in this PRZM-3 file (0=not simulated, 1=simulated)
col: 48-48	ISPRAY	flag indicating whether spray drift occurred (0=no,1=yes)
col: 53-72	SOLFRC	fractions of three sediment sizes
RECORD 8a	**FORMAT**	**I5,F10.0**
Repeat this record NTRIB times		
col: 1-5	WASPID	identification of the WASP segment
col: 6-15	TEMP	tributary area associated with this PRZM-3 file corresponding to WASP segment number (ha)
RECORD 8b	**FORMAT**	**3F10.0**
Repeat this record TNAPP times		
col: 1-30	MSPRAY	total mass of the chemical in spray drift that falls on the WASP segment for each chemical in each application associated with this PRZM-3 file (kg/ha)

9.2.2 Application Procedure

PRZWASP is a small, stand-alone program, which can be copied (using the DOS copy command) from the program disk to the directory where it will be used. The only requirements are a 386/486 computer and extended memory. The program has been structured to consider most scenarios that can take place in terms of connections between PRZM-3 and WASP models. Before the user can run the bridge program, a careful layout of the WASP simulation scenario is necessary to prepare the input parameter file. Most of the information for this file is extracted from the PRZM-3 simulation runs; hence it is imperative that the PRZM-3 runs be entirely consistent with the PRZM-3/WASP scenario.

To execute the bridge program, an input parameter file is required. The input file contains information on the WASP start date, number of segments and systems to be considered in the WASP model, description of the systems, and PRZM-3 information. PRZM-3 information consists of all the PRZM-3 generated files for EXAMS, the total number of chemical applications in each, erosion information if simulated, and details on the amount of chemical deposited by spray drift for each application. If erosion is being simulated, data for up to three solid fractions namely, sand, silt, and clay can be input.

The PRZM-3 program disk contains the executable code for PRZWASP, an example test run input parameter file and the resulting output. The program disk also contains the PRZM-3 output files used in the example input file. To invoke the program, type PRZWASP at the command prompt. The user will be prompted to enter the input parameter filename and the names of the output nonpoint source and runoff files. All of the PRZM-3 generated files should be present in the same directory, or else the path must be specified. A detailed description of the example input parameter file and test run is given in the following section.

Users of the bridge code should be mindful that the nature of a 'bridge' from a model that computes unit area fluxes to a second model that requires information on both connectivity and areal extent of these fluxes does not allow a mass balance computation for the entire system that is evaluated by the combined models. In the absence of a mass balance computation, the person defining the bridge code parameters has a heightened responsibility to assure an appropriate linkage between the two models.

9.2.3 Example Input and Test Run

Figure 9.1 shows a schematic of an example test run. In the stream section AA', the area receiving nonpoint source load from PRZM-3 segments to be simulated by the WASP model is subdivided equally into six WASP surface water segments. The WASP surface water segments identified from 1 to 6, receive loads from three PRZM-3 runs, namely PRZM1, PRZM2, and PRZM3. The PRZM1 output file provides unit area daily loads (i.e. kg/cm^2/day) for the areas shown as A_1, and A'_1; PRZM2 file provides the unit loads for A_2, and A'_2; and PRZM3 file is for A_3, A'_3, and A''_3. The area A'_2 of segment PRZM2 also contributes to WASP surface water segment 2. Thus, a single PRZM output file can provide unit loads to multiple WASP segments.

(Note: There are always four water column segments considered in the WASP model. The surface water (segment 1), subsurface water (segment 2), upper benthic (segment 3), and lower benthic (segment 4) segment. Here we are dealing with only the surface water segments.)

The surface area of each WASP surface water segment must be known to calculate the mass of the pesticide deposited from spray drift. A_1 through A_3, and A'_1 through A''_3 are the segment areas associated with each PRZM-3 output file, providing loads corresponding to respective WASP segments, as illustrated in Figure 9.1 by arrows. Three pesticides atrazine, metolachlor, and alachlor were simulated in this example. Three PRZM-3 simulations running consecutively for three years from 1978, were considered. Two sediment fractions, sand and silt, were simulated along with the chemicals. The areas of PRZM-3 and WASP segments, the flags to indicate spray drift, the solid fractions, and the mass of chemical deposited from spray drift are entered in the input file as shown in Table 9.4.

Tables 9.5 and 9.6 contain a representative portion of the output nonpoint source file and the runoff information file for the test run shown in Table 9.4. The nonpoint source file is in a format which can be directly read by the WASP model, whereas the runoff file contains volumetric water in cubic meters due to runoff and precipitation entering

each WASP segment on a daily basis; this latter file can be utilized as an external flow file in a hydrodynamic model, e.g. RIVMOD.

Table 9.4 Example Input File for PRZWASP

```
1978 01 01
    6    1    5
    1       2.0
    2       3.0
    3       2.0
    4       3.0
    5       4.0
    6       5.0
    1    5    6    2    3
ATRAZINE
METOLACHLOR
ALACHLOR
SAND
SILT
    3    3
 PRZMF   NTRIB TNAPP  ISED ICHEM ICHEM ICHEM ISPRY SOLFRC  SOLFRC  SOLFRC
PRZM1EXA  2      3     1     1     1     0     1     0.30    0.70    0.00
    1      60.0
    2      40.0
      0.01      0.05      0.00
      0.02      0.03      0.00
      0.03      0.01      0.00
PRZM2EXA  2      3     1     1     1     1     1     0.20   0.80     0.00
    2      10.0
    3      40.0
      0.10      0.20      0.03
      0.02      0.20      0.03
      0.03      0.20      0.03
 PRZMF   NTRIB TNAPP  ISED ICHEM ICHEM ICHEM ISPRY SOLFRC  SOLFRC  SOLFRC
PRZM3EXA  3      3     1     0     1     1     0     0.50    0.50    0.00
    4      55.0
    5      45.0
    6      35.0
```

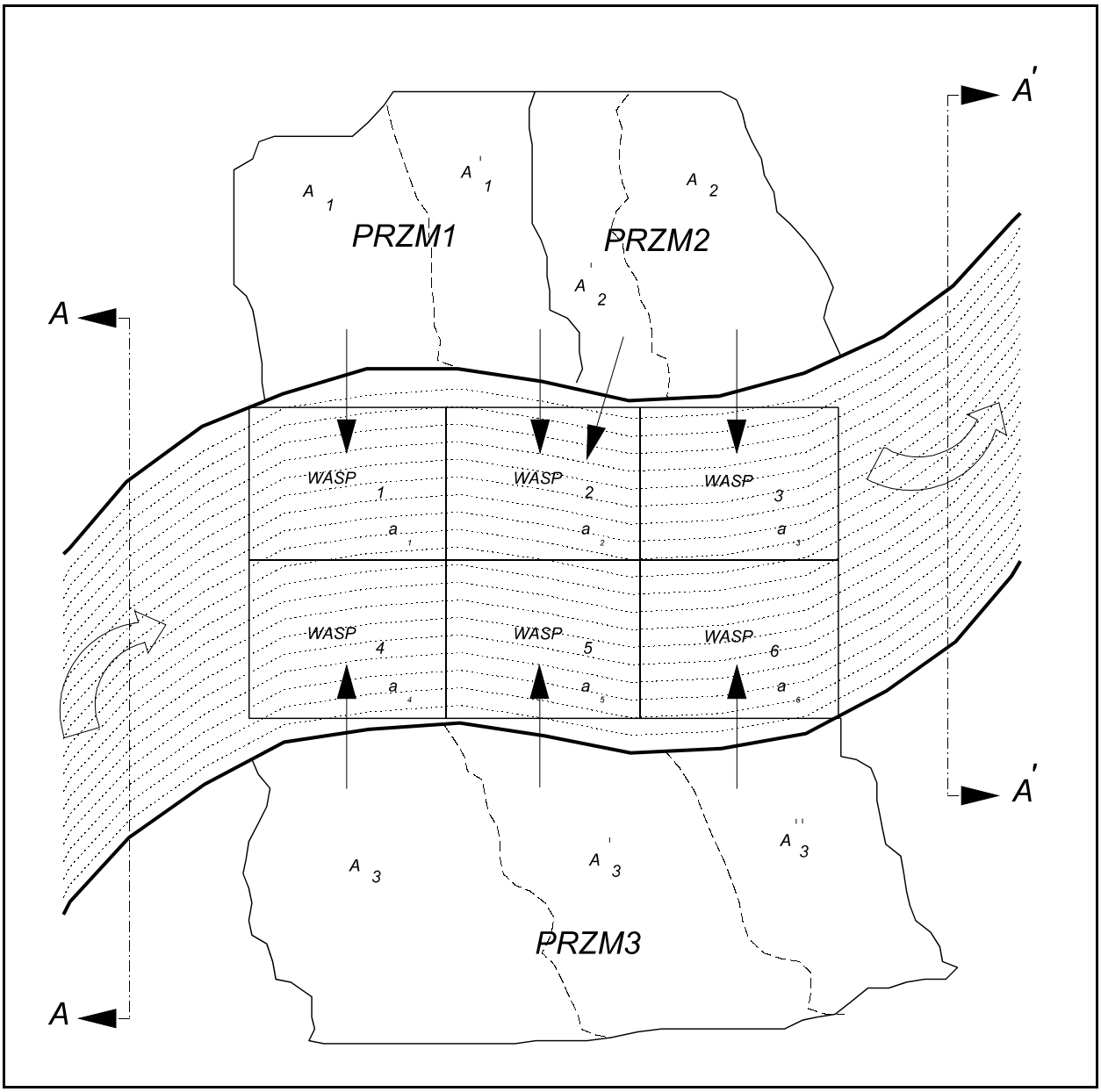


Figure 9.1 Schematic of an example PRZWASP test run.

PRZM1 through PRZM3 - PRZM-3 segments (i.e. separate output files)
$WASP_1$ through $WASP_6$ - Identification of WASP surface water segments
A_1 and A'_1 - Tributary areas associated with PRZM1, ha
A_2 and A'_2 - Tributary areas associated with PRZM2, ha
A_3, A'_3, A''_3 - Tributary areas associated with PRZM3, ha
a_1 through a_6 - Surface area of each WASP segment, ha

Table 9.5 Output Nonpoint Source File for PRZWASP Test Run[1]

```
PRZM2              6    1    5
    1
    2
    3
    4
    5
    6
    1    5    6    2    3
ATRAZINE
METOLACHLOR
ALACHLOR
SAND
SILT
   80.0000
ATRAZINE        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
METOLACHLOR     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ALACHLOR        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
SAND            2.594E+03 2.017E+03 1.153E+03 3.963E+03 3.242E+03 2.522E+03
SILT            6.052E+03 5.188E+03 4.611E+03 3.963E+03 3.242E+03 2.522E+03
   81.0000
ATRAZINE        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
METOLACHLOR     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ALACHLOR        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
SAND            2.936E+03 2.283E+03 1.305E+03 4.485E+03 3.670E+03 2.854E+03
SILT            6.850E+03 5.872E+03 5.219E+03 4.485E+03 3.670E+03 2.854E+03
   95.0000
ATRAZINE        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
METOLACHLOR     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
ALACHLOR        0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
SAND            6.264E+03 4.872E+03 2.784E+03 9.570E+03 7.830E+03 6.090E+03
SILT            1.462E+04 1.253E+04 1.114E+04 9.570E+03 7.830E+03 6.090E+03
..........
```

[1] Output is truncated to conserve space

Table 9.6 Output Runoff Information File for PRZWASP Test Run[1]

```
   80.0000
RUNOFF-M3       2.273E+03 1.894E+03 1.515E+03 2.083E+03 1.705E+03 1.326E+03
PRECIP-M3       0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   81.0000
RUNOFF-M3       2.590E+03 2.158E+03 1.726E+03 2.374E+03 1.942E+03 1.511E+03
PRECIP-M3       0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   95.0000
RUNOFF-M3       5.278E+03 4.398E+03 3.518E+03 4.838E+03 3.958E+03 3.079E+03
PRECIP-M3       5.240E+02 7.860E+02 5.240E+02 7.860E+02 1.048E+03 1.310E+03
..........
```

[1] Output is truncated to conserve space

9.3 On-site Wastewater Disposal System (OSWDS)

In order to enable PRZM-3 to be used as a tool for evaluating rural wellhead protection strategies for nitrates, a stand-alone program that allows simplistic modeling of inputs of septic effluent nitrogen species to the PRZM soil column has been developed (Imhoff et al. 1995). The On-site Wastewater Disposal System (OSWDS) module offers an appropriate level of detail for representing inflows/processes/outflows by implementing a generalized module (i.e., one not dependent on specific reaction kinetics) comprised of two treatment units (Figure 9.2). The first treatment unit always represents the septic tank; the second treatment unit represents all transformations/ losses that occur between the outlet of the septic tank and the inflow into the unaltered subsurface soil. (For our purposes "unaltered" means below or beyond the area that has been modified for purposes of wastewater distribution and/or treatment.)

The user has the option of whether to consider only the first treatment unit, or both treatment units. If only one treatment unit is modeled, the output flow and N concentrations from the unit are directly input into the appropriate PRZM-3 soil compartment. The PRZM-3 soil horizon into which OSWDS outflow is introduced is specified by the user based on knowledge of the effluent depth compared to the soil horizon depths. If only one treatment unit is modeled, this depth corresponds to the depth below the ground surface of the tank outlet; if two treatment units are modeled, the effluent depth typically corresponds to the bottom depth of the area modified for wastewater distribution/treatment.

Effluent is assumed to be homogeneously distributed throughout the horizon into which it is introduced.

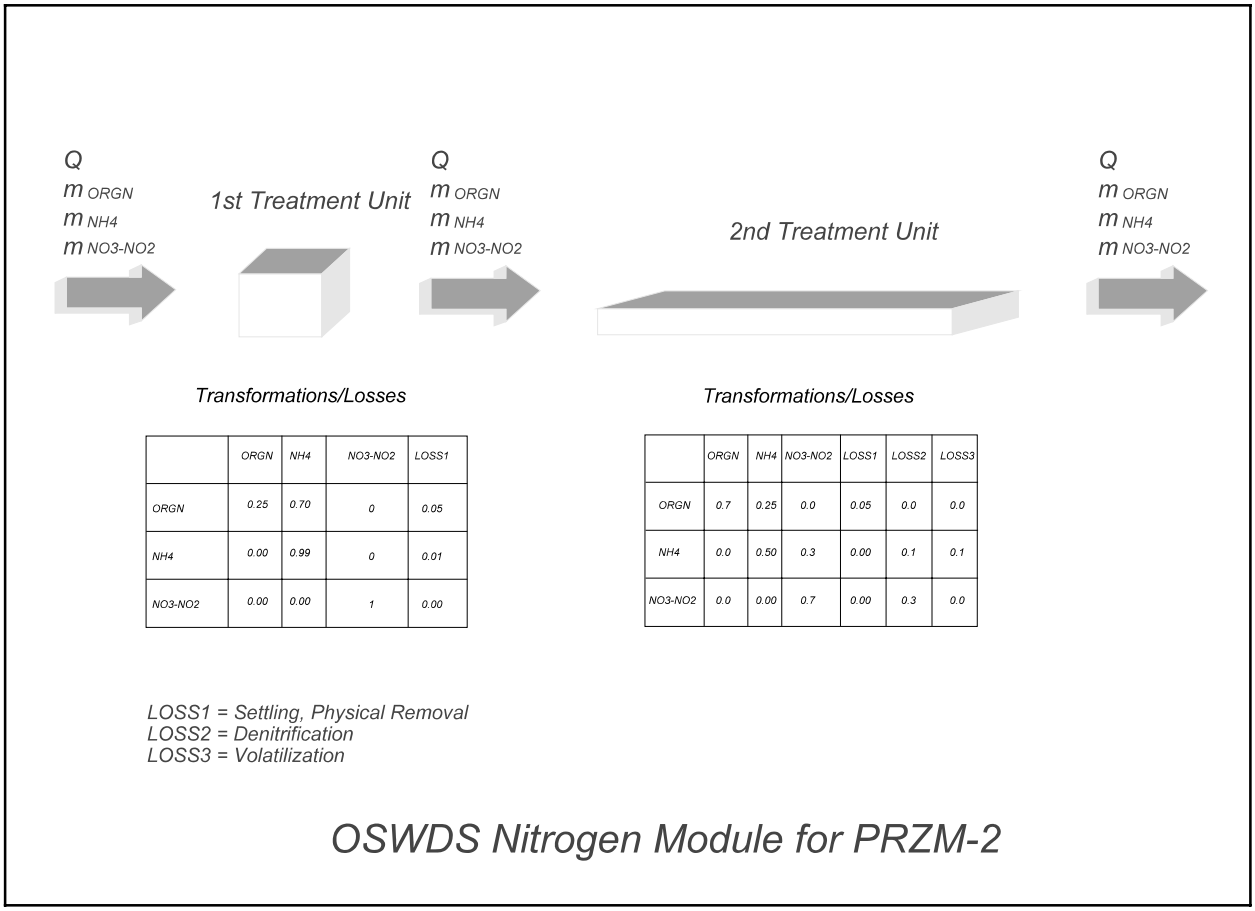
Wastewater influent to the first treatment unit is characterized according to the following scheme:

(1) The user defines a "base" timeseries of wastewater flow (gal/day) and concentrations of associated nitrogen species (mg/l). The base wastewater flow is defined by assigning a value for per person wastewater generation (gal/capita), and one or more seasonal occupancy rates (# of persons serviced by the On-site Wastewater Disposal System OSWDS).

(2) The ability to define seasonal occupancy is enabled. The user specifies the number of "occupancy seasons" during the calendar year, the starting date of each season, and the number of occupants serviced by the OSWDS.

(3) The modeling scheme assumes that the nitrogen species concentrations associated with a particular OSWDS remain constant over time (i.e., the flows can vary seasonally, but the concentrations do not vary with time). The user defines the concentrations of N species in the influent; reasonable default values gleaned from the literature for residential systems are provided in Table 9.7.

(4) Nitrogen species that are modeled in the influent wastewater are total organic N, ammonium, and nitrate-nitrite. While the literature consistently reports negligible amounts of nitrate-nitrite in typical wastewater influent, for the sake of flexibility combined nitrate-nitrite is included as a possible wastewater constituent for atypical situations. Given that the modeling of N transformations within the OSWDS module is not mechanistic, there is no benefit to differentiating between particulate and dissolved organic N, or between labile and refractory organic N. However, this distinction is needed prior to input to the soil region represented by PRZM-3 (see discussion below).



	ORGN	NH4	NO3-NO2	LOSS1
ORGN	0.25	0.70	0	0.05
NH4	0.00	0.99	0	0.01
NO3-NO2	0.00	0.00	1	0.00

	ORGN	NH4	NO3-NO2	LOSS1	LOSS2	LOSS3
ORGN	0.7	0.25	0.0	0.05	0.0	0.0
NH4	0.0	0.50	0.3	0.00	0.1	0.1
NO3-NO2	0.0	0.00	0.7	0.00	0.3	0.0

Figure 9.2 Schematic Representation of the On-site Wastewater Disposal System (OSWDS) Nitrogen Module.

Table 9.7 Typical Mean Concentration Values (mg/l) for Nitrogen Species in Septic Tank Effluent

	EPA (1980)	**Reneau (1989)**	**NVPDC (1990)**
Total N	46	40-80	72
NH_4^+-N		30-60	60
NO_3^--N		<1	<1
Dissolved Org. N		10-20	12
Particulate Org. N		<1	<1

The treatment effects of the **septic tank** are modeled as follows:

(5) The efficiency of the septic tank is defined by the user by (*I*) assigning values for a series of transformation factors between N species and (*ii*) defining a physical loss term for organic N due to settling/storage within the tank and tank maintenance activities (i.e., pumping).

(6) N species that are modeled within the septic tank are total organic-N, ammonium, and nitrate-nitrite. (Nitrate-nitrite concentrations are consistently reported at insignificant levels within septic tanks, but nonetheless, for the sake of generality, we will include transformation factors that allow user-controlled specification of this constituent.

The treatment effects of the **second treatment unit** are modeled as follows:

(7) As in the first treatment unit, the efficiency of the second unit is defined by the user by (*I*) assigning values for a series of transformation factors between N species and (*ii*) defining a physical loss term for organic N. The transformation factors are expanded to allow representation of the production, and loss of, elemental nitrogen via denitrification, and ammonia via volatilization. (Literature suggests that transformation of ammonium to nitrate-nitrite can be significant within the distribution/treatment area outside the septic tank, particularly in systems engineered to facilitate nitrification/denitrification.) The physical loss term represents the sum of loss due to settling, clogging, complexation or any other process that results in permanent physical arrest of nitrogen species within the confines of the distribution/treatment area.

(8) N species that are modeled as state variables within the second treatment unit are total organic-N, ammonium, and nitrate-nitrite.

Regarding the N constituent linkage between the OSWDS module and the PRZM-3 soil compartment, the modeling strategy is borrowed from that used for modeling sediment in the HSPF model (Bicknell et al. 1993). In the same manner that sediment is modeled as a single constituent in the HSPF land surface module (PERLND) and then divided into sand, silt and clay fractions (via user input) prior to its input in the HSPF instream module (RCHRES), total organic N is modeled as a single constituent throughout the OSWDS module, and capabilities are implemented for user-defined allocation of total N into particulate labile and particulate refractory, (we have assumed that all organic N effluent is particulate) to parallel the N species scheme that are used in the PRZM-3 soil compartments.

The modeling approach assumes that <u>all</u> OSWDSs are located in the subsurface area that is represented by the PRZM component of PRZM-3 (i.e., septic tanks do not generate direct fluxes to VADOFT). The linkage has required the development of capabilities for representing lateral influxes of both water and chemical constituents into specific PRZM-3 compartments. The soil horizon into which the lateral flows occur is user-defined. Specification of effluent flow into a soil layer that is below the area modeled using the PRZM component (i.e., in the area modeled using VADOFT) is not allowed, and results in an error message and termination of the run.

The OSWDS module has been implemented with the dual capability to (1) write to user-defined files, or (2) to interact with the ANNIE/WDM capabilities for timeseries management and display of relevant flow and nitrogen species. Users are able to provide the timeseries influent to the first treatment unit of the OSWDS module by defining flows and concentrations in the module input sequence. Users are able to provide the timeseries influent to the second treatment unit of the OSWDS module by direct use of values generated by the simulation of the first treatment unit. The design assumes that all interactions between the OSWDS module and the PRZM-3 model occur via PRZM-3 reading OSWDS module output files to obtain input to the soil compartment(s). These files contain flow/chemical mass flux data derived from one of two different run options: (1) results generated by a simulation that only considered the first treatment unit, (2) results generated by simulating both treatment units. Running the OSWDS module “stand-alone” allows the user to develop scenarios related to different septic tank influent conditions (e.g., occupancy rates, seasonal occupancy) and/or treatment options (e.g., nitrification/denitrification schemes); store the results of the scenarios; and use the results at a later date as input to various PRZM-3 soil horizon conditions.

A detailed description of the OSWDS input variables and an example of an input file are provided in Tables 9.8 and 9.9.

Table 9.8 Input Guide for On-site Wastewater Disposal System (OSWDS) Module

RECORD 1 - Control Parameters

Format (I5,F8.0,2I5,2(2X,2I2,I4),F8.0)

NSEA	number of seasonal occupancies
UVOL	unit volume (l/person/day)
NTR	number of treatments (1 <= NTR <=2)
OFLG	output flag (1 - WDM, 2 - Flat file)
SEDAT	start/end date of simulation (ddmmyyyy)
LCHSIZ	leach field size (m^2)

RECORD 2 - Influent Volume Input

Format (2I2,I4,F8.1)

start date, number of occupants, (2I2,I4,F8.1)

RECORD 3 - Influent Concentrations

Format (3F8.2)

Organic N, Ammonia, Nitrate/Nitrite (kg/l)

RECORD 4 - Primary Treatment Transformations/Losses

Format (4F8.2)

For each constituent, specify fraction resulting in:

Org N, Ammonia, Nitrate/Nitrite, Settling/Removal

RECORD 5 - Secondary Treatment Transformations/Losses

Format (6F8.2)

For each constituent, specify fraction resulting in:

Org N, Ammonia, Nitrate/Nitrite, Settling/Removal, Denitrification, Volatilization

Table 9.8	Input Guide for On-site Wastewater Disposal System (OSWDS) Module

RECORD 6 - Output File

IF OFLG = 1,

WDM file name, data-set numbers, (A32,4I5)

ELSE IF OFLG = 2,

Flat file name, (A32)

Table 9.9 Example Input File for On-site Wastewater Disposal System (OSWDS) Module

```
    1   170.0    2    2  01011957  31121966        60.0
01011957     4.0
    52.0    11.0     0.0
   0.288   0.654     0.0   0.058
     0.0     1.0     0.0     0.0
     0.0     0.0     1.0     0.0
     1.0     0.0     0.0     0.0     0.0     0.0
     0.0     1.0     0.0     0.0     0.0     0.0
     0.0     0.0     1.0     0.0     0.0     0.0
SEPTIC.OUT
```

SECTION 10
REFERENCES

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SECTION 11
Appendices

11.1 Error Messages and Warnings

The PRZM-3 code contains a number of error and warning messages that indicate either fatal or non-fatal routine conditions. A list of the current error (fatal) and warning (non-fatal) conditions that are recognized by the code is given in Table 11.1. Along with each message, troubleshooting approaches are described. Error or warning messages originating in PRZM-3 (the main code) are numbered beginning with 1000; PRZM pesticide routines, 2000; VADOFT, 3000; PRZM nitrogen routines, 4000; and the Monte Carlo module, 5000. Note that error numbers less than 1000 may appear. These numbers are being supplied by the Fortran compiler that was used to compile PRZM-3 and its associated modules. These errors will probably be associated with reading input data; e.g., problems such as inappropriate characters in an input field that the code is attempting to interpret as an integer or a disk drive being unavailable for reading data. Consult the compiler errors list for the exact cause.

Note also that, if the compiler uses numbers in the range of 1000 to 5000 for these file access errors, an error number may appear that seems to be an EXESUP/PRZM/VADOFT error. The error message however, will not, correspond to the messages in Table 11.1. The message will be something such as: "Error in attempting to open file [<file name>]" or "Error in input....". Again, check the compiler's run time error list for the exact cause.

When errors and warnings are reported in the output echo file, three lines of information are provided. The first line reports the number and whether the condition was an error (fatal) or warning (non-fatal). The second line supplies the associated message. The third line supplies a subroutine trace to indicate where the error occurred. For example, the third line might be: 'PRZM3>INPREA>VADINP'. This indicates that the error occurred in the subroutine VADINP (the VADOFT input routine), which was called from subroutine INPREA, which was called from the PRZM-3 main program. This third line will not appear if an error occurs in the routine INITEM, which is the routine to read the PRZM3.RUN file and initialize the simulation.

11.2 Variable Glossary

This section presents the major variables used in the PRZM-3 code, as well as variables for the bridge codes that link PRZM-3 to the HSPF and WASP models (see Sections 9.1 and 9.2). Table 11.2 presents variables used in the EXESUP module, Table 11.3 presents all PRZM variables other than those specific to nitrogen simulation, Table 11.4 presents PRZM nitrogen simulation variables, Table 11.5 presents VADOFT variables, Table 11.6 presents variables used in the Monte Carlo module, Table 11.7 presents PZ2HSPF bridge code variables, and Table 11.8 presents variables used in the PRZWASP bridge code.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches

	Error or Warning	Troubleshooting Approach/Explanation
1010	Water table is above vadose zone	The water table has accumulated to above the top of the vadose zone. Use higher conductivities or increase the thickness of the vadose zone.
1020	Water table is above root zone	The water table is above the top of the root zone. Use higher conductivities or increase the thickness of the root zone.
1050	Zero or negative mass in VADOFT/PRZM nodes below the water table	This is a warning only, the concentration values in the VADOFT or PRZM nodes below the water table will not be adjusted for the current timestep. If this warning appears repeatedly, the VADOFT or PRZM geometry might have to be adjusted.
1070	Error in the file name input, line with...	An incorrect (or misspelled) identifier was supplied for a file.
1090	Bad value [nnnn] for number of chemicals	The number of chemicals must be between 1 and inclusive. Change the number in the global data group of PRZM-3 input file.
1092	Bad index [nnnn] of chemical	An invalid index was provided for input record EXESUP3 with ANAME = 'PARENT OF'. Values less than 1 or greater than NCHEM are not valid.
1100	Bad value [nnnn] for chemical parent species	Check input values. Chemical 1 can have a parent of 0 only. Chemical 2 can have a parent of 0 or 1. Chemical 3 can have a parent of 0, 1, or 2.
1190	Bad identifier reading global data [<value>]	An invalid label appears in the global data section (EXESUP) of the PRZM3.RUN input file.
1200	End date is before start date	Check the 'START DATE' and 'END DATE' records of PRZM3.RUN input file.
1202	End date and start date are the same	Check the 'START DATE' and 'END DATE' records of PRZM3.RUN input file.
1210	Unrecognized label [<label>] while attempting to read ECHO or TRACE	A record in the PRZM3.RUN file appears after the 'ENDDATA' record before the 'ECHO' or 'TRACE' records.
1220	Echo level not defined; set to 5 [or 1]	No output echo level was specified in the global parameter file. The value was set to 5 if MONTE CARLO was not selected or 1 if MONTE CARLO was selected.
1230	Trace level not defined; set to 0	No subroutine trace level was specified in the global parameter file. The value was set to the default value of 0.
1240	End of file on PRZM-3 run file	Recheck the global data group of the PRZM-3 input file. There is an error in the input sequence; an option was set which required more lines of data than supplied.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches		
	Error or Warning	**Troubleshooting Approach/Explanation**
1250	Error reading PRZM-3 run file...	Error in reading PRZM-3 input data, most likely there are inappropriate characters in a data field that is attempting to be interpreted as integer data.
1260	File type [‘nn’] has already been specified	A file with the same unit number has been open while PRZM-3 is running. Should never occur in current version of PRAM-3.
1270	Too many files requested to be open at once	The maximum number of files allowed (defined in the include file IOUNITS.PAR) is too small a number for the (recently modified) version of PRAM-3. This error should not appear in the current version of PRAM-3.
1280	ENDFILE statement present before file [nn] was opened	An input file, which is required for the current PRZM-3 simulation configuration, has not been identified in the file group of the PRAM-3 input file.
1290	Request to close file [nn] which was not open	Should never occur in current version of PRAM-3. Implies that recent code modifications have been made which did not properly account for which files were open.
1300	Unknown unit number to open file	Implies that recent code modifications have been made which did not properly account for which files were open.
1310	Too many lines required for Trace option	Should never occur in current version of PRAM-3. Implies that recent code modifications have been made resulting in a very high level of subroutine nesting.
1320	Argument [<value>] too large for EXP	Attempt to take the exponential of too large a real number.
1330	Negative or zero argument [<value>]	Attempt to take the log of a zero or negative argument.
1350	Single precision overflow	A mathematical operation resulted in a number too large for the real value being calculated.
1360	Negative argument [<value>] to SQRT	Attempt to take the square root of a negative number. Subroutine trace accompanying error message will show in which routine the error occurred.
1390	Invalid index [nnnn]in reading record [<record number>]	A bad index value in a VADOFT read, probably initial condition data.
1400	Error reading PRZM data	Probable causes are inappropriate characters in an input field for integer or real reads.
1500	ENDDATA before starting end day was provided	The label 'ENDDATA' appears in the global day was provided parameters section of PRZM3.RUN file before the record was provided.
1510	ENDDATA before end day was provided	The label 'ENDDATA' appears in the global parameters section of PRZM3.RUN file before the 'END DATE' record was provided.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches

	Error or Warning	Troubleshooting Approach/Explanation
1530	ENDDATA before number of chemicals was provided	The label 'ENDDATA' appears in the global parameters section of PRZM3.RUN file (with TRNSIM = 'ON') before the 'NUMBER OF CHEMICALS' record was provided. The 'NUMBER OF CHEMICALS' record is required for a transport simulation.
1540	ENDDATA before the parent of chemical n was provided	The label 'ENDDATA' appears in the global parameters section of PRZM3.RUN file (with TRNSIM = 'ON' and NUMBER OF CHEMICALS greater than 1) before the 'PARENT OF n' record was provided.
1550	dd/mm/yy - Invalid START (or END) DATE	An invalid date has been entered in the global parameters section of the PRZM3.RUN input file. Check to see whether the month being specified had the number of days which is being implied (e.g., 31/02/88 is not valid).
1560	End of file [<file identifier>] encountered	The end of the file specified was reached while still attempting to read data.
1570	Monte Carlo simulation - Level reset to 1	If an echo level greater than 3 is Echo requested with Monte Carlo on, the echo level will be reset to 1. No action required.
2000	Simulation date (dd/mm/yy), meteorological date (dd/mm/yy) do not match	The meteorological data file is not aligned with the simulation data. There is probably a missing match record in the data file or the simulation start and end dates specified in PRZM3.RUN do not correspond to the dates in the meteorological data file.
2010	Number of chemicals in PRZM [NN] <> number of chemicals in EXESUP [nn]	The value supplied to the PRZM input file for the number of chemicals being simulated does not agree with the number supplied to the PRZM3.RUN input file.
2020	ERFLAG has invalid value	ERFLAG (Erosion method) may only take on values of 0, 2, 3, or 4 (see ERFLAG in Chapter 11)
2040	NPI [nnnn] + NEW [nnnn] is greater than NPII [nnnn]	Decrease the number of PRZM compartments or increase the parameter NPII. If the latter, in subroutine MOC recompile the code. This error only occurs if the MOC rather than backward difference transportsolution technique is used.
2050	Solution for tridiagonal matrix not found, previous day's values used	If this message appears repeatedly, the PRZM problem definition geometry should be reevaluated.
2060	NDC [nnnn] is greater than NC [nnnn]	Change PRZM problem definition geometry so that the input value of NDC is less than or equal to the parameter NC or change the value of NC and recompile.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches		
	Error or Warning	**Troubleshooting Approach/Explanation**
2065	CROPNO [n] not found in ICNCN(1:NDC): n_1 n_2 ... n_{NDC}	The crop number (CROPNO, record 9A) does not match any of the crop numbers in ICNCN (record 9). CROPNO should be present in one of the ICNCN of the (multiple) records 9.
2070	NCPDS [nnnn] is greater than NC [nnnn]	Change PRZM problem definition geometry so that the input value of NCPDS is less than or equal to the parameter NC or change the value of NC and recompile.
2080	NAPS [nnnn] is greater than NAPP [nnnn]	Change PRZM problem definition geometry so that the input value of NAPS is less than or equal to the parameter NAPP or change the value of NAPP and recompile.
2090	NHORIZ [nnnn] is greater than NCMPTS [nnnn]	Change PRZM problem definition geometry so that the input value of NHORIZ is less than or equal to the parameter NCMPTS or change the value of NCMPTS and recompile.
2100	NCOM2+1 [n] is greater than NCMPTS [n]	The total number of compartments NCOM2(roughly, Sum(Ceiling(THKNS/DPN))) is greater than NCMPTS, the dimension of the array DelX. Change PRZM problem definition geometry so that the value of NCOM2 is less than the parameter NCMPTS or change the value of NCMPTS and recompile.
2110	NPLOTS [nnnn] is greater than 7	Reduce the number of requested plots.
2120	Sum of horizon thicknesses exceeds depth	Change PRZM problem definition geometry so that the sum of horizon thickness is equal to the user supplied total depth.
2130	Soil profile description is incomplete, data available for xx.xx of xx.xx cm	Change PRZM problem definition file so that profile data are supplied for the entire depth.
2140	Calculated field capacity water content exceeds the saturation value	Either decrease the soil bulk density or adjust the parameters for calculating field capacity water content (if THFLAG=1) or lower the supplied value of field capacity water content (if THFLAG=0).
2150	Application [nn] failed to meet ideal soil conditions	The specified pesticide application did not meet soil moisture criteria before the WINDAY value expired. Currently this error will halt execution.
2160	WINDAY [nn] for application [nn] is too large	The value for WINDAY, specified in the PRZM input sequence, causes overlap on a proceeding application date. Reduce the value for WINDAY to a value lesser than the difference of application dates.
2170	Horizon into which septic effluent is to be introduced > number of horizons.	Execution is halted.
2180	DEPI(<n>,<n>) changed from <value> to <value> because CAM is equal to <n>.	If CAM is equal to 1, 2, or 3, and DEPI is not equal to the default value (4 cm), then DEPI is set to the default value. Execution continues.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches		
	Error or Warning	**Troubleshooting Approach/Explanation**
2190	DEPI(<n>,<n>) changed from <value> to <value> because CAM is equal to <n>.	See section 4, Record 16: if CAM == 4-10, then DEPI >= DPN(1). Execution continues.
2200	CAM(<n>,<n>) == <n> is out of the valid range 1-10	See section 4, Record 16 for the valid range. Execution is halted.
2210	PCDEPL changed from <value> to 0.5	See section 4, Record 27 for the valid range. Execution continues.
2220	Sum(THKNS(1:NHORIZ)) [n] is less than Max(AMXDR(1:NDC)) [n]	The maximum root zone depth is greater than the soil's total thickness. The difference was added to the last compartment and the user data adjusted. Execution continues.
2230	IBGN [n] is greater than NCMPTS [n]	The total number of compartments IBGN (roughly, Sum(Ceiling(THKNS/DPN))) is greater than NCMPTS, the dimension of the array DelX. Execution is halted.
3000	Fatal error in HFINTP, interpolation failed	The current time in VADOFT exceeds the supplied values of the interpolation time vector in attempting to interpolate head or flux values. This error should not occur when running VADOFT in linked mode. If running VADOFT alone, increase the number of time periods of the interpolation time and head/flux vectors.
3010	VARCAL - timestep nnn solution fails to converge after nnn reductions	The maximum number of time refinements was exceeded due to non-convergence. Relax the converge criterion, change the iterative scheme or revise VADOFT parameters.
3020	Attempt to run VADOFT w/PRZM on and ITRANS.ne.1	The user has attempted to run VADOFT with PRZM on and ITRANS not equal to one. Set ITRANS to 1 and make the appropriate changes to the VADOFT parameter file.
3030 3040	Incorrect value for IMODL in VADOFT input	An incorrect value has been entered for IMODL in the VADOFT input file. Check the values entered; IMODL = 0 for transport, IMODL = 1 for flow.
3050	Requested value of NOBSND [nnnn] greater than MXPRT [nnnn]	The value entered for the number of observation nodes in VADOFT (NOBSND) exceeds the maximum (MXPRT). Reduce the number of observation nodes or increase MXPRT in the PARAMETER statement. If the latter, recompile the model.
3060	Transport simulation, NVREAD reset to 1	The value of NVREAD supplied by the user was reset to 1 since a transport simulation was requested; no action required.
3070	PRZM is on; IVSTED reset to 1	The value of IVSTED supplied by the user was reset to 1; no action required.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches

	Error or Warning	Troubleshooting Approach/Explanation
3080	PRZM is on; flow boundary conditions will be over-written	If PRZM is on and linked to VADOFT, a prescribed flux b.c. will be used at the VADOFT top node. Daily values of water and solute flux are generated by PRZM. Related boundary conditions in the VADOFT impact file are overwritten. IBTND1 is set to 0; no action required.
3090	PRZM is on; transient data at top node ignored	If PRZM is on, any transient flow data relevant to VADOFT's upper boundary is overwritten. ITCND1 is set to 0; no action required.
3120	PRZM is on; transport boundary conditions will	PRZM output will overwrite VADOFT upper boundary condition for solute transport. PRZM generates be overwritten daily volume of solute flux. IBTNDI is set to 0. No action required.
3130	PRZM is on; transient data at top node ignored	If PRZM is on, any transient solute flux data the user has input for the upper boundary in VADOFT is ignored. ITCNDN is set to 0. No action required.
3170	Invalid index [nnn] in reading PINT	An invalid index (less than 1 or greater than the parameter NP) was supplied for an initial condition value. Supply proper value.
3190	ITMGEN<>1 in linked mode, results may be unpredictable	The user is supplying output marker time values that, potentially, could result in a read error of Darcy velocities during the VADOFT transport simulation.
3210	End of file reading VADOFT Darcy velocities	Check to see whether warning 3190 occurred prior to this fatal error. Make necessary changes to VADOFT input file.
4000	The horizon number specified to receive septic influent [n] does not exist	The horizon number into which the septic effluent is to be introduced does not exist. This number must be between 1 and NHORIZ (See Record 32 of the PRZM input defns.)
4010	If FIXNFG is 1, NUPTFG must be 1. As NUPTFG is 0, FIXNFG will be set to 0	The flag FIXNFG is set to 1, indicating nitrogen fixation is to be simulated, but the flag NUPTFG is set to zero. In order for nitrogen fixation to be simulated, the yield-based algorithm for nitrogen uptake (NUPTFG =1) must be used.
4020	Sum of monthly plant uptake fractions over the year [n] do not sum to 1	The monthly fractions for yield-based plant uptake of nitrogen must sum to unity across the calendar year.
4030	Sum of layered plant uptake fractions [n] do not sum to 1 in month [n]	The monthly fractions for yield-based plant uptake of nitrogen from soil layers must sum to one across the number of horizons being simulated for each month.
4040	Sum of fraction of nitrogen uptake from nitrate & ammonium [n] is not 1	The input parameters which designate the fraction of nitrogen uptake that comes from nitrate and ammonium must sum to unity.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches		
	Error or Warning	**Troubleshooting Approach/Explanation**
5000	Format error in reading Monte Carlo input file	Check Monte Carlo input file. Illegal characters are in inappropriate data file columns.
5010	Premature end of Monte Carlo input file	Check Monte Carlo input file. Insufficient data lines have been provided given the users problem definition.
5020	Uniform random number could not be generated for exponential distribution	Random exponential distribution variates could not be generated. Probable cause is inappropriate distribution parameters being supplied in the Monte Carlo input file.
5030	Cannot have a negative mean for a log normal distribution. Mean equals <value>	A negative mean was calculated for a log normal distribution. Check distribution parameters supplied in the Monte Carlo input file.
5040	Subroutine DECOMP terminated, matrix BBT is not positive definite	Monte Carlo solution matrix could not be decomposed. Check distribution parameters supplied in Monte Carlo input file.
5050	The number of [MONTE CARLO RUNS] is greater than maximum of <value>	Too large a value was chosen for the number of Monte Carlo runs. Reduce number In input file or change NRMAX in parameter file and recompile.
5060	The number of [MONTE CARLO VARIABLES] is greater than maximum of <value>	Reduce number in input file or change MCMAX and recompile.
5070	The number of [EMPIRICAL DIST. DATA POINTS] is greater than maximum of <value>	Reduce number in input file or change NEMP and recompile.
5080	The number of [MONTE CARLO OUTPUT VARIABLES] is greater than maximum of <value>	Reduce number in input file or change NMAX and recompile.
5090	The number of [DAYS IN OUTPUT AVG. PERIOD] is greater than maximum of <value>	Reduce number in input file or change NPMAX and recompile.
5100	The number of [REQUESTED OUTPUT CDFS] is greater than maximum of <value>	Reduce number in input file or change NCMAX and recompile.
5110	First element for horizon [<value>] not found	The PRZM horizon value provided for a variable defined in the Monte Carlo input file is probably invalid (does not match the PRZM horizon/element number description provided in the PRZM file).
6010	INFIL subroutine. (d+hf)*dw ≤ 0	The solution of the integrated Green-Ampt equation requires (d+hf)*dw > 0 (see equations 6.121 and 6.19). Execution is halted.
6020	Subroutine INFIL. Value out of range.	See discussion in the PRZM manual regarding the Green-Ampt equation. The variable *z* is outside the range of $-e^{-1} \leq z < 0$. Execution is halted.

Table 11.1 PRZM-3 Error Messages, Warnings, and Troubleshooting Approaches		
	Error or Warning	**Troubleshooting Approach/Explanation**
6120	Subroutine Get_Crop_Params: Crop Height is outside the nominal range 0.0 m < ZCH < 25 m.	See discussion in the PRZM manual regarding the Volatilization Flux. Execution is halted.
6130	ITFLAG [#] was not 0, 1 or 2.	See PRZM input file record 20. Execution is halted.
6140	MSFLG(n_1) [n_2] was not 1 or 2.	See PRZM input file record 32B. Execution is halted.
6150	Errors detected. PRZM stopped.	Several fatal errors were detected. Execution is halted.

Table 11.2 EXESUP Program Variables

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
BASEND	--	Scalar	Number of bottom PRAM node within a given PRZM zone.	EXESUP	--	M
BOTFLX	cm day^{-1}	Array	Water flux from VADOFT base node for each timestep.	EXESUP	VADSTO	M
DAFLUX	q cm^{-2}	Array day^{-1}	Dispersive-advective flux at each PRZM node in each zone for each chemical (positive).	EXESUP	PRZSTO	M
DAVFLX	ppm cm day^{-1}	Array	Nodal values of dispersive advective flux from VADOFT.	EXESUP	VADSTO	M
DISUNS	ppm (q cm^{-3})	Array	Temporary storage of VADOFT (or PRZM) nodal concentrations for mass correction computations.	EXESUP	--	M
EDAT	--	Array	Ending day, month, year of PRZM simulation.	EXESUP	--	M
FLOSIM	--	Logical	Flow simulation indicator.	EXESUP	--	M
ICHEM	--	Scalar	Counter for number of chemicals.	EXESUP	--	M
IDAY~~O~~	--	Scalar	Starting day of PRZM simulation.	EXESUP	--	M
ILDLT	--	Scalar	Counter for PRZM or VADOFT timesteps.	EXESUP	--	M
IMON~~O~~	--	Scalar	Starting month of PRZM simulation.	EXESUP	--	M
IPRZM	--	Scalar	Counter for number of PRZM zones.	EXESUP	--	M
IPZONE	--	Scalar	Counter for VADOFT zones.	EXESUP	--	M
IYR~~O~~	--	Scalar	Starting year of PRZM simulation.	EXESUP	--	M
LLSTS	days	Scalar	Number of days in final timestep.	EXESUP INITEM	--	I O
NCHEM	--	Scalar	Number of chemicals.	EXESUP INPREA INITEM	--	I I O

Table 11.2 EXESUP Program Variables

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NDAYS	days	Scalar	Number of days in a timestep minus one.	EXESUP	--	M
NLDLT	--	Scalar	Number of PRZM or VADOFT timesteps.	EXESUP INPREA INITEM	--	I I O
NP	--	Scalar	Total number of nodes.	EXESUP	CONTR2	I
NPNARY	--	Array	Number of VADOFT nodes in all VADOFT zones.	EXESUP	--	M
NPRZM	--	Scalar	Number of PRZM zones.	EXESUP INPREA INITEM	--	I I O
NPV	--	Scalar	Number of VADOFT nodes in a given zone.	EXESUP	--	I
NPZONE	--	Scalar	Number of VADOFT zones.	EXESUP INPREA INITEM	--	I I O
NPZ	--	Scalar	Temporary storage for the amount number of PRZM or VADOFT nodes.	EXESUP	--	M
PINT	L M/L^3	Array	VADOFT corrected values of head or concentration.	EXESUP	VADSTO	M
PRZMON	--	Logical	PRZM on indicator.	EXESUP INPREA INITEM	--	I I O
PRZMPF	q cm^{-2} day^{-1}	Array	Daily chemical flux from the base of PRZM.	EXESUP	PRZSTO	M
PRZMWF	cm day^{-1}	Array	Daily water flux from the base of PRZM.	EXESUP	PRZSTO	M
P2VWHT	--	Array	Weighting factors for transfer of water or chemical flux from PRZM to VADOFT.	EXESUP	ZONWHT	M
REDAT	--	Array	Ending day, month, year of PRZM simulation within a timestep.	EXESUP	--	M
RSDAT	--	Array	Starting day, month, year of PRZM simulation within timestep.	EXESUP	--	M

Table 11.2 EXESUP Program Variables

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
RSTFG	--	Scalar	PRZM restart flag, 1 if first time through, 2 thereafter.	EXESUP	--	M
SAVCNC	ppm	Array	Concentrations at each VADOFT node from previous timestep.	EXESUP	VADSTO	M
SAVHED	cm	Array	Previous timestep VADOFT heads by node	EXESUP	VADSTO	M
SDAT	--	Array	Starting day, month, year of PRZM simulation	EXESUP	--	M
TOPFLX	cm day^{-1} (g cm^{-2} day^{-1})	Array	Weighted water (or pesticide) flux leaving the base of PRZM.	EXESUP	VADSTO	M
TOWFLX	cm day^{-1}	Array	Water flux from PRZM to top of VADOFT for each timestep.	EXESUP	VADSTO	M
TRNSIM	--	Logical	Indicator for flow and transport simulation.	EXESUP INPREA INITEM	--	I I O
VADFON	--	Logical	VADOFT on indicator.	EXESUP INPREA INITEM	--	I I O
VD2TC	--	Array	VADOFT correction factors for converting from dissolved to total solute concentration	EXESUP	VADSTO	M
WHGT	--	Scalar	Temporary variable for storing flux weighting factors.	EXESUP	--	M
ZPESTR	g cm^{-2} day^{-1}	Array	PRZM chemical flux by zone, compartment, time period, and chemical.	EXESUP	PRZSTO	M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
A	day^{-1}	Array	Lower Diagonal Element of Solution Matrix (I-1)	SLPEST TRDIAG	PEST	O I
AAA	cm^{-1}	Scalar	A Variable Used to Calculate the Average Temperature Gradient in the Top Compartment	SLTEMP		M
ABSOIL	fraction	Scalar	Daily Value of Soil Surface Albedo	SLTEMP		M
AD	day^{-1}	Array	Soil Horizon Drainage Parameter	READ ECHO INITL HYDR2	HYDR	O I I I
ADFLUZ	$g\ cm^{-2}\ day^{-1}$	Array	Advective Flux of Pesticide	SLPEST MASBAL OUTPST OUTTSR	PEST	O I I I
ADL	day^{-2}	Scalar	Lateral Drainage Time Constant	READ ECHO INITL HYDR2	HYDR	O I I I
ADS	$mg\ kg^{-1}$	Array	Adsorbed Portion of Pesticide in Each Compartment	OUTCNC		
AFIELD	ha	Scalar	Area of Field	READ EROSN	HYDR	O
AINF	cm	Array	Percolation Into Each Soil Compartment	HYDROL HYDR1 HYDR2	HYDR	O I I
AIRDEN	$gm\ cm^{-3}$	Scalar	Density of Air at Ambient Temperature	SLTEMP		M
AIRLMD	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Scalar	Thermal Conductivity of Air	SLTEMP		
AKAY	--	Array	K-Factor in the Soil Thermal Conductivity Equation	SLTEMP		M
ALAMDA	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Array	Thermal Conductivity of Soil Constituent	SLTEMP		
ALBEDO	fraction	Array	Soil Surface Albedo at Start of Each Month	READ SLTEMP	MET	O I
AMXDR	cm	Scalar	Maximum Rooting Depth of Each Crop	READ INITL PLGROW	CROP	O I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
ANETD	cm	Scalar	Minimum Depth from Which ET is Extracted Year Around	READ INITL	CROP	O I
ANUM	cm	Scalar	Total Available Water in Profile	EVPOTR		
APD	--	Scalar	Day of Month of Pesticide Application	READ		
APDEP	cm	Scalar	Depth of irrigation water applied to soil	IRRIG	--	O
APM	--	Scalar	Month of Pesticide Application	READ		
ATEMP	°C	Array	Air Temperature	Main		O
AVSTOR	$cm^3\ cm^{-3}$	Scalar	Available Water Storage	HYDR2		
AW	--	Scalar	Fraction of Soil Voids Occupied by Water	EVPOTR		
B	day^{-1}	Array	Diagonal Element of Solution Matrix (I)	SLPEST	PEST	O
BBB	$°K\ cm^{-1}$	Scalar	A Variable Used to Calculate the Average Temperature Gradient in the Top Compartment	SLTEMP		M
BBT	°C	Array	Bottom Boundary Temperature at Start of Each Month	READ SLTEMP	MET	O I
BD	$g\ cm^{-3}$	Array	Mineral Soil Bulk Density	SLTEMP	HYDR	I
BDFLAG	--	Scalar	Bulk Density Flag (0 = Whole Soil BD Entered, 1 = Mineral BD and OC Entered)	READ ECHO INITL		O I I
BFLO	cm	Array	Monthly Baseflow Runoff Accumulated for Output Table	OUTHYD	TABLE	O
BT	m	Scalar	Bottom width of furrows	FURROW IRREAD	IRGT	I
C	day^{-1}	Array	Upper Diagonal Element of Solution Matrix (I+1)	SLPEST TRDIAG	PEST	O I
CB	$kg\ ha^{-1}$	Scalar	Cumulative Pesticide Balance Error	OUTPST		
CC	g	Array	Total mass associated with a moving point	MOC1 INITL	PEST	M
CELLBG	--	Scalar	First location in a compartment	INITL		M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
CEVAP	cm	Scalar	Current Daily Canopy Evaporation Depth	EVPOTR MASBAL OUTHYD OUTTSR	HYDR	O I I I
CFLAG	--	Scalar	Conversion Flag for Initial Pesticide Input	READ INITL	MISC	O I
CHANGE	g	Array	Change in total pesticide mass per compartment	MOC1		M
CINT	cm	Scalar	Current Crop Interception Storage	INITL HYDROL EVPOTR MASBAL OUTHYD OUTTSR	HYDR	O I I I I I
CINTB	cm	Scalar	Crop Interception From Previous Time Step	PMAIN MASBAL OUTHYD	HYDR	O I I
CINTCP	cm	Array	Maximum Interception Storage of Each Crop	READ ECHO PLGROW	CROP	O I I
CLAY	percent	Array	Percent Clay in Each Soil Horizon	SLTEMP	HYDR	I
CONC	--	Alpha - numeric	Flag for Output of Soil Pesticide Concentration Profile	PMAIN		
CONDUC	cm day^{-1}	Scalar	Canopy Conductance Including Boundary Layer's Conductance	MAIN SLPST0 SLPST1	PEST	O I I
CONST	--	Scalar	Constant Values Used to Multiply Each Time Series Output	READ ECHO OUTTSR		O I I
CORED	cm	Scalar	Total Depth of Soil Profile	READ ECHO INITL	HYDR	O I I
COVER	fraction	Scalar	Current Areal Cover of Crop Canopy	SLTEMP	CROP	I
COUNT	--	Array	Number of moving points in a compartment	MOC1		M
COVMAX	fraction	Array	Maximum Areal Coverage of Each Crop at Full Canopy Development	READ ECHO INITL PLGROW	CROP	O I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
CN	--	Array	Runoff Curve Numbers for Antecedent Soil Moisture Condition II	READ ECHO HYDROL	HYDR	O I I
CNCPOND	g cm^{-3}	Scalar	Concentration of pesticide in inflowing water	MOC1 INITL	PEST	I
CNDBDY	cm day^{-1}	Scalar	Boundary Layer's Conductance	MAIN		O
CNDM	--	Array	Accumulated Number of Days in Each Month (With and w/o Leap Year)	PMAIN		
CNDMO	--	Array	Accumulated Number of Days in Each Month	SLTEMP	MISC	I
CPBAL	g cm^{-2}	Scalar	Cumulative Pesticide Balance Error	MASBAL OUTPST	PEST	M I
CRC	day m^{-1}	Array	Canopy Resistance	CANOPY		O
CRCNC	day m^{-1}	Array	Canopy Resistance	MAIN OUTPST	PEST	O I
CTOT	g	Scalar	Concentration of consolidated points	MOC	-	M
CURVN	--	Scalar	Current Value of Runoff Curve Number	HYDROL		
CWBAL	cm	Scalar	Cumulative Water Balance Error	MASBAL OUTHYD	HYDR	O I
D	m	Scalar	Zero Displacement Height	CANOPY SLTEMP		O M
DAIR	cm^2 day^{-1}	Scalar	Molecular Diffusivity in the Air	ECHO MAIN READ SLPST0 SLPST1	PEST	I I O I I
DAY	--	Alpha-numeric	Flag for Daily Output of Water or Pesticide Summary	PMAIN		
DELT	day	Scalar	Time Step	INITL HYDR2 PLPEST SLPEST MASBAL	MISC	O I I I I
DELTA	°K	Scalar	Convergence Criteria in the Newton-Raphson Solution Technique	SLTEMP		M
DELX	cm	Array	Compartment Thickness	SLTEMP	HYDR	I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
DELXSQ	cm^{-2}	Scalar	Compartment Thickness Squared	INITL SLPEST	HKYDR	O
DEN	--	Array	Point density. The number of points in the horizon divided by the depth of the horizon.	INITL	HYDR	M
DENOM	cm	Scalar	Total Voids in the Soil Profile	EVPOTR		
DENOM	$cm\ hr^{-1}$	Scalar	Available Water for Runoff During a Storm	EROSN		
DEPI	cm	Array	Depth of Pesticide Incorporation	READ ECHO PESTAP	PEST	O I
DFFLUX	$g\ cm^{-2}\ day^{-1}$	Array	Diffusive/Dispersive Flux of Pesticide Leaving Each Soil Compartment	SLPEST OUTPST OUTTSR	PEST	O I I
DGAIR	$cm^2\ day^{-1}$	Array	Molecular Diffusivity in the Soil Air Pore	SLPST0 SLPST1		I I
DGRATE	day^{-1}	Array	First Order Decay Rate for Vapor-Phase Pesticide	ECHO INITL READ SLPST0 SLPST1	PEST	I I O I I
DIFFCH	$m^2\ day^{-1}$	Scalar	Eddy Diffusivity at Canopy Height	CANOPY		O
DIFFCO	$cm^2\ day^{-1}$	Array	Diffusivity of Soil Compartment	SLTEMP		M
DIFK	$m^2\ day^{-1}$	Scalar	Eddy Diffusivity	CANOPY		O
DIN	cm	Scalar	Current Plant Canopy Interception Potential	PLGROW HYDROL OUTHYD	HYDR	O I I
DISP	$cm^2\ day^{-1}$	Array	Dispersion/Diffusion Coefficient	READ ECHO INITL SLPEST	PEST	O I I I
DISS	$mg\ l^{-1}$	Array	Dissolved Portion of Pesticide in Each Compartment	OUTCNC		
DKFLUX	$g\ cm^{-2}$	Array	Decay Flux of Pesticide From Each Compartment	SLPEST MASBAL OUTPST OUTTSR	PEST	O I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
DKRATE	day^{-1}	Array	Pesticide Decay Rate in Each Soil Horizon	READ ECHO INITL SLPEST	PEST	O I I I
DKRT12	day^{-1}	Array	Transformation Rate from Parent Pesticide to First Daughter Product	ECHO READ INITL PSTLNK	PEST	I O O I
DKRT13	day^{-1}	Array	Transformation Rate from Parent Pesticide to Second Daughter Product	ECHO READ INITL PSTLNK	PEST	I O O I
DKRT23	day^{-1}	Array	Transformation Rate from First Daughter Product to Second Daughter Product	ECHO READ INITL PSTLNK	PEST	I O O I
DOM	--	Scalar	Number of Current Day of Month of Simulation	SLTEMP	MISC	I
DPN	cm	Array	Layer Depth in Each Horizon	ECHO READ	HYDR	I O
DT	hr	Array	Average Hours of Daylight for a Day Falling in Each Month	READ ECHO EVPOTR	MET	O I I
DVF	kg ha^{-1} day^{-1}	Scalar	Daily Foliage Pesticide Volatilization Flux	OUTPST		O
DW	Fraction	Scalar	Available porosity in soil column	IRRIG FURROW	IRGT	O
DX	m	Scalar	Spatial stop used in furrow finite difference model	FURROW IRRIG	IRGT	M I
EF	kg ha^{-1}	Scalar	Daily Erosion Flux	OUTPST		
ELTERM	day^{-1}	Scalar	Erosion Loss Term for Pesticide Balance	EROSN SLPEST	PEST	O I
EMD	--	Scalar	Day of Month of Crop Emergence	READ ECHO		
EMM	--	Scalar	Month of Crop Emergence	READ ECHO		
EMMISS	fraction	Scalar	Infrared Emissivity of Soil Surface	READ SLTEMP	MET	O I
EN	--	Scalar	Manning's roughness coefficient for furrows	FURROW IRREAD	IRGT	I O

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
ENDYEAR	--	Scalar	Ending Year of Simulation Used to Loop for Output Table	INITEM	TABLE	O
ENP	Kcal $mole^{-1}$	Scalar	Enthalpy of Vaporization	KHCORR		
ENPY	Kcal $mole^{-1}$	Array	Enthalpy of Vaporization	ECHO MAIN READ	PEST	I I O
ENRICH	--	Scalar	Enrichment Ratio for Organic Matter	EROSN		
ERFLAG	--	Scalar	Erosion Flag (0 = Not Calculated, 1 is Not Used, 2 = Calculated by MUSLE, 3 = Calculated by MUST, 4 = Calculated by MUSS)	READ PMAIN	HYDR	O I
ERFLUX	g cm^{-2}	Scalar	Erosion Flux of Pesticide From Soil Surface	SLPEST MASBAL OUTPST	PEST	O I I
ERPST	g cm^{-2}	Array	Total Erosion Pesticide Load Used for Output Table	OUTPST OUTNIT	TABLE	O O
EVAP	cm day^{-1}	Scalar	Daily Evaporation from the Top 5 cm of Soil After Adjusting for Crop evapotranspiration	SLTEMP		M
EVPO	cm	Array	Monthly Evapotranspiration Accumulated for Output Table	OUTHYD	TABLE	O
EXTRA	cm^3 cm^{-3}	Scalar	Extra Water Occurring in a Compartment Over the Allowed Saturation Amount	OUTTSR HYDR2		I
F	g cm^{-2} day^{-1}	Array	Vector of Source Terms for Each Compartment (Tri-diagonal Matrix)	SLPEST TRDIAG	PEST	O I
F0/	kg ha^{-1}	Scalar	Current Foliar Pesticide Storage	OUTPST		
FAIH	--	Scalar	Stability Function for Sensible Heat	CANOPY		O
FAIM	--	Scalar	Stability Function for Momentum	CANOPY		O
FAM	--	Scalar	Pesticide Application Flag (1= Soil, 2= Linear Foliar, 3= Exponential Foliar)	READ ECHO PESTAP	PEST	O I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
FC	cm	Array	Field Capacity Water Depth in Soil Compartment	INITL EVPOTR	HYDR	O
FCV	--	Array	Regression Coefficients for Prediction of Field Capacity Soil Water Content	THCALLC		
FDAY	--	Scalar	Loop Limit, First Day	PMAIN		
FEXTRC	cm^{-1}	Scalar	Foliar Extraction Coefficient for Foliar Wash off Model	READ ECHO PLPEST	PEST	O I I
FILTRA	$m^2\ kg^{-1}$	Scalar	Filtration Parameter for Exponential Foliar Application Model	READ ECHO PESTAP	PEST	O I I
FIRST	--	Scalar	Index of first point under interface with Ratio greater than 2	MOC	HYDR	M
FL	$kg\ ha^{-1}$	Scalar	Foliar Pesticide Decay Loss	OUTPST		
FLEACH	Fraction	Scalar	Leaching factor, as fraction of soil moisture deficit	IRRIG IRREAD	IRGT	I O
FOLP0/	$g\ cm^{-2}$	Scalar	Foliar Pesticide Storage From Previous Time Step	PLPEST MASBAL OUTPST PMAIN	PEST	O I I I
FP	$kg\ ha^{-1}$	Scalar	Current Daily Foliar Pesticide Storage	OUTPST		
FPDLOS	$g\ cm^{-2}$	Scalar	Current Daily Foliar Pesticide Decay Loss	PLPEST MASBAL OUTPST OUTTSR	PEST	O I I I
FPVLOS	$g\ cm^{-2}\ day^{-1}$	Array	Daily Foliage Pesticide Volatilization Flux	MASBAL OUTPST PLPEST	PEST	I I O
FPWLOS	$g\ cm^{-2}$	Scalar	Current Daily Pesticide Washoff Loss	PLPEST		
FRAC	--	Scalar	Fraction of the Distance a Curve Number is Between Increments of Ten	READ		
FRAC	--	Scalar	Fraction of the Current Crop Growing Season Completed	PLGROW		
FRAC	--	Array	Number of Compartments Available to Extraction of ET	EVPOTR		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
FRACOM	--	Scalar	Fraction of Layer Attributed to the Current Horizon	INITL		
FS	m	Array	Infiltration depth at each station in furrow	FURROW IRRIG	IRGT	O I
FX1	$°K^4$	Scalar	Fourth Order Energy Balance Equation in Terms of Soil Surface Temperature	SLTEMP		M
FX2	$°K^3$	Scalar	Derivative of Energy Balance Equation in Terms of Soil Surface Temperature	SLTEMP		M
GAMMA	--	Array	Pesticide Uptake Efficiency by Plant	PLGROW SLPEST	PEST	O I
GEE	Fraction	Array	Depolarization Factors of Soil Constituent in Three Dimensions	SLTEMP		M
GFLD	Fraction	Scalar	Depolarization Factor of Entrapped Air at Field Capacity Water Content	SLTEMP		M
GRADT	$°C\ m^{-1}$	Scalar	Temperature Gradient	CANOPY		O
GRADW	day^1	Scalar	Wind Speed Gradient	CANOPY		O
HAD	--	Scalar	Day of Month of Crop Harvest	READ ECHO		
HAM	--	Scalar	Month of Crop Harvest	READ ECHO		
HEIGHT	cm	Scalar	Canopy Height	MAIN OUTPST PLGROW SLTEMP	CROP	I I O I
HENRY	$cm^3\ cm^{-3}$	Scalar	Henry's Constant	KHCORR		I
HENRYK	$cm^3\ cm^{-3}$	Array	Henry's Constant	ECHO MAIN READ	PEST	I I O
HF	m	Scalar	Green-Ampt Suction head parameter	FURROW INFIL IRREAD	IRGT	I I O
HGT	m	Scalar	Thickness of Each Layer in the Canopy	CANOPY		O

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
HORIZN	--	Array	Soil Horizon Number	READ ECHO INITL OUTHYD OUTPST OUTCNC	MISC	O I I I I I
HSWZT	--	Scalar	Hydraulics Flag (O= Free Draining Soils, 1= Restricted Drainage)	READ ECHO INITL PMAIN		O I I I
HTEMP	°C	Scalar	Average Air Temperature	CANOPY		O
HTITLE	--	Alpha-numeric	Comment Line to Enter Information about Hydrology Parameters	READ ECHO		
HTMAX	cm	Array	Maximum Canopy Height	ECHO PLGROW READ	CROP	I M O
I	--	Scalar	Loop Counter	SLTEMP KHCORR CANOPY		
IAPDY	--	Array	Julian Day of Pesticide Application	READ ECHO PMAIN	MISC	O I I
IAPYR	--	Array	Year of Pesticide Application	READ ECHO PMAIN	MISC	O I I
IARG	--	Array	Argument of Variable Identified by 'PLNAME’	READ ECHO OUTTSR	MISC	O I I
IARG1	--	Scalar	Argument of Variable Identified by 'PLNAME'	OUTTSR		
IB	--	Scalar	Backward Loop Index	INITL HYDR2		
IBM1	--	Scalar	Counter	INITL		
ICNAH	--	Array	Soil Surface Condition After Harvest	READ ECHO PLGROW	HYDR	O I I
ICNCN	--	Array	Crop Number	READ ECHO INITL	CROP	O I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
ICROSS	--	Scalar	Number of horizon interfaces where points need to be consolidated, i.e. Ratio greater than 2.	INITL MOC	HYDR	M
IDEL	--	Scalar	Number of points which are consolidated	MOC	-	M
IDFLAG	--	Scalar	Flag to Identify if Soil Thermal Conductivity and Heat Capacity are Input or Simulated in the Model	ECHO READ SLTEMP OUTCNC	MET	I O I I
IEDAY	--	Scalar	Ending Day of Simulation	READ PMAIN ECHO	MISC	O I I
IEDY	--	Scalar	Counter	INITL		
IEMER	--	Array	Julian Day of Crop Emergence	READ ECHO INITL PLGROW	CROP	O I I I
IEMON	--	Scalar	Ending Month of Simulation	READ ECHO PMAIN	MISC	O I I
IEND	--	Scalar	Index of point at which consolidation ends	MOC	-	M
IERROR	--	Scalar	Error Flag if Tri-Diagonal Matrix Cannot be Saved	SLPEST TRDIAG		
IEYR	--	Scalar	Ending Year of Simulation	READ ECHO PMAIN	MISC	O I I
IFIRST	--	Scalar	Flag to Print Output Heading and Initialize Output Array	OUTTSR		
IFLO	cm	Array	Monthly Interflow Runoff Accumulated for Output Table	OUTHYD	TABLE	O
IHAR	--	Array	Julian Day of Crop Harvest	READ ECHO INITL PLGROW	CROP	O I I I
II	--	Scalar	Loop Counter	OUTPST		
IJ	--	Scalar	Loop Counter	PMAIN		
ILP	--	Scalar	Initial Level of Pesticide Flag (O= No Pesticide, 1= Initial Pesticide)	READ ECHO	MISC	O I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
INABS	cm	Scalar	Initial Abstraction of Water from Potential Surface Runoff	HYDROL EROSN	HYDR	O I
INCROP	--	Array	Crop Growing in Current Cropping Period	READ ECHO INITL PLGROW OUTHYD OUTPST	CROP	O I I I I
INICRP	--	Scalar	Initial Crop Number if Simulation Starting Date is Before First Crop Emergence Date	READ ECHO INITL	CROP	O I I
INTFC	--	Scalar	Whole Layer(s) Attributed to the Current Horizon	INITL		
IOUT	--	Scalar	Index of first point outside flow domain	MOC1		M
IPEIND	--	Scalar	Pan Evaporation Indicator Flag (O= Data Read In, 1= Calculated)	READ ECHO	MET	O I
IPSCND	--	Scalar	Foliage Pesticide Condition after Harvest: 1. Surface Applied 2. Removed 3. Surface Residue	ECHO PLGROW READ	CROP	O M I
IRTYPE	--	Scalar	Irrigation type flag: 0=No irrigation 1=Flood irrigation 2=Furrow irrigation 3=Over-canopy sprinklers 4=Under-canopy sprinklers 5=Over-canopy without runoff 6=Over-canopy, user-defined rates, with runoff 7=Over-canopy, user-defined rates, without runoff	IRRIG IRREAD	IRGT	I O
ISCOND	--	Scalar	Surface Condition After Harvest Corresponding to 'INICRP'	READ ECHO PLGROW HYDROL EROSN	HYDR	O I I I I
ISDAY	--	Scalar	Starting Day of Simulation	READ ECHO INITL PMAIN	MISC	O I I I
ISDY	--	Scalar	Counter	INITL		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
ISMON	--	Scalar	Starting Month of Simulation	READ ECHO INITL PMAIN	MISC	O I I I
ISTART	--	Scalar	Index of point at which consolidation starts	MOC	-	M
ISTYR	--	Scalar	Starting Year of Simulation	READ ECHO INITL PMAIN	MISC	O I I I
ITEM1	--	Alpha-numeric	Hydrology Output Summary Indicator	READ ECHO OUTHYD	MISC	O I I
ITEM2	--	Alpha-numeric	Pesticide Output Summary Indicator	READ ECHO OUTPST	MISC	O I I
ITEM3	--	Alpha-numeric	Soil Pesticide Concentration Profile Output Indicator	READ ECHO PMAIN	MISC	O I I
ITEMP	°C	Scalar	Mean Daily Temperature Rounded to Next Lowest Whole Number	EVPOTR	MISC	O
ITFLAG	--	Scalar	Soil Temperature Flag	ECHO MAIN OUTCNC READ	MET	I I I O
ITMP	--	Scalar	Number of Compartments Pesticide is Applied to When Incorporated	PESTAP		
IY	--		Annual Loop Counter	PMAIN PLGROW OUTHYD OUTPST OUTTSR OUTCNC		I I I I I I
IYEAR	--	Scalar	Number of Simulation Years Used to Make Output Table	OUTPST OUTHYD OUTNIT		O O O
IYREM	--	Array	Year of Crop Emergence	READ ECHO INITL PLGROW	CROP	O I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
IYRHAR	--	Array	Year of Crop Harvest	READ ECHO INITL PLGROW	CROP	O I I I
IYRMAT	--	Array	Year of Crop Maturation	READ ECHO INITL PLGROW	CROP	O I I I
J	--	Scalar	Loop Counter	PMAIN READ ECHO INITL PLGROW OUTHYD OUTPST		
JJ	--	Scalar	Loop Counter	READ		
JP1	--	Scalar	Counter (J+1)	READ		
JP1T10	--	Scalar	Counter (JP1*10)	READ		
JT10	--	Scalar	Counter (J*10)	READ		
JULDAY	--	Scalar	Julian Day	PMAIN PLGROW OUTHYD OUTPST	MISC	O I I I
K	--	Scalar	Loop Counter	SLTEMP		
KD	$cm^3\ g^{-1}$	Array	Adsorption/partition Coefficient for Soil Compartment	READ ECHO INITL KDCALC PESTAP SLPEST MASBAL OUTPST OUTTSR OUTCNC	PEST	O I I O I I I O I I
KDFLAG	--	Scalar	Partition Coefficient Flag (O= Kd Read In, 1= Kd Calculated)	READ ECHO PMAIN		O I I
KH	$cm^3\ cm^{-3}$	Array	Henry's Constant at Current Time	MAIN SLPST0 SLPST1	PEST	O I I
KK	--	Scalar	Loop Counter	READ		I
KOC	$cm^3\ g^{-1}$ -oc	Scalar	Organic Carbon Partition Coefficient	KDCALC		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
KS	m/s	Scalar	Saturated hydraulic conductivity of soil	FURROW INFIL IRREAD	IRGT	I I O
L	--	Scalar	Loop Counter	SLTEMP		
LA	kg ha^{-1}	Scalar	Daily Lateral Pesticide Flux For Each Pesticide Used for Output Table	OUTPST		O
LATFLX	g cm^{-2} day^{-1}	Array	Daily Lateral Pesticide Flux For Each Pesticide from the Entire Soil Column	INIACC SLPSTO MASBAL OUTPST OUTTSR	PEST	O O I I I
LAYERS	--	Scalar	Number of Layers in Canopy	CANOPY		O
LBTEMP	°C	Scalar	Daily Value of Bottom Boundary Temperature	SLTEMP		M
LDAY	--	Scalar	Loop Limit (Last Day)	PMAIN		
LEAP	--	Scalar	Additional Day Flag for Leap Year	SLTEMP		I
LFREQ1	--	Scalar	Frequency of Soil Compartment Reporting in Water Output Summary	READ OUTHYD	MISC	O I
LFREQ2	--	Scalar	Frequency of Soil Compartment Reporting in Pesticide Output Summary	READ OUTPST	MISC	O I
LFREQ3	--	Scalar	Frequency of Soil Compartment Reporting in Concentration Profile Output Summary	READ OUTCNC	MISC	O I
LL	--	Scalar	Loop counter	MOC1		
LOGD	--	Scalar	Logarithm of Zero Displacement Height	CANOPY		O
LOGKOC	--	Scalar	Natural Log of Koc	KDCALC		
LOGZO	--	Scalar	Logarithm of Roughness Length	CANOPY		O
LTFLUX	g cm^{-2} day^{-1}	Array	Daily Lateral Pesticide Flux For Each Pesticide from Each Soil Compartment	SLPST0 OUTPST	PEST	O I
M	--	Scalar	Loop counter	MOC1		
MAD	--	Scalar	Day of Month of Crop Maturation	READ ECHO		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
MAM	--	Scalar	Month of Crop Maturation	READ ECHO		
MASS	g	Array	Current pesticide mass in compartment	MOC1		M
MASSO	g	Array	Total pesticide mass in each compartment at previous time step	MOC1 INITL	PEST	M
MAT		Array	Julian Day of Crop Maturation	READ ECHO INITL PLGROW	MISC	O I I I
MCFLAG	--	Scalar	Transport solution technique flag (0 = PRZM, 1= MOCPRZM)	ECHO READ PMAIN	PEST	I
MD	--	Scalar	Number of Day Read from Meteorologic File	PMAIN		
MDOUT	kg ha^{-1}	Array	Monthly Pesticide Decay from Each Compartment	OUTPST	ACCUM	M
MEOUTW	cm	Array	Monthly ET from Each Soil Compartment	OUTHYD	ACCUM	M
MINPP	kg ha^{-1}	Array	Monthly Advection/Dispersion Flux from Each Compartment	OUTPST	ACCUM	M
MINPP1	kg ha^{-1}	Scalar	Monthly Foliar Applied Pesticide	OUTPST	ACCUM	M
MINPP2	kg ha^{-1}	Scalar	Monthly Soil Applied Pesticide	OUTPST	ACCUM	M
MINPW	cm	Array	Monthly Infiltration into Each Soil Compartment	OUTHYD	ACCUM	M
MINPW1	cm	Scalar	Monthly Precipitation	OUTHYD	ACCUM	M
MINPW2	cm	Scalar	Monthly Snowfall	OUTHYD	ACCUM	M
MINTH	--	Alpha-numeric	Flag for Monthly Output Summary (for Either Water or Pesticide)	PMAIN		
MLOUT	g cm^{-2} day^{-1}	Array	Monthly Lateral Pesticide Outflow From Each Soil Compartment For Each Pesticide	INIACC OUTPST	ACCUM	O
MM	--	Scalar	Number of Month Read from Meteorologic File	PMAIN		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
MNTHP1	--	Scalar	Current Month Plus 1 (Month + 1)	OUTHYD		
MODFC	--	Scalar	Fraction Multiplier	INITL		
MONTH	--	Scalar	Number of Current Month of Simulation	SLTEMP	MISC	I
MOUTP	kg ha^{-1}	Array	Monthly Pesticide Uptake from Each Compartment	OUTPST	ACCUM	M
MOUTP1	kg ha^{-1}	Scalar	Monthly Pesticide Washoff Flux	OUTPST	ACCUM	M
MOUTP2	kg ha^{-1}	Scalar	Monthly Pesticide Runoff Flux	OUTPST	ACCUM	M
MOUTP3	kg ha^{-1}	Scalar	Monthly Pesticide Erosion Flux	OUTPST	ACCUM	M
MOUTP4	kg ha^{-1}	Scalar	Monthly Foliar Pesticide Decay Loss	OUTPST	ACCUM	M
MOUTP5	kg ha^{-1}	Scalar	Monthly Pesticide Uptake Flux from Profile	OUTPST	ACCUM	M
MOUTP6	kg ha^{-1}	Scalar	Monthly Pesticide Decay	OUTPST	ACCUM	M
MOUTP9	g cm^{-2} day^{-1}	Array	Monthly Lateral Pesticide Outflow From the Entire Soil Column For Each Pesticide	INIACC OUTPST	ACCUM	O
MOUTW	cm	Array	Monthly Exfiltration from Each Compartment	OUTHYD	ACCUM	M
MOUTW1	cm	Scalar	Monthly Canopy Evaporation	OUTHYD	ACCUM	M
MOUTW2	cm	Scalar	Monthly Thrufall	OUTHYD	ACCUM	M
MOUTW3	cm	Scalar	Monthly Runoff	OUTHYD	ACCUM	M
MOUTW4	cm	Scalar	Monthly Snowmelt	OUTHYD	ACCUM	M
MOUTW5	cm	Scalar	Monthly Evapotranspiration	OUTHYD	ACCUM	M
MOUTW6	MTonne	Scalar	Total Monthly Sediment Loss	OUTHYD	ACCUM	
MSTART	--	Scalar	Flag for Positioning Meteorologic File	PMAIN		
MSTR	cm	Array	Previous Month Storage of Water in Each Soil Compartment	OUTHYD	ACCUM	M
MSTR1	cm	Scalar	Monthly Canopy Interception	OUTHYD	ACCUM	M
MSTR2	cm	Scalar	Monthly Accumulation of Snow	OUTHYD	ACCUM	M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
MSTRP	kg ha^{-1}	Array	Storage of Pesticide from Previous Month in Each Soil Compartment	OUTPST	ACCUM	M
MSTRP1	kg ha^{-1}	Scalar	Storage of Foliar Pesticide from Previous Month	OUTPST	ACCUM	M
MY	--	Scalar	Number of Year Read from Meteorologic File	PMAIN		
N	--	Scalar	Loop Counter	CANOPY SLTEMP		
NAPPC	--	Scalar	Pesticide Application Counter	PMAINPES TAP	PEST	O I
NAPS		Scalar	Number of Pesticide Applications in the Simulation	READ ECHO INITL PMAIN	PEST	O I I I
NBYR	--	Scalar	Beginning Year of Crop Growth for Current Crop (Loop Limit)	INITL PLGROW		
NCELL	--	Scalar	Compartment number in which a point is located	MOC1 INITL		M
NCOM0/	--	Scalar	Number of Compartments from Which ET is Extracted Year Round	INITL PLGROW	HYDR	O I
NCOM1	--	Scalar	Current Number of Compartments, that ET is Extracted From	PLGROW EVPOTR OUTHYD	HYDR	O I I
NCOM2	--	Scalar	Number of Compartments in Soil Profile	SLTEMP	HYDR	I
NCOM2M	--	Scalar	Number of Compartments in Soil Profile minus 1 (NCOM2 - 1)	INITL SLPEST	HYDR	O I
NCOMRZ	--	Scalar	Number of Compartments in the Root Zone	INITL SLPEST OUTHYD OUTPST	CROP	O I I I
NCP	--	Scalar	Number of Current Cropping Period	INITL PLGROW	CROP	O I
NCPDS	--	Scalar	Number of Cropping Periods in the Simulation	READ ECHO INITL PLGROW	CROP	O I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
NCROP	--	Scalar	Number of Current Crop	INITL PLGROW HYDROL EROSN	CROP	O I I I
NDC	--	Scalar	Number of Different Crops in Simulation	READ ECHO INITL PLGROW	CROP	O I I I
NDCNT	--	Scalar	Number of Days Since Crop Emergence for Current Crop	INITL PLGROW	MISC	O I
NDYRS	--	Scalar	Number of Years Between Emergence and Maturation of a Crop	INITL PLGROW		
NET	g	Array	Net change in mass due to advection	MOC1		M
NEW	--	Scalar	Number of new points entering the flow domain	MOC1		M
NEWK	$cm^3\ cm^{-3}$	Array	Henry's Constant	KHCORR		O
NEXDAY	--	Scalar	Extra Day Added for Leap Year	PLGROW		
NEYR	--	Scalar	Ending Year of Crop Growth for Current Crop	INITL PLGROW		
NHORIZ	--	Scalar	Total Number of Soil Horizons	READ ECHO INITL KDCALC	MISC	O I I I
NLINES	--	Scalar	Numbers of Lines for Listing Initial Pesticides in Profile (Loop Limit)	ECHO		
NM1	--	Scalar	Number of Compartments in Profile Minus 1 (NCOM2 - 1)	TRDIAG		
NOPRT	--	Scalar	Print Flag	OUTHYD OUTPST		
NPI	--	Scalar	Current Number of Moving Points in Soil Profile	MOC1 INITL	HYDR	M
NPLOTS	--	Scalar	Number of Time Series to be Output (Maximum of 7)	READ ECHO PMAIN OUTTSR	MISC	O I I I
NRZCOM	--	Scalar	Current Number of Layers in Root Zone	PLGROW		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
NSPACE	--	Scalar	Number of furrow stations for finite difference	FURROW IRRIG	IRGT	M I
NSUM	--	Scalar	Cumulative Sum of Compartment Numbers	EVPOTR		
NSUMM	--	Scalar	Termination Loop Index for Summary Output	OUTHYD OUTPST		
NUM	--	Scalar	Number of Soil Compartment	KHCORR		I
NUM	--	Scalar	Initial number of moving points per compartment	MOC1 INITL	HYDR	I
NUMDYS	--	Scalar	Number of Days in a Month	SLTEMP		M
OC	percent	Array	Organic Carbon in Each Soil Horizon	SLTEMP	PEST	I
OKH	$cm^3\ cm^{-3}$	Array	Henry's Constant at Previous Time	INITL MAIN SLPST0 SLPST1	PEST	O I I I
ORGM	percent	Scalar	Organic Matter Content of a Soil Horizon	INITL		
OSNOW	cm	Scalar	Snow Accumulated at the End of the Previous Time Step	PMAIN HYDROL MASBAL	HYDR	O I I
OUTFLO	$cm\ day^{-1}$	Array	Lateral Outflow of Water from Each Soil Compartment	OUTSTR		O
OUTPUT	--	Array	Output Array for Time Series	OUTTSR		
PA	$kg\ ha^{-1}$	Scalar	Daily Foliar Pesticide Application	OUTPST		
PB	$kg\ ha^{-1}$	Scalar	Pesticide Balance	OUTPST		
PBAL	$g\ cm^{-2}$	Scalar	Current Pesticide Balance Error	MASBAL OUTPST	PEST	O
PCDEPL	Fraction	Scalar	Fraction of available water capacity where irrigation is triggered (range 0.0 - 0.9)	IRRIG IRREAD	IRGT	I O
PCMC	--	Scalar	Partition Coefficient Model Flag (1= Karick hoff, 2= Kenega, 3= Chiou)	READ KDCALC	MISC	O I
PCOUNT	--	Array	Number of points crossing an interface with Ratio greater than 2.	INITL MOC	HYDR	M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
PESTR	g cm^{-2}	Array	Total Pesticide in Each Soil Compartment	READ ECHO INITL PMAIN PESTAP MASBAL OUTPST	PEST	O I I I I I I
PET	cm	Scalar	Total Daily Potential Evapotranspiration	EVPOTR		
PETP	cm	Scalar	Running Total of Available Evapotranspiration	EVPOTR		
PEVP	cm	Scalar	Pan Evaporation	PMAIN EVPOTR	MET	O I
PFAC	--	Scalar	Pan Factor for ET	READ ECHO EVPOTR	MET	O I I
PI	--	Scalar	3.1415926	CANOPY		
PLDKRT	day^{-1}	Array	Foliar Pesticide Decay Rate	READ ECHO PLPEST	PEST	O I I
PLNAME	--	Alpha-numeric	Time Series Output Identifier (Options Listed in User's Guide)	READ OUTTSR	MISC	O I
PLNTAP	g cm^{-2}	Scalar	Pesticide Applied to Crop Canopy	PESTAP OUTPST OUTTSR	PEST	O I I
PLVKRT	day^{-1}	Array	Foliage Pesticide Volatilization Rate	ECHO PLPEST READ	PEST	I I O
PNBRN	--	Array	Output Array for Time Series	OUTTSR		
PRDPTH	cm	Scalar	Depth Used in the Extraction of Pesticide Flux in Runoff	SLPST0 SLPST1		M M
PRECIP	cm	Scalar	Precipitation	PMAIN HYDROL EROSN MASBAL OUTHYD OUTTSR	MET	O I I I I I
PTEMP	g cm^{-3}	Array	Temporary storage of total pesticide mass per cc water after advection step	MOC1		M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
PTITLE	--	Alpha-numeric	Comment Line to Input Information About Pesticide Parameters	READ ECHO	MISC	O I
PVFLUX	g cm^{-2} day^{-1}	Array	Daily Soil Pesticide Volatilization Flux	MASBAL OUTPST OUTRPT OUTTSR SLPST0 SLPST1	PEST	I I I I O O
PWIND	m day^{-1}	Array	Wind Velocity	MAIN		O
Q	m^3	Scalar	Runoff Volume	EROSN		
QC1	cal cm^{-2} day^{-1} °K^{-1}	Scalar	Sensible Heat Flux Term	SLTEMP		M
QEVF	cal cm^{-2} day^{-1}	Scalar	Evaporation Heat Flux	SLTEMP		M
QGHF	cal cm^{-1} day^{-1} °K^{-1}	Scalar	Soil Heat Flux Term	SLTEMP		M
QLW1	cal cm^{-2} day^{-1} °K^{-4}	Scalar	Atmospheric Longwave Radiation Component Term	SLTEMP		M
QLW2	cal cm^{-2} day^{-1} °K^{-1}	Scalar	Longwave Radiation Flux Term Emitted by Soil Surface	SLTEMP		M
QO	m^3/s	Scalar	Flow rate entering head of furrow	FURROW IRREAD	IRGT	I O
QQP	m^6 sec^{-1}	Scalar	Runoff Energy Factor	EROSN		
QS	m^3/s	Array	Flow rate in furrow at each downstream station	FURROW	IRGT	M
QSWR	cal cm^{-2} day^{-1}	Scalar	Net Shortwave Radiation Flux Term	SLTEMP		M
RAIN	cm	Array	Monthly Precipitation Accumulated for Output Table	OUTHYD	TABLE	O
RATIO	--	Array	The ratio of point densities between adjacent horizons	INITL MOC	HYDR	M
RETEAP	cm/hr	Scalar	Maximum rate of water that sprinklers can deliver	IRRIG IRREAD	IRGT	I O
RF	kg ha^{-1}	Scalar	Pesticide Runoff Flux	OUTPST		
RINUM	--	Scalar	Richardson Number	CANOPY		O
RMULT	--	Scalar	Multiplication Factor for Time Series Output	OUTTSR		

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
RMULT1	--	Scalar	Multiplication Factor for Curve Number AMC I	READ		
RMULT3	--	Scalar	Multiplication Factor for Curve Number AMC III	READ		
RNSUM	--	Scalar	Converts NSUM to a Real Number	EVPOTR		
RNUM	ha cm^{-2}	Scalar	Numerator of Peak Runoff Rate	EROSN		
RODPTH	--	Scalar	Number of Soil Compartments that Affect Runoff	HYDROL		
ROFLUX	g cm^{-2} day^{-1}	Scalar	Runoff Flux of Pesticide From Land Surface	SLPEST MASBAL OUTHYD OUTTSR	PEST	O I I I
ROPST	g cm^{-2}	Array	Total Runoff Pesticide Load Used for Output Table	OUTPST	TABLE	O
RTR	day^{-1}	Array	Transformation Term from Daughter Product Consideration	PSTLNK SLPST0 SLPST1	PEST	O I I
RUNOF	cm	Scalar	Current Runoff Depth	HYDROL PMAIN EROSN SLPEST MASBAL OUTHYD OUTTSR	HYDR	O I I I I I I
RVEL	--	Array	Retarded solute velocity	MOC1		M
RZD	cm	Scalar	Maximum Root Zone Depth for All Crops	INITL OUTHYD		
RZFLUX	g cm^{-2}	Scalar	Dispersive/Advective Flux of Pesticide Past the Bottom Root Zone Compartment	SLPEST OUTTSR	PEST	O I
RZI	--	Scalar	Active Root Zone Flag	INITL PLGROW	MISC	O I
SA	kg ha^{-1}	Scalar	Application of Pesticide to the Soil	OUTPST		
SAIM	--	Scalar	Integrated Momentum Stability Parameter	CANOPY		O
SAND	percent	Array	Percent Sand in Each Soil Horizon	SLTEMP	HYDR	I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
SD	kg ha^{-1}	Scalar	Sum of the Decay Fluxes From All Compartments in Soil Profile	OUTPST		
SDKFLX	g cm^{-2} day^{-1}	Scalar	Sum of the Decay fluxes From All Compartments in Soil Profile	SLPEST OUTPST	PEST	O I
SEDI	kg ha^{-1}	Array	Monthly Erosion Accumulated For Output Table	OUTHYD	TABLE	O
SEDL	MTonne day^{-1}	Scalar	Erosion Sediment Loss	PMAIN EROSN OUTHYD	HYDR	O M O
SF	Fraction	Scalar	Slope of furrow channel (vertical/horizontal)	FURROW IRREAD	IRGT	I O
SFAC	cm $°C^{-1}$	Scalar	Snowmelt Factor	READ ECHO HYDROL	MET	O I I
SIGMA0	--	Scalar	Summation Variable Used to Calculate K Factor in the Soil Thermal Conductivity Equation	SLTEMP		M
SIGMA1	cal cm^{-1} $°C$ day^{-1}	Scalar	Total Numerator Value in the Soil Thermal Conductivity Equation	SLTEMP		M
SIGMA2	--	Scalar	Total Denominator Value in the Soil Thermal Conductivity Equation	SLTEMP		M
SJDAY	--	Scalar	Starting Day of Simulation	INITL		
SLKGHA	kg ha^{-1} day^{-1}	Scalar	Erosion Sediment Loss	EROSN		
SMDEF	cm	Scalar	Soil moisture deficit requiring irrigation	IRRIG	IRGT	O
SMELT	cm	Scalar	Current Daily Snowmelt Depth	HYDROL EROSN OUTHYD	HYDR	O
SNOW	cm	Scalar	Snowpack Accumulation Depth	SLTEMP	HYDR	I
SNOWFL	cm	Scalar	Current Snowfall Depth	HYDROL MASBAL OUTHYD OUTTSR	MET	O I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
SOILAP	g cm^{-2}	Array	Pesticide Applied to the Soil	PESTAP PMAIN OUTPST OUTTSR	PEST	O I I I
SOL	mole fraction mg 1^{-1} umoles 1^{-1}	Scalar	Pesticide Solubility - Karickhoff Model Kenaga Model Chiou Model	READ KDCALC		O I
SOLRAD	cal cm^{-2} day^{-1}	Scalar	Shortwave Solar Radiation	READ SLTEMP	MET	O I
SPESTR	g cm^{-3}	Array	Dissolved Pesticide in Each Soil Compartment	INITL PMAIN PESTAP SLPEST	PEST	O I I I
SPT	°C	Array	Temperature of Soil in Each Compartment	SLTEMP MAIN	MET	O I
SPTEMP	g cm^{-3}	Array	Temporary storage of dissolved pesticide mass per cc water after advection step	MOC1 SLPST1 INITL	PEST	M
SRC	g cm^{-3} day^{-1}	Array	Source Term from Daughter Product Consideration	PSTLNK SLPST0 SLPST1	PEST	O I I
SRCFLX	g cm^{-2} day^{-1}	Array	Source Flux of Pesticide from Each Soil Compartment	SLPST0 SLPST1 OUTPST	PEST	O O I
STARTYR	--	Scalar	Starting Year of Simulation Used to Loop for Output Table	INITEM OUTPST OUTHYD	TABLE	O I I
STEMP	°C	Array	Soil Compartment Temperature	KHCORR		I
STEP1	--	Alpha-numeric	Time Step of Water Output Summary	READ ECHO OUTHYD	MISC	O I I
STEP2	--	Alpha-numeric	Time Step of Pesticide Output Summary	READ ECHO OUTPST	MISC	O I I
STEP3	--	Alpha-numeric	Time Step of Concentration Profile Output Summary	READ ECHO OUTCNC	MISC	O I I
STITLE	--	Alpha-numeric	Comment Line to Input Information About Soil Parameters	READ ECHO	MISC	O I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
STK	°K	Scalar	Soil Surface Temperature in Kelvin Scale	SLTEMP		M
STTDET	cm day^{-1}	Scalar	Daily Evaporation from the Top 5cm of Soil	SLTEMP EVPOTR	MET	I O
SU	kg ha^{-1}	Scalar	Sum of the Uptake Fluxes From All Soil Compartments	OUTPST		
SUMC	g	Array	Sum of mass in a compartment	MOC1		M
SUMXP	kg ha^{-1}	Scalar	Sum of Soluble Pesticide in Profile	OUTPST		
SUPFLX	g cm^{-2} day^{-1}	Scalar	Sum of the Uptake Fluxes From All Soil Compartments	SLPEST OUTPST OUTTSR	PEST	O I I
SURF	cm	Array	Monthly Surface Runoff Accumulated for Output Table	OUTHYD	TABLE	O
SV	kg ha^{-1} day^{-1}	Scalar	Daily Soil Pesticide Volatilization Flux	OUTPST		O
SW	cm	Array	Current Water Depth in Each Soil Compartment	INITL HYDROL EVPOTR HYDR1 HYDR2 SLPEST OUTTSR	HYDR	O I I I I I I
T	--	Scalar	Fraction Compartment Check	INITL		
TA	day^{-1}	Array	Lower Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TAPP	g cm^{-2}	Array	Total Pesticide Applied Per Application	READ ECHO INITL PESTAP	PEST	O I I I
TB	day^{-1}	Array	Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TC	day^{-1}	Array	Upper Diagonal Element of Tridiagonal Matrix	SLTEMP		M
TCNC	g cm^{-3}	Array	Average Pesticide Concentration in Canopy	OUTPST		O
TCORR	mole cal^{-1}	Scalar	Temperature Correction Factor	KHCORR		M
TEMP	°C	Scalar	Ambient Air Temperature	SLTEMP	MET	I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
TEMPK	K	Scalar	Air Temperature in Kelvin Scale	SLTEMP		M
TEND	day	Scalar	Time required for point to move to compartment boundary	MOC1		M
TERM	--	Scalar	Exponential Pesticide Washoff Term	PLPEST		
TERM1	--	Scalar	Exponential Pesticide Decay Term	PLPEST		
TERM2	--	Scalar	Product of Washoff and Decay Terms	PLPEST		
EF	°C	Array	Vector of Previous Time Step Soil Compartment Temperature	SLTEMP		M
IFLO	cm	Array	Monthly Total Runoff Accumulated for Output Table	OUTHYD	TABLE	O
FRAC	--	Scalar	Total Fraction of Compartments Available for Evapotranspiration Extraction	EVPOTR		
THEIR	$cm^3\ cm^{-3}$	Array	Volumetric Air Content	SLPST0 SLPST1		O
THCOND	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Array	Thermal Conductivity of Soil Compartment	SLTEMP		M
THEFC	$cm^3\ cm^{-3}$	Array	Field Capacity Water Content for Each Soil Horizon	SLTEMP	HYDR	I
THETAS	$cm^3\ cm^{-3}$	Array	Soil Compartment Water Content at Saturation	SLTEMP	HYDR	I
THETH	$cm^3\ cm^{-3}$	Scalar	Soil Moisture Content Half Way Between Wilting Point and Field Capacity in the Top Soil Compartments	INITL HYDROL	HYDR	O I
THETN	$cm^3\ cm^{-3}$	Array	Soil Water Content at the End of the Current Day for Each Soil Compartment	HYDR1 HYDR2 PMAIN SLPEST MASBAL OUTHYD OUTPST OUTTSR OUTCNC	HYDR	O O I I I I I I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
THETO	$cm^3\ cm^{-3}$	Array	Soil Water Content at the End of the Previous Day for Each Soil Compartment	SLTEMP	HYDR	I
THEWP	$cm^3\ cm^{-3}$	Array	Wilting Point Water Content for Each Soil Horizon	SLTEMP	HYDR	I
THFLAG	--	Scalar	Soil Water Content Flag (O= Field Capacity and Wilting Point are Input, 1= Field Capacity and Wilting Point are Calculated)	READ ECHO PMAIN	MISC	O I I
THKLY1	cm	Scalar	Thickness of Top Compartment	SLTEMP		
THKNS	cm	Array	Soil Horizon Thickness	READ ECHO INITL HYDROL	MISC	O I I I
THRUFL	cm	Scalar	Precipitation that Falls Past the Crop Canopy to the Soil Surface	HYDROL OUTHYD OUTTSR	MET	O I I
THZERO	$cal\ cm^{-1}\ day^{-1}\ °C^{-1}$	Array	Thermal Conductivity of Soil at Water Content and Wilting Point	SLTEMP		M
TITLE	--	Alpha-numeric	Title of the Simulation (User Supplied)	READ ECHO	MISC	O I
TLEFT	day	Scalar	Travel time left in current time step	MOC1		M
TMPK	K	Scalar	Soil Temperature	KHCORR		M
TNDGS	day	Array	Total Number of Days in Each Growing Season	INITL PLGROW	CROP	O I
TOL	--	Scalar	Fraction Compartment Check	INITL		
TOP	--	Array	Location of top compartment in horizon where points are consolidated	INITL MOC	HYDR	M
TOT	$day\ m^{-1}$	Scalar	Canopy Resistance	CANOPY		O
TOTAL	$mg\ kg^{-1}$	Array	Total Pesticide in Each Compartment	OUTCNC		
TOTR	$day\ m^{-1}$	Scalar	Total Canopy Resistance	CANOPY		O
TR	hr	Scalar	Duration of Average Erosive Storm Event	READ ECHO EROSN	MET	O I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
TRFLUX	g cm^{-2} day^{-1}	Array	Transformation Flux of Pesticide from Each Soil Compartment	SLPST0 SLPST1 OUTPST	PEST	O I I
TS	cm^3 cm^{-3}	Array	Previous Soil Compartment Water Content Minus Evapotranspiration	HYDR2		
TSRCFX	g cm^{-2} day^{-1}	Array	Sum of the Source Flux from All Compartments in Soil Profile	SLPST0 SLPST1 OUTPST	PEST	O O I
TSW	cm	Scalar	Total Soil Water in Compartments Available for Evapotranspiration Extraction	EVPOTR		
TTHKNS	cm	Scalar	Total Thickness of Soil Profile (For Computational Check)	INITL		
TTRFLX	g cm^{-2} day^{-1}	Array	Sum of the Transformation Flux from All Compartments in Soil Profile	SLPST0 SLPST1 OUTPST	PEST	O O I
TWLVL	cm cm^{-1}	Scalar	Fraction of Water to Soil Depth for Runoff Calculation	HYDROL		
TWP	cm	Scalar	Total Wilting Point Depth in Compartments Available for Evapotranspiration Extraction	EVPOTR		
U	--	Array	Upper Decomposed Matrix	TRDIAG		
UBT	°C	Scalar	Upper Boundary or Soil Surface Temperature	SLTEMP		M
UPF	kg ha^{-1}	Scalar	Daily Pesticide Uptake Flux in Profile	OUTPST		
UPFLUX	g cm^{-2}	Array	Uptake Flux of Pesticide From Each Soil Compartment	SLPEST OUTPST	PEST	O I
UPTKF	--	Scalar	Plant Pesticide Uptake Efficiency Factor	READ ECHO PLGROW	PEST	O I I
URH	m day^{-1}	Scalar	Wind Velocity at Reference Height	CANOPY MAIN		I O
USLEC	--	Array	Universal Soil Loss Equation 'C' Factor	READ ECHO EROSN	HYDR	O I I
USLEK	--	Scalar	Universal Soil Loss Equation 'K' Factor	READ ECHO EROSN	HYDR	O I I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
USLELS	--	Scalar	Universal Soil Loss Equation 'Ls' Factor	READ ECHO EROSN	HYDR	O I I
USLEP	--	Scalar	Universal Soil Loss Equation 'P' Factor	READ ECHO EROSN	HYDR	O I I
USTAR	m day^{-1}	Scalar	Friction Velocity	CANOPY		O
UTEMP	°C	Array	Air Temperature	CANOPY		I
UWIND	m day^{-1}	Array	Wind Velocity	CANOPY		I
VAPLMD	cal cm^{-1} day^{-1} $°C^{-1}$	Scalar	Thermal Conductivity of Vapor in the Soil Pores	SLTEMP		
VAR1	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Into a Compartment	OUTPST		
VAR2	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Out of a Compartment	OUTPST		
VAR2D	cm	Scalar	Water Storage in a Single Compartment for thePrevious Day	OUTHYD		
VAR2M	cm	Scalar	Water Storage in a Single Compartment for the Previous Month	OUTHYD		
VAR2RZ	kg ha^{-1}	Scalar	Daily Advection/Dispersion Flux of Pesticide Out of the Root Zone	OUTPST		
VAR2Y	cm	Scalar	Water Storage in a Single Compartment for the Previous Year	OUTHYD		
VAR3	kg ha^{-1}	Scalar	Pesticide Storage in a Single Compartment for the Previous Day	OUTPST		
VEL	cm day^{-1}	Array	Water Velocity in Each Soil Compartment	HYDR1 HYDR2 SLPEST	HYDR	O I I
VHTCAP	cal cm^{-3} $°C^{-1}$	Array	Heat Capacity Per Unit Volume of Soil	SLTEMP		M
VLFLAG	--	Scalar	Advection flux flag (0 = all soil water velocities are zero, 1 = soil water velocity is nonzero)	HYDR1 PMAIN HYDR2	HYDR	I

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
VOLCOR	--	Scalar	A Variable Used to Convert Weight Percents of Soil Constituents to Volume Fractions of Bulk Volume	SLTEMP		
WBAL	cm	Scalar	Current Water Balance Error	MASBAL OUTHYD	HYDR	O I
WEIGHT	kg m^{-2}	Scalar	Current Plant Dry Foliage Weight	PLGROW PESTAP	CROP	O I
WF	kg ha^{-1}	Scalar	Daily Pesticide Washoff Flux	OUTPST		
WFMAX	kg m^{-2}	Array	Maximum Plant Dry Foliage Weight at Full Canopy	READ ECHO INITL	CROP	O I I
WIND	cm sec^{-1}	Scalar	Wind Speed	READ SLTEMP MAIN	MET	O I I
WLVL	cm	Scalar	Total Soil Water in the Compartments that Affect Runoff	HYDROL		
WOFLUX	g cm^{-2} day^{-1}	Scalar	Washoff Flux of Pesticide From Plant Foliage	SLPEST OUTPST	PEST	O I
WP	cm	Array	Wilting Point Water Depth in a Soil Compartment	EVPOTR	HYDR	O
WPV	--	Array	Regression Coefficients for Prediction of Wilting Point Soil Water Content	THCALC		
WTERM	g cm^{-2}	Scalar	Current Daily Pesticide Washoff Loss	PLPEST SLPEST	PEST	O I
X	g cm^{-3}	Array	Dissolved Pesticide in Each Soil Compartment	TRDIAG SLPEST MASBAL OUTPST OUTTSR OUTCNC PMAIN	PEST PEST	O I I I I I I
XFRAC	Fraction	Scalar	Location in furrow where infiltration is to be used in PRZM transport calculations (as fraction of total furrow length)	IRRIG IRREAD	IRGT	I O
XL	m	Scalar	Length of furrows	IRRIG FURROW IRREAD	IRGT	I I O

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
XP	g cm^{-3}	Array	Total Pesticide in Each Soil Compartment	MASBAL		
XVOL	fraction	Array	Volume Fraction of Soil Constituent	SLTEMP		
Y	--	Array	Intermediate Matrix Solution Array	TRDIAG		
YDOUT	kg ha^{-1}	Array	Annual Pesticide Decay From Each Soil Compartment	OUTPST	ACCUM	M
YEAR	--	Alpha-numeric	Flag for Annual Water and Pesticide Summary Output	PMAIN		
YEOUTW	cm	Array	Annual Evapotranspiration From Each Soil Compartment	OUTHYD	ACCUM	M
YINPP	kg ha^{-1}	Array	Annual Advective/Dispersive Flux Into Each Soil Compartment	OUTPST	ACCUM	M
YINPP1	kg ha^{-1}	Scalar	Annual Pesticide Applied to Foliage	OUTPST	ACCUM	M
YINPP2	kg ha^{-1}	Scalar	Annual Pesticide Applied to Soil	OUTPST	ACCUM	M
YINPW	cm	Array	Annual Infiltration Into Each Soil Compartment	OUTHYD	ACCUM	M
YINPW1	cm	Scalar	Annual Precipitation	OUTHYD	ACCUM	M
YINPW2	cm	Scalar	Annual Snowfall	OUTHYD	ACCUM	M
YLOUT	g cm^{-2}	Array	Annual Lateral Pesticide Outflow From Each Soil Compartment For Each Pesticide	INIACC OUTPST	ACCUM	O O
YOUTP	kg ha^{-1}	Array	Annual Pesticide Uptake From Each Soil Compartment	OUTPST	ACCUM	M
YOUTP1	kg ha^{-1}	Scalar	Annual Pesticide Washoff Flux	OUTPST	ACCUM	M
YOUTP2	kg ha^{-1}	Scalar	Annual Pesticide Runoff Flux	OUTPST	ACCUM	M
YOUTP3	kg ha^{-1}	Scalar	Annual Pesticide Erosion Flux	OUTPST	ACCUM	M
YOUTP4	kg ha^{-1}	Scalar	Annual Foliar Pesticide Decay Flux	OUTPST	ACCUM	M
YOUTP5	kg ha^{-1}	Scalar	Total Annual Pesticide Uptake Flux	OUTPST	ACCUM	M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
YOUTP6	kg ha^{-1}	Scalar	Total Annual Pesticide Soil Decay Flux	OUTPST	ACCUM	M
YOUTP9	g cm^{-2}	Array	Annual Lateral Pesticide Outflow From the Entire Soil Column for Each Pesticide	INIACC OUTPST	ACCUM	O O
YOUTW	cm	Array	Annual Exfiltration From Compartment	OUTHYD	ACCUM	M
YOUTW1	cm	Scalar	Annual Canopy Evaporation	OUTHYD	ACCUM	M
YOUTW2	cm	Scalar	Annual Thrufall	OUTHYD	ACCUM	M
YOUTW3	cm	Scalar	Annual Runoff	OUTHYD	ACCUM	M
YOUTW4	cm	Scalar	Annual Snowmelt	OUTHYD	ACCUM	M
YOUTW5	cm	Scalar	Total Annual Evapotrans piration	OUTHYD	ACCUM	M
YOUTW6	MTonne	Scalar	Total Annual Sediment Loss	OUTHYD	ACCUM	M
YSTR	cm	Array	Previous Year Storage of Water in Each Soil Compartment	OUTHYD	ACCUM	M
YSTR1	cm	Scalar	Annual Canopy Interception	OUTHYD	ACCUM	M
YSTR2	cm	Scalar	Annual Snow Accumulation	OUTHYD	ACCUM	M
YSTRP	kg ha^{-1}	Array	Storage of Pesticide From Previous Year in Each Soil Compartment	OUTHYD	ACCUM	M
YSTRP1	kg ha^{-1}	Scalar	Storage of Foliar Pesticide	OUTHYD	ACCUM	M
Z	Fraction	Scalar	Side slope of furrow channel walls (horizontal/vertical)	FURROW IRREAD	IRGT	I O
Z	--	Array	Location of moving points	MOC1 INITL	HYDR	M
ZC	--	Array	Location of fixed compartment center	MOC1 INITL	HYDR	M
ZCH	m	Scalar	Canopy Height	CANOPY MAIN SLTEMP		I O M
ZCTOT	--	Scalar	Concentration weighted locations of consolidated points	MOC		M
ZIN	--	Array	Temporary storage of new point locations	MOC1		M
ZO	m	Scalar	Roughness Height	CANOPY SLTEMP		O M

Table 11.3 PRZM Program Variables, Units, Location, and Variable Designation

Variable	Units	Type	Description	Subroutine	Common Block	I,M, O
ZRH	m	Scalar	Reference Height	CANOPY MAIN		I O
ZTOT	--	Scalar	Location of consolidated Points	MOC		M
ZWIND	m	Scalar	Distance Above the Ground Where Wind Speed was Measured	READ MAIN SLTEMP		O O I

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
AGKPRN	day^{-1}	Scalar	Above-ground plant return rate	PRZNRD NITR	CNITR	O M
AGPLTN	kg/ha	Scalar	Above-ground plant N storage	PRZNRD NITR	CNITR	O M
ALPNFG	--	Scalar	Flag for above-ground and litter simulation	PRZNRD NITR	CNITR	O I
AMIMB/ NCFX8	kg/ha	Array	Ammonia immobilization flux from each compartment	NITR	CNITR	M
AMMINF	kg/ha	Array	Inflow of septic ammonia in each compartment	SEPTIN NITBAL	CSPTIC	O I
AMMON	g/cm^2	Scalar	Daily inflow of septic ammonia	GETMET SEPTIN	CSPTIC	O I
AMNIT/ NCFX7	kg/ha	Array	Ammonia nitrification flux from each compartment	NITR	CNITR	M
AMUPA/ NCFX21	kg/ha	Array	Above-ground ammonia uptake flux from each compartment	NITR	CNITR	M
AMUPB/ NCFX23	kg/ha	Array	Below-ground ammonia uptake flux from each compartment	NITR	CNITR	M
AMVOFG	--	Scalar	Flag for ammonia volatilization simulation	PRZNRD NITR NITRXN	CNITR	O I
AMVOL/ NCFX18	kg/ha	Array	Ammonia volatilization flux from each compartment	NITRXN NITBAL	CNITR	M I
ANUFM	--	Array	Monthly above-ground uptake fraction for each compartment	PRZNRD NITR	CNITR	O I
ANUTF	--	Array	Above-ground plant uptake fraction for each compartment	PRZNRD NITR NITRXN	CNITR	O M I
BGNPRF	--	Scalar	Plant return refractory fraction	PRZNRD NITR NITRXN	CNITR	O M I
BNPRFM	--	Array	Monthly below-ground plant return refractory fraction	PRZNRD NITR	CNITR	O I

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
CNIT	--	Array	Concentration of nitrogen constituents for each compartment	NITMOV	CNITR	M
CRPDAT	--	Array	Plant and harvest dates for each crop	NITR CRDYFR YUPINI YUPTGT	CNITR	O I I I
CRPDAY	--	Array	Number of days each month for each crop	CRDYFR YUPINI YUPTGT	CNITR	O I I
CRPFRC	--	Array	Fraction of monthly plant uptake per crop	CRDYFR YUPINI YUPTGT	CNITR	O I I
DENIF/ NCFX6	kg/ha	Array	Denitrification from each compartment	NITR NITBAL	CNITR	M I
DNTHRS	--	Array	Fraction of water saturation when denitrification begins for each compartment	PRZNRD NITR	CNITR	O I
FIXNFG	--	Scalar	Flag for nitrogen fixation simulation	PRZNRD NITR NITRXN	CNITR	O I
FORAFG	--	Scalar	Ammonia adsorption/desorption calculation method	PRZNRD NITRXN	CNITR	O I
GNPM	--	Array	General nitrogen parameters (nitrate/ammonium uptake fractions,temp coeffs., max solubility of ammonium)	PRZNRD NITRXN	CNITR	O I
INFLOW	cm	Scalar	Daily inflow of septic water	GETMET SEPTIN	CSPTIC	O I
ITMAXA	--	Scalar	Max iterations for Freundlich solution	PRZNRD NITRXN SV	CNITR	O I I
KPLN	day^{-1}	Array	Plant uptake rate per compartment	PRZNRD NITR NITRXN	CNITR	O M I
KPLNM	day^{-1}	Array	Monthly plant uptake rate per compartment	PRZNRD NITR NITRXN	CNITR	O M I

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
KRBNM	day^{-1}	Array	Monthly below-ground plant return rate per compartment	PRZNRD NITR	CNITR	O I
KRANM	day^{-1}	Array	Monthly above-ground plant return rate	PRZNRD NITR	CNITR	O I
KRETAN	day^{-1}	Array	Litter return rate for compartments in first horizon	PRZNRD NITR	CNITR	O M
KRETBN	day^{-1}	Array	Below-ground plant return rate for each compartment	PRZNRD NITR NITRXN	CNITR	O M I
KRLNM	day^{-1}	Array	Monthly litter return rate	PRZNRD NITR	CNITR	O I
KVOL	day^{-1}	Array	Ammonia volatilization rates for each compartment	PRZNRD NITRXN	CNITR	O I
LINF	cm	Array	Inflow of septic water in each compartment	SEPTIN HYDR1 HYDR2	CSPTIC	O I I
LINPRF	--	Scalar	Litter return refractory fraction	PRZNRD NITR	CNITR	O M
LITTRN	kg/ha	Scalar	Litter N storage	PRZNRD NITR	CNITR	O M
LNPRFM	--	Array	Monthly litter return refractory fraction	PRZNRD NITR	CNITR	O I
NAPFRC	--	Array	Fraction of organic N application that becomes refractory	PRZNRD NITRAP	CNITR	O I
NBUFF	--	Array	Data buffer for atmospheric deposition time-series values	GETMET	CNITR	O
NC1	--	Scalar	Number of compartments in first horizon	PRZNRD NITR	CNITR	O M
NCRP	--	Scalar	Number of crop periods each year	NITR	CNITR	O
NDFC	kg/ha	Array	Yield-based plant uptake deficit for each compartment	NITRXN YUPTGT	CNITR	M M
NECNT	–	Array	Counter for error messages	NITRXN SV	CNITR	M

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NFIXFX/ NCFX12	kg/ha	Array	Nitrogen fixation flux for each compartment	NITRXN NITBAL	CNITR	M I
NIACNM	kg/ha	Array	Monthly dry atmospheric deposition flux values	PRZNRD GETMET	CNITR	O I
NIADDR/ NCFX10	kg/ha	Array	Dry atmospheric deposition fluxes	GETMET NITR NITBAL	CNITR	O I I
NIADWT/ NCFX11	kg/ha	Array	Wet atmospheric deposition fluxes	GETMET NITR NITBAL	CNITR	O I I
NIADFG	--	Array	Atmospheric deposition flags	PRZNRD GETMET	CNITR	O I
NIAFXM	kg/ha	Array	Monthly wet atmospheric deposition flux values	PRZNRD GETMET	CNITR	O I
NIIMB/ NCFX17	kg/ha	Array	Nitrate immobilization flux from each compartment	NITR	CNITR	M
NIT	kg/ha	Array	Storage of nitrogen constituents for each compartment	PRZNRD NITR NITRXN SEPTIN NITRAP	CNITR	O M M M M
NITINF	kg/ha	Array	Inflow of septic nitrate in each compartment	SEPTIN NITBAL	CSPTIC	O I
NITR	g/cm^2	Scalar	Daily inflow of septic nitrate	GETMET SEPTIN	CSPTIC	O I
NIUPA/ NCFX20	kg/ha	Array	Above-ground nitrate uptake flux from each compartment	NITR	CNITR	M
NIUPB/ NCFX22	kg/ha	Array	Below-ground nitrate uptake flux from each compartment	NITR	CNITR	M
NMXRAT	--	Scalar	Ratio of max uptake to target uptake	PRZNRD NITRXN	CNITR	O I
NPM	day^{-1}	Array	First order rates for each compartment, ammonium absorption parameters	PRZNRD NITRXN	CNITR	O I
NRXF	kg/ha	Array	Daily reaction fluxes for each compartment	NITRXN	CNITR	M

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NUPTFG	--	Scalar	Flag for plant uptake method	PRZNRD NITR NITRXN	CNITR	O I I
NUPTFM	--	Array	Monthly fraction of annual yield-based uptake target	PRZNRD YUPINI YUPTGT	CNITR	O I I
NUPTG	day^{-1}	Array	Yield-based plant uptake target for each compartment	YUPTGT NITRXN	CNITR	O I
NUPTGT	--	Scalar	Annual yield-based plant uptake target	PRZNRD YUPINI YUPTGT	CNITR	O I I
NUPTM	--	Array	Fraction of monthly yield-based uptake target from each compartment	PRZNRD YUPINI YUPTGT	CNITR	O I I
NWCNT	--	Array	Counter for warning messages	NITRXN OMSG	CNITR	M
ORGINF	kg/ha	Array	Inflow of septic organic N in each compartment	SEPTIN NITBAL	CSPTIC	O I
ORGN	g/cm^2	Scalar	Daily inflow of septic organic N	GETMET SEPTIN	CSPTIC	O I
ORGRFC	--	Scalar	Fraction of septic organic N that becomes refractory	PRZNRDSE PTIN	CSPTIC	O I
ORNMN/ NCFX9	kg/ha	Array	Mineralization flux from each compartment	NITR	CNITR	M
ORNPM	--	Array	Organic N parameters for each compartment	PRZNRD NITRXN	CNITR	O I
OSAMS/ NCFX3	kg/ha	Array	Solution ammonia lateral outflow from each compartment	NITMOV NITBAL	CNITR	M I
OSNO3/ NCFX5	kg/ha	Array	Nitrate lateral outflow from each compartment	NITMOV NITBAL	CNITR	M I
OSSLN/ NCFX14	kg/ha	Array	Labile organic N lateral outflow from each compartment	NITMOV NITR NITBAL	CNITR	M M I
OSSRN/ NCFX16	kg/ha	Array	Refractory organic N lateral outflow from each compartment	NITMOV NITR NITBAL	CNITR	M M I

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
PNUTG	day^{-1}	Array	Yield-based plant uptake target from each compartment for end of previous month	YUPINI YUPTGT	CNITR	O M
PSAMS/ NCFX2	kg/ha	Array	Solution ammonia leaching output from each compartment	NITMOV NITBAL	CNITR	M I
PSNO3/ NCFX4	kg/ha	Array	Nitrate leaching output from each compartment	NITMOV NITBAL	CNITR	M I
PSSLN/ NCFX13	kg/ha	Array	Labile organic N leaching output from each compartment	NITMOV NITBAL	CNITR	M I
PSSRN/ NCFX15	kg/ha	Array	Refractory organic N leaching output from each compartment	NITMOV NITBAL	CNITR	M I
REFRON/ NCFX19	kg/ha	Array	Labile to refractory conversion flux for each compartment	NITR	CNITR	M
RETAGN/ NCFX24	kg/ha	Array	Above-ground plant return to litter flux	NITR	CNITR	M
RTLLN/ NCFX25	kg/ha	Array	Litter return to labile organic N in first horizon's compartments	NITR	CNITR	M
RTRLN/ NCFX26	kg/ha	Array	Litter return to refractory organic N in first horizon's compartments	NITR	CNITR	M
RTLBN/ NCFX27	kg/ha	Array	Below-ground plant return to labile organic N for each compartment	NITR	CNITR	M
RTRBN/ NCFX28	kg/ha	Array	Below-ground plant return to refractory organic N for each compartment	NITR	CNITR	M
SBUFF	--	Array	Data buffer for septic effluent time-series values	GETMET	CSPTIC	O
SEDN/ NCFX1	kg/ha	Array	Sediment and runoff loss fluxes	NITMOV	CNITR	M
SEPDSN	--	Array	Data-set numbers for septic effluent time-series values	PRZNRD GETMET	CSPTIC	O I

Table 11.4 PRZM Nitrogen Simulation Variables, Units, Location, and Variable Designations						
Variable	**Units**	**Type**	**Description**	**Subroutine**	**Common Block**	**I,M,O**
SEPHZN	--	Scalar	Horizon number for septic effluent	PRZNRD SEPTIN	CSPTIC	O I
THVOL	--	Scalar	Temperature correction coeff for ammonia volatilization	PRZNRD NITRXN	CNITR	O I
TNIT	kg/ha	Array	Total storage of nitrogen constituents in soil profile	NITR	CNITR	M
TOTNIT	kg/ha	Scalar	Total nitrogen storage in soil profile	PRZNRD NITR NITBAL	CNITR	O M I
TONIT0	kg/ha	Scalar	Total nitrogen storage in soil profile for previous day	PRZNRD NITBAL	CNITR	O M
TRFVOL	ºC	Scalar	Reference temperature for ammonia volatilization	PRZNRD NITRXN	CNITR	O I
VNPRFG	--	Scalar	Flag for time-varying plant return	PRZNRD NITR	CNITR	O I
VNUTFG	--	Scalar	Flag for time-varying plant uptake	PRZNRD NITR	CNITR	O I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations						
Variable	**Units**	**Type**	**Description**	**Subroutine**	**Common Block**	**I,M,O**
A	--	Array	Left Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
ASTORN	--	Scalar	Value of A(NP) Where NP=Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M
B	--	Array	Main Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
BALSTO	--	Array	Array Containing Mass Balance Information	MAIN BALCHK		M O
BSTOR1	--	Scalar	Value of B(1)	ASSEMF ASSEMT BALCHK	WORKA	M
BSTORN	--	Scalar	Value of B(NP) Where NP=Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
C	--	Array	Right Diagonal of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
CORD	L	Array	Nodal Coordinates	MAIN VSWCOM	CORD	I
CSTOR1	--	Scalar	Value of C(1)	ASSEMF ASSEMT BALCHK	WORKA	M
CTRFAC	--	Array	Coordinate Transform ation Factors for Different Soil Materials	CONVER DSWFUN MAIN	WORKN	M
D	--	Array	Right-Hand-Side Vector of a Tridiagonal Matrix	ASSEMF ASSEMT	ASOLV	M
DETAND	--	Array	Nodal Storage Factor	ASSEMF	WELEM	M
DIS	L M/L^3	Array	Current Nodal Value of Head of Concentration	MAIN ASSEMF BALCHK VARCAL VSWCOM	BSOLV	M O
DLAMDA	1/t	Scalar	Value of Decay Constant for the Node Currently Being Evaluated	MAIN ASSEMT VARCAL	CONTR	M
DLAMND	1/t	Scalar	Nodal Value of Decay Constant	MAIN ASSEMT BALCHK VARCAL		I
DPKND	L/t	Array	Nodal Values of Hyd. Conductivity Increment	ASSEMF	WELEM	M
DPKRAV	L^2	Scalar	Value of Rel. Perm. for Node Currently Being Solved	ASSEMF PKWFUN		M
DSTOR1	--	Scalar	The Value of D(1)	ASSEMF ASSEMT BALCHK	WORKA	M
DSTORN	--	Scalar	The Value of D(NP) Where NP = Number of Nodes	ASSEMF ASSEMT BALCHK	WORKA	M
DTEPS	--	Scalar	Time Step Tolerance Parameter	MAIN		M
DTMARK	--	Scalar	Marker Time Increment	MAIN		M
DX	--	Scalar	DX = THL(I) NEL	MAIN		M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
EL	L	Scalar	Elemental Values for Finite-Element Element Length Formulation	MAIN ASSEMF ASSEMT BALCHK VARCAL		M
ETAND	--	Array	Nodal Values of Fluid Storage Factor	ASSEMF ASSEMT BALCHK	WELEM	M
FLX1	L^3/t	Scalar	Value of Fluid Flux Entering Node 1 (for Flow FLX1 = 0.0)	MAIN ASSEMT HFINTP VARCAL	CONTR	M
FLXN	L^3/t	Scalar	Value of Fluid Flux Entering the Last Node (for Flow FLX1 = 0.0)	MAIN ASSEMT HFINTP VARCAL	CONTR	M
FVAL	--	Array	Functional Coefficient Values for the Soil Moisture Relationship	MAIN ASSEMT HFINTP SWFUN CONVER DSWFUN	MDATA	M
HAVE	L	Scalar	Average Head Value	ASSEMF SWFUN DSWFUN		M
HCAP	L	Array	Value of Pressure Head on Press. Head vs. Sat. Curve	MAIN ASSEMF INTERP	SWHDA	M
HCRIT	L	Scalar	Critical Head Value	ASSEMF SWFUN DSWFUN		I
HDOBS	$L\ M\ L^{-3}$	Array	Head or Concentration of Observation Node for Current Time	MAIN	DAOBS	M O
HINV	$L\ M\ L^{-3}$	Scalar	Default Value of Initial Head or Concentration	MAIN		I
HTOL	L	Scalar	Head Tolerance Allowed for Nonlinear Solution	MAIN ASSEMF VARCAL DSWFUN	CONTR	I
HVTM	L	Array	Value of function corresponding to Time Values (TMHV)	MAIN HFINTP		M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
IBTND1	--	Scalar	Last Node Boundary Condition Code (1=1st type, 0=3rd type)	MAIN ASSEMF ASSEMT VARCAL		I
IBTNDN	--	Scalar	Last Node Boundary Condition Code (1=1st Type, 0=3rd type)	ASSEMF MAIN ASSEMT VARCAL		I
ICONVG	--	Scalar	Convergence Flag (1=Converged, 0=Not Converged)	MAIN VARCAL		I
IHORIZ	--	Scalar	Simulation Orientation Indicator (0=Vertical, 1=Horizontal)	MAIN		I
IKALL	--	Scalar	Time Stepping Scheme Indicator (1=Backward, 0=Central)	MAIN		I
ILAYR	--	Scalar	Current Layer Number	MAIN		I
IMAT	--	Scalar	Counter Used in Looping with Respect to Materials	MAIN ASSEMF ASSEMT INTERP PKWFUN SWFUN CONVER DSWFUN		I
IMATL	--	Scalar	Material Identifying Number for Current Layer	MAIN		I
IMBAL	--	Scalar	Mass Balance Computation Indicating Parameter	MAIN	CONTR	I
IMOD	--	Scalar	For Modified Newton Raphson Solution Procedure	MAIN DSWFUN	CONTR1	I
IMODL	--	Scalar	Simulation Identifier (Flow or Transport)	MAIN BALCHK VARCAL	CONTR	I
INEWT	--	Scalar	Nonlinear Iterative Procedure Flag (1=Newton, 0=Picard)	MAIN ASSEMF VARCAL	CONTR	I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations						
Variable	**Units**	**Type**	**Description**	**Subroutine**	**Common Block**	**I,M,O**
INOCTS	--	Scalar	Number of Computation Time Steps Required to Simulate This Target Time Step	MAIN VARCAL		I
INPFL	--	Scalar	Unit Number for Input File	MAIN		I
INTSPC	--	Scalar	Initial Condition Specifier for Head Conversion Convert Initial Head Values (1=Yes, 0=No)	MAIN		I
IOBSND	--	Scalar	Observation Node Index	WORKA		I
IPRCHK			Print Check Flag (Triggers Additional Diagnostic Output)	MAIN ASSEMF ASSEMT BALCHK VARCAL CONVER		I
IPROP	--	Array	Generated Material Property Identifiers	MAIN ASSEMF ASSEMT	MDATA	I
IREP	--	Scalar	Time Step Refinement Counter	MAIN VARCAL		M
IREPMX	--	Scalar	Maximum Number of Nonlinear Solution Cycles	MAIN VARCAL		I
IRESOL	--	Scalar	Maximum Number of Time Step Refinements	MAIN VARCAL		I
IRLTYP	--	Scalar	Flag for the Type of Relative Function Being Evaluated	ASSEMF	INTERP	I
ITCND1	--	Scalar	Node 1 Boundary Condition Flag (1 = Transient, 0 = Steady State)	MAIN HFINTP		I
ITCNDN	--	Scalar	Node 1 Boundary Condition Flag (1 = Transient, 0 = Steady State)	MAIN HFINTP		I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
ITER	--	Scalar	Iterative Counter (Current Iteration Number)	MAIN ASSEMF ASSEMT BALCHK VARCAL VSWCOM		M
ITMARK	--	Scalar	Backup File Output Indicator	MAIN VSWCOM		M
ITMFC	--	Scalar	Marker Time Increasing Parameter	MAIN VSWCOM		M
ITMGEN	--	Scalar	Marker Time Value Generation Indicator	MAIN		I
ITRANS	--	Scalar	Transient Steady-State Flag (1=TR, 0=SS)	MAIN ASSEMF VARCAL	CONTR	I
ITSGN	--	Scalar	Time Step Generation Indicator	MAIN		I
ITSTH	--	Array	Identifies Location of Previous Time Value of Time Graph	MAIN HFINTP		I
IVSTED	--	Scalar	Steady-State Velocity Field Indicator	MAIN		I
KPROP	--	Scalar	Flag for Perm-Saturation and Pressure Head-Saturation Curves (1=Functional, 0=Tabulated)	MAIN ASSEMF VARCAL		I
MARK	--	Scalar	Flow Direction Flag (1=Vertical, 0=Horizontal)	MAIN ASSEMF VARCAL VSHCOM	CONTR	I
MM	--	Scalar	Place Holder for Loop Incrementer			M
MXMAT	--	Scalar	Maximum Number of Materials Allowed (Due to the Size of Arrays)	MAIN ASSEMF ASSEMT INTERP SWFUN DSWFUN		I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
MXNODE	--	Scalar	Maximum Number of Nodes Allowed (Due to the Size of Some Arrays)	MAIN ASSEMF ASSEMT BALCHK TRIDIA VARCAL VSWCOM		I
MXTMV	t	Scalar	Maximum Time Value to be Interpolated	MAIN HFINTP		I
NDCOUN	--	Scalar	Material Number Temporary Counter	MAIN		M
NDM1	--	Scalar	Counter Minus One NDM1 = NDCOUN	MAIN		M
NDOBS	--	Array	Nodal Values of Observation Nodes	MAIN	DAOBS	I
NE	--	Scalar	Number of Elements in the Linear Representation	MAIN VSWCOM	CONTR	I
NEL	--	Scalar	Storage Location for the Number of Finite Elements in the Current Layer NELM(I)	MAIN		M
NELM	--	Array	Number of Finite Elements in the Current Layer	MAIN		I
NITMAX	--	Scalar	Maximum Number of Nonlinear Iterations Allowed per Time Step	MAIN VARCAL	CONTR	I
NLAYRG	--	Scalar	Number of Layers That Need to be Discritized	MAIN		I
NMAT	--	Scalar	Number of Soil Materials	MAIN CONVER		I
NOBSND	--	Scalar	Number of Observation Nodes in the Simulation	MAIN		I
NONU	--	Scalar	Nonuniform Initial Condition Indicator	MAIN		I
NOWRIT	--	Scalar	Restart Data Writing Indicator	MAIN		I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
NP	--	Scalar	Total Number of Nodal Points	MAIN ASSEMF ASSEMT BALCHK TRIDIA VARCAL VSWCOM	CONTR	I
NPIN	--	Scalar	Number of Non-default Initial Values	MAIN		I
NPROB	--	Scalar	Number of Simulations to be Made	MAIN		I
NSTEP	--	Scalar	Nodal Value Printout Control Parameter	MAIN BALCHK	CONTR	I
NTN1	--	Scalar	Storage Location for NTSNDH(1)	MAIN		M
NTNP	--	Scalar	Storage Location for NTSNDH(NP)	MAIN		M
NTOMT	--	Scalar	Number of Backup File Output Marker Time Values	MAIN VSWCOM		I
NTS	--	Scalar	Number of Time Steps in This Simulation	MAIN		M
NTSNDH	--	Array	Number of Time Values on the Time Graph ([1]=CONC, [2]=HEAD)	MAIN HFINTP		I
NUMK	--	Array	Values of Permeability from the Permeability vs Saturation Table for Each Material	MAIN ASSEMF INTERP	SWHDA	I
NUMP	--	Array	Number of Pressure Head vs. Saturation Values for Each Material	MAIN ASSEMF INTERP	SWHDA	I
NUMT	--	Scalar	Time Step incrementer	MAIN		I
NVPR	--	Scalar	Velocity Printout Control Parameter	MAIN VSWCOM	CONTR	I
NVREAD	--	Scalar	Velocity Reading Indicator	MAIN		I

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
OUTFL	--	Scalar	Output File Unit Number	MAIN ASSEMF ASSEMT BALCHK INTERP VARCAL VSWCOM		I
PCUR	$L\ M\ L^{-3}$	Array	Current Value of Pressure Head or Concentration for the Current Time Step	ASSEMF VARCAL	BSOLV	M
PINT	$L\ M\ L^{-3}$	Array	Initial Value of Pressure Head or Concentration	MAIN ASSEMF ASSEMT BALCHK VARCAL	BSOLV	I
PKND	L/t	Array	Nodal Values of Hydraulic Conductivity	MAIN ASSEMF VSWCOM	WELEM	M
PKRW	L^2	Array	Value of Relative Permeability (on Perm. vs. Sat. Curve)	MAIN ASSEMF INTERP	SWHDA	M
PKWOUT	L^2	Scalar	Relative Permeability Computed Using Function Then Passed Back	PKWFUN		M
PROP	--	Array	Saturated Material Properties (Flow or Transport) Flow-Hydraulic Conductivity Porosity, Specific Storage Air Entry Pressure Transport-Dispersivity, Porosity, Retardation Diffusion	MAIN ASSEMF ASSEMT	MDATA	I
QVTM	L^3/t	Array	Volumetric Water Flux Values Corresponding to Time Values	MAIN HFINTP		M
SLOPE	--	Scalar	Slope of the Line Between the Points Being Interpolated	HFINTP INTERP		M
SSWV	--	Array	Value of Water Phase Saturation (on Press. Head vs Sat. Curve)	ASSEMF INTERP	SWHDA	M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
STMARK	t	Scalar	Starting Marker Time Value	MAIN		M
SWAVE	--	Scalar	Average Water Saturation	ASSEMF PKWFUN		M
SWDFI	--	Array	Default Value of Water Saturation for the Current Material	MAIN		I
SWND	--	Array	Current Water Saturation at the Node Being Evaluated	MAIN ASSEMF ASSEMT VARCAL VSWCOM		M
SWNDPT	--	Array	Water Saturation for the Node at Previous Time Step	MAIN VSWCOM		M
SWRKP	--	Array	Temporary Working Array	CONVER	WORKN	M
SWV	--	Array	Value of Water Phase Saturation (on Perm. vs. Sat. Curve)	MAIN ASSEMF INTERP	SWHDA	M
TAP8	--	Scalar	Unit Number for Restart File	MAIN		I
TAP10	--	Scalar	Unit Number of Flow-to-Transport File (Darcy Vel. & Water Sat.)	MAIN VSWCOM	MDATA	I
TDIFF	t		TDIFF=TMCUR-TMVECX	MAIN		M
TERIFL	--	Scalar	Unit Number for Input File	MAIN		I
TEROFL	--	Scalar	Unit Number for Output File	MAIN		I
TFAC	--	Scalar	Time Step Multiplier	MAIN		I
THETA	--	Scalar	Value Used in the Time Stepping Scheme (Theta=0.5 for Central Difference Scheme, Theta=1.0 for Backward Difference Scheme)	MAIN ASSEMT BALCHK VARCAL		M
THETM1	--	Scalar	Theta Minus One	MAIN ASSEMT BALCHK VARCAL		M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
THL	L	Array	Thickness of Current Layer	MAIN		M
TIN	t	Scalar	Value of Initial Time Step	MAIN ASSEMF ASSEMT BALCHK VARCAL	CONTR	I
TIMA	t	Scalar	Initial Time Value of the Simulation	MAIN VSWCOM	CONTR	I
TIMAKP	t	Scalar	Storage Location for the Value of Time Where Iteration Computation is Taking Place	MAIN		M I
TITLE		Alpha-Numeric	Title of Simulation	MAIN		I
TMACCU	L^3 M	Scalar	Quantitative Storage Water Volume or Solute Mass	MAIN BALCHK	CONTR	M
TMAX	t	Scalar	Maximum Time Step Size	MAIN		I
TMCUR	t	Scalar	Current Time Value	MAIN VSWCOM		M
TMDCAY	M	Scalar	Cumulative Solute Mass Decay	MAIN BALCHK	CONTR	M
TMFOMT	t	Array	Time Values for Output to the Backup File	MAIN VSWCOM		I
TMHV	t	Array	Time Values at the Interpolation Points ([1]=CONC, [2]=HEAD)	MAIN HFINTP		M
TMVEC	t	Array	Values of Time Generated by the Code, to be Used in the Simulation	MAIN BALCHK		I M
TMVECX	t	Scalar	Extra Time Value Due to the Reduction of a Time Step When Solution is not Converging	MAIN BALCHK HFINTP VARCAL		M
UWF	--	Scalar	Value of Upstream Weighting Factor for the Node Currently Being Evaluated	MAIN ASSEMT VARCAL	CONTR	M

Table 11.5 VADOFT Program Variables, Units, Location, and Variable Designations

Variable	Units	Type	Description	Subroutine	Common Block	I,M,O
UWFI	--	Array	Value of Upstream-Weighting Factor for the Current Material	MAIN	TPDEF	M
VALND1	--	Scalar	Value of First Node (Depending on: Type of Run & Type of Boundary)	MAIN ASSEMF ASSEMT HFINTP VARCAL		M
VALNDN	--	Scalar	Value of Last Node (Depending on: Type of Run & Type of Boundary)	MAIN ASSEMF ASSEMT HFINTP VARCAL		M
VDAR	L/t	Array	Darcy Velocity for Each Node	MAIN ASSEMF BALCHK VARCAL VSWCOM		M O
VDARPT	L/t	Array	Nodal Darcy Velocities at Previous Time	MAIN VSWCOM		M
VDFI	L/t	Array	Default Value of Darcy Velocity for Current Material	MAIN		I
XX	--	Scalar	The *X* value Passed in INTERP (to be Used in the Interpolation)	INTERP		M
YY	--	Scalar	The *Y* Value Passed in INTERP (to be Used in the Interpolation)	INTERP		M

Table 11.6 Monte Carlo Program Variables

Variable	Units	Description	Subroutine
BBT	Double Precision	Correlation matrix for Monte-Carlo inputs.	Main program READM INITMC
CORR	Double Precision Array	Array of correlation terms for summary output variables.	Main Program STATIS OUTPUT
DECOM	Integer	Decomposed correlation matrix for Monte-Carlo inputs.	Main Program INITMC RANDOM
DIST	Real Array	Array storing empirical distributions.	Main Program READM Random
IN2	Integer	Monte-Carlo input file number.	Main Program READM
IOUT	Integer	Monte-Carlo summary output file unit number.	Main Program READM OUTPUT
IOUT2	Integer	Output file unit number for results of each Monte-Carlo run.	Main Program STATIS
IRUN	Integer	Do loop counter for Monte-Carlo runs.	Main Program STATIS
IVAR	Integer	Do loop counter for variable number.	Main Program
LARR	Integer Array	Array storing array addresses for random input variables.	Main Program READM INITMC
MCMAX	Integer	Maximum possible number of random input variables.	Main Program
MCVAR	Integer	Number of random input variables.	Main Program READM INITMC RANDOM
NCMAX	Integer	Maximum possible number of variables for which cumulative distributions can be plotted.	Main Program
NDAT	Integer Array	Number of values in empirical distributions.	Main Program READM RANDOM
NEMP	Integer	Maximum number of empirical distribution value-probability pairs.	Main Program READM RANDOM
NMAX	Integer	Maximum possible number of variables for which summary statistics can be printed.	Main Program

Table 11.6 Monte Carlo Program Variables

Variable	Units	Description	Subroutine
NRMAX	Integer	Maximum number of Monte-Carlo runs allowed.	Main Program
NRUNS	Integer	Number of Monte-Carlo Runs.	Main Program READM OUTPUT
NVAR		Number of summary output variables.	Main Program
PNAME	Character Array	Input labels used to flag random input variables.	Main Program READM INITMC
RMC	Real Array	Array of randomly-generated numbers.	Main Program RANDOM
SNAME	Character Array	Input labels used to flag summary output variables.	Main Program READM OUTPUT
STAT	Double Precision Array	Array of summary statistics for output variables.	Main Program STATIS OUTPUT
VAR	Real Array	Array storing distribution parameters for random input variables.	Main Program READM INITMC RANDOM
XCDF	Real Array	Array storing values of selected variables for plotting cumulative distributions.	Main Program STATIS OUTPUT
XMC	Real Array	Array storing values of summary output variables.	Main Program STATIS

Table 11.7 PZ2HSPF Bridge Program Variables

Variable	Description
CRPAREA	Area of crop treated with pesticide (ha)
CRPNAM	Name of crop (20 characters)
DECERO	Total mass of pesticide lost due to decay in erosion (mass units)
DECGW	Total mass of pesticide lost due to decay in groundwater (mass units)
DECLAT	Total mass of pesticide lost due to decay in lateral flow (mass units)
DECSUR	Total mass of pesticide lost due to decay in surface flow (mass units)
DESCRP	Description of run (80 characters)
DGRATE	Groundwater-associated pesticide decay rate (/day) (array of values for each pesticide)
DGW	Total mass of pesticide in groundwater flow lost due to delivery ratio (mass units)
DLRATE	Interflow-associated pesticide decay rate (/day) (array of values for each pesticide)
DRERO	Total mass of pesticide in erosion lost due to delivery ratio (mass units)
DRLAT	Total mass of pesticide in lateral flow lost due to delivery ratio (mass units)
DRRATE	Surface runoff-associated pesticide decay rates (/day) (array of values for each pesticide)
DSRATE	Sediment-associated pesticide decay rates (/day) (array of values for each pesticide)
ENDATE	Simulation ending date (array containing year, month, day, hour, minute, and second; user enters year, month, day)
ERFLUX	Total mass of pesticide in erosion after losses (mass units)
EROFLX	Mass of chemical associated with erosion; array of values for each chemical and each day; units are mass units/ha/day for input and mass units/day for output
EROMB	Mass balance on total pesticide in erosion (mass before losses - losses - mass after losses) (mass units)
GROFLX	Mass of chemical associated with groundwater runoff; array of values for each chemical and each day; units are mass units/ha/day for input and mass units/day for output
GWFLUX	Total mass of pesticide in groundwater flow after losses (mass units)
GWMB	Mass balance on total pesticide in groundwater flow (mass before losses - losses - mass after losses) (mass units)
GWRAT	Groundwater "delivery ratio" (array of values for each pesticide)
INFLNM	Input file name (20 characters)
INPDSN	Array of dataset numbers containing the input data, i.e. the fluxes by soil layer generated by PRAM-3 (erosion, surface runoff, interflow and groundwater pesticide fluxes)
INPFL	Unit number of input file for PZ2HSPF bridge program
LAGERO	Total mass of pesticide lost due to lag of erosion (mass units)
LAGGW	Total mass of pesticide lost due to lag of groundwater flow (mass units)

Table 11.7 PZ2HSPF Bridge Program Variables	
Variable	**Description**
LAGLAT	Total mass of pesticide lost due to lag of lateral flow (mass units)
LAGSUR	Total mass of pesticide lost due to lag of surface flow (mass units)
LATFLX	Mass of chemical associated with lateral runoff; array of values for each chemical and each day; units are mass units/ha/day for input and mass units/day for output
LATMB	Mass balance on total pesticide in lateral flow (mass before losses - losses - mass after losses) (mass units)
LATRAT	Interflow "delivery ratio" (array of values for each pesticide)
LTFLUX	Total mass of pesticide in lateral flow after losses (mass units)
MXDAYS	Maximum number of days that program can process in a run (current value = 1470)
MXPEST	Maximum number of pesticides or chemicals that program can process in a run (current value = 3)
NUMDAY	Number of days in simulation run span
NUMPST	Number of pesticides or chemicals to be processed by the program
OPTFLG	Option flag for writing to WDM file; program writes to WDM if > 1
OUFLNM	Output file name (20 characters)
OUTDSN	Array of dataset numbers containing the output data, i.e. the data transformed by PZ2HSPF bridge program and used as input to HSPF (erosion, surface runoff, interflow, groundwater and total aqueous runoff pesticide fluxes)
OUTFL	Unit number of output file for PZ2HSPF bridge program
PBAL	Mass balance on total pesticide (sum of EROMB, SURMB, LATMB, and GWMB) (mass units)
PSTNAM	Names of pesticides (array of 20-character names)
SEDRAT	Sediment delivery ratio (array of values for each pesticide)
SEGNUM	Model segment ID number
STDATE	Simulation starting date (array containing year, month, day, hour, minute, and second; user enters year, month, day)
SUFLUX	Total mass of pesticide in surface flow after losses (mass units)
SURFLX	Mass of chemical associated with surface runoff; array of values for each chemical and each day; units are mass units/ha/day for input and mass units/day for output
SURMB	Mass balance on total pesticide in surface flow (mass before losses - losses - mass after losses) (mass units)
TERO	Sediment-associated pesticide time lag from field to stream (days or fraction of a day)
TGW	Groundwater-associated pesticide time lag from field to stream (days or fraction of a day)
TLAT	Interflow-associated pesticide time lag from field to stream (days or fraction of a day)
TOTERO	Total mass of pesticide in erosion before losses (mass units)

Table 11.7 PZ2HSPF Bridge Program Variables	
Variable	**Description**
TOTFLX	Total mass of chemical input to stream; array of values for each chemical and each day (mass units/day)
TOTGW	Total mass of pesticide in groundwater flow before losses (mass units)
TOTLAT	Total mass of pesticide in lateral flow before losses (mass units)
TOTSUR	Total mass of pesticide in surface flow before losses (mass units)
TSUR	Surface runoff-associated pesticide time lag from field to stream (days or fraction of a day)
WDFLNM	WDM file name (20 characters)
WDMSFL	Unit number of WDM file

Table 11.8 PRZWASP Bridge Program Variables	
Variable	**Description**
APPCTR	Application counter for the chemical
APDAY	Date of pesticide application as JULIAN day
CALYR	Calendar year determined from the WASP start date
CHMNUM	Number of chemicals simulated in a PRAM-3 run
CLINE	Character line specified to skip header of PRZM-3 file
DOM	Day of the month as output by PRZM-3
ERFLUX	Erosion flux of pesticide, $g/cm^2/day$
EDAY	Ending day of WASP simulation for output
FDAY	Beginning day of WASP simulation for output
HISEG	Last segment number for output on current line
IAPM	Month of pesticide application
IAPD	Date of pesticide application
ICHEM	Flag to specify which chemical is being simulated in each PRAM-3 run
INP	Unit number for the input file name to be read in by the main program PRZWASP
INPFNM	Name of the input parameter file
INPS	Flag to check if chemicals or sediment are simulated
INTOPT	Interpolation option; 1 = step function (only one in code now)
ISED	Flag to specify if erosion is being simulated (0=No, 1=Yes)
ISDFRC	Flag to specify which solid fractions are considered
ISPRAY	Flag to specify if spray drift is simulated (0=No, 1=Yes)

Table 11.8 PRZWASP Bridge Program Variables	
Variable	**Description**
JULIAN	Function to calculate julian day from a given calendar date
LEN	Length of a PRZM-3 file name
LDAY	Loading day counter
LPYEAR	Subroutine to determine if the simulation year is a leap year
LOSEG	Beginning segment number for output on current line
MSPRAY	Mass of pesticide considered as spray drift, kg/ha
MXSYST	Maximum number of systems possible
MXAPPS	Maximum number of pesticide applications
MXCHEM	Maximum number of chemicals that can be simulated
MXSYST	Maximum number of systems that can be simulated
MXWSEG	Maximum number of WASP segments that can be simulated
MXPRZM	Maximum number of PRZM-3 segments that can be simulated
MXSOLD	Maximum number of solid fractions that can be simulated
NLINES	Number of lines per loading day required for WASP output
NUMSYS	Number of WASP systems receiving nonpoint source loads (see WASP5.0 documentation for detail)
NPSFNM	Unit number of NPS file for WASP
NPSSEG	WASP segment number receiving load
NPSSYS	WASP system numbers receiving loads
NPSNAME	Name or description of WASP systems receiving loads
NUMPRZ	Number of PRZM-3 segments considered
NUMPYR	Number of years PRZM-3 runs have been made
NUMSEG	Number of segments receiving nonpoint source loads
NPSTYP	Name or description of the nonpoint source model or method of generation; this is echoed to the output file
NPS	Unit number for the nonpoint source file
NPSLOAD	Nonpoint source load which each WASP segment receives on each day of a calendar year, kg/day
NTRIB	Number of tributary areas of PRZM-3 contributing loads to a WASP segment
OUTFLG	Flag to prompt generation of output on a nonzero loading day, (0=No, 1=Yes)
PRX	Unit number for the PRZM-3 output file for EXAMS
PRZMFILE	Name of the PRZM-3 output file for EXAMS

Table 11.8 PRZWASP Bridge Program Variables	
Variable	**Description**
PRECIP	Precipitation, cm/day
RDAY	Day as real
RNF	Unit number for the runoff output file
RNFFNM	Name of the bridge program output runoff file
RUNOF	Surface runoff depth generated by PRZM-3, cm/day
ROFLUX	Surface runoff flux, $g/cm^2/day$
SEGAREA	Surface area of the WASP segment, ha
SOLFRC	Solids fraction in the sediment
SLTNHA	Soil loss, tonnes/ha
TOTTRB	Total tributary area contributing to each WASP segment from all PRAM-3 segments, ha
TNAPP	Total number of pesticide applications in a PRZM-3 run
TRIBA	Tributary area of each PRZM-3 segment contributing to each WASP segment, ha
WSDATE	WASP simulation start date (year, month, day)
WASPID	WASP segment ID number
WATNAM	Names of the two water systems namely, runoff and precipitation
YREXT	Year extension at the end of a PRZM-3 file

11.3 PRZM and VADOFT Example Input Files

The following pages contain examples using different options in PRZM and VADOFT. Below each example file is a brief summary of the scenario illustrated.

```
1 CHEMICAL, 1 HORIZON, TEMP CORRECTION, BACKGROUND LEVELS HYDROLOGY PARAMETERS
(CROP DATA FROM USDA NO.283 HANDBOOK)
                    0.72      0.03      0         15.000   1         1
                    0
                    1
                    1    0.00      20.0          80.000   1         86        78        82        0.0       0.0       0.0
          60.0
                    1
                    110582  300982  151082  1
PESTICIDE TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
                    1    1    0
ALDICARB
                    120582  0    1.0  1.00
                    1    1
SOILS PARAMETERS
                    20.0      0.3  0    0         0         0         0         0         1         1         0
                    4.3E03  1.0E-7   5.5E-3
 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.97 10.0
 8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3
                    1
                    1    20.0      1.32          0.330    0.0       0.0
                         0.012     0.011         0.000
                         1.0  .330      .133      1.0       0.3
                         8.3  10.0      60.0      0.0       0.0
                    1    1
                    0.000     0.000     0.000     0.000     0.000     0.000                       0.000                 0.000
                    0.000     0.000     0.010     0.020     0.030     0.040                       0.050                 1.000
                    0.050     0.040     0.030     0.020
                    WATR  YEAR  1         PEST     YEAR  1                   CONC                YEAR  1
                    5    YEAR
                    TUPX1  TSER    1.0E05
                    RZFX1  TSER    1.0E05
                    CHGT   TSER
                    PRCP   TSER
                    VFLX1  TCUM   1.0E05
SPECIAL ACTIONS
                    120682  KD 1    0.5
                    170682        SNAPSHOT
```

This PRZM input file represents a scenario where one chemical is applied and background levels are present at the bottom compartments of the root zone. Volatilization is simulated through the entire root zone. Plant uptake is simulated until crop harvest. One soil horizon is specified of 20 cm with a compartment thickness of 1 cm. Output is reported on a yearly basis for hydrology, flux, and concentration. Special actions are implemented following chemical application.

```
1 CHEMICAL, NO TEMPERATURE CORRECTION, PRZM INPUT FOR ZONE 1
HYDROLOGY PARAMETERS (CROP DATA FROM USDA NO.283 HANDBOOK)
                0.00    0.00    0       15.000  1       1
                0
                1
                1   0.15    20.0        80.000  1       86      78      82      0.0     0.0     0.0
        0.0
                1
                110582  300982  151082  1
PESTICIDE TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
                1   1   0
ALDICARB
                120582  0   2.5  1.00
                1   1
SOILS PARAMETERS
                20.0    0.0  0   0       0       0       0       0       0       0       0
                0.0E0   0.0E00  0.0E00
                1
                1   20.0    1.45        0.233   0.0     0.0
                    0.012   0.012       0.000
                    2.5  .233   .050    1.0     1
                0   0
                WATR  YEAR  1       PEST    YEAR  1               CONC            YEAR  1
                3   YEAR
                RFLX1 TSER  1.0E05
                RUNF  TSER
                INFL  TSER  12
```

This PRZM input file represents one chemical being applied 2.5 cm deep at a rate of 1.0 kg/ha. The soil horizon is 20 cm deep with a compartment thickness of 2.5 cm. This is an example of a basic sequence without any options.

```
3 CHEMICALS, 2 HORIZONS, EROSION, IRRIGATION, PRZM INPUT FOR ZONE 1
HYDROLOGY PARAMETERS (CROP DATA FROM USDA NO.283 HANDBOOK)
                0.72    0.00    2       0.000   1       3
                9.6  9.7  12.2    13.6    15.4    15.5
                15.7    14.5    12.5    11.3    9.5     9.0
                1
                0.15    0.14    1.0     2.0     5.8
                1
                1   0.15    30.0        80.000  3       86      78      82      0.1     0.1     0.1
        60.0
                1
                110582  300982  151082  1
PESTICIDE TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
                2   3   0
ALDICARB                    ATRAZINE            CARBOFURAN
                120582  0   2.5  1.0     2.5     2.00    1.00    2.00
                120682  0   2.5  1.0     2.5     1.00    0.00    1.00
                1   1
SOILS PARAMETERS
                45.0    0.3  0   0       0       0       0       1               1       1       0
                4.3E3   1.0E-7  2.5E-7  1.4E-7              5.5E-5          5.5E-3
                    5.5E-5
        3       0.25    0.55    .78
 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.97 10.0
 8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3
```

```
2
1       15.0    1.45    0.233   0.0     0.0     0.0     0.0
            0.012   0.000       0.000   0.010   0.010   0.000   0.015   0.015   0.000
            0.5 .233    .050    1.0     .1      1.      .3
            8.3 10.0    60.0    0.0     0.0
            0.000   0.000       0.000
        2   30.0    1.45        0.233   0.0     0.0     0.0     0.0
            0.012   0.000       0.000   0.005   0.005   0.000   0.015   0.015   0.000
            2.5 .233    .050    0.5     .1      .5      .1
            8.3 10.0    60.0    0.0     0.0
            0.000   0.000       0.000
        0   0
        WATR    YEAR    1       PEST    YEAR    1               CONC            YEAR    1
        2   YEAR
RFLX1   TSER    1.0E05
        RUNF    TSER
```

This PRZM input file represents 3 chemicals being applied at various incorporation depths and various applications simultaneously. Erosion losses are calculated. Irrigation is triggered when water capacity falls below 55 percent during the cropping period. Two soil horizons represent the 45 cm root zone with the first horizon occupying the first 15 cm and the second horizon the lower 30 cm. Pesticide runoff flux and runoff depth are plotted to a time series file.

```
1 CHEMICAL, 2 HORIZONS, NO VOLATILIZATION, BIODEGRADATION, BACKGROUND LEVELS
HYDROLOGY PARAMETERS (CROP DATA FROM USDA NO.283 HANDBOOK)
                    0.00      0.00      2          0.000    1          3
   9.6    9.7   12.2   13.6   15.4   15.5
  15.7   14.5   12.5   11.3    9.5    9.0
     0
     1
     1   0.00   45.0  80.000      3  50  50  50 0.0 0.0 0.0          60.0
     1
 110581  300981  151081      1
PESTICIDE TRANSPORT AND TRANSFORMATION AND APPLICATION PARAMETERS
     2      1      0
ALDICARB
 120281      0    0.5   0.00
 120581      0    0.5   0.00
     1      1
SOILS PARAMETERS
   45.0    0.0   0   0   0   0   0   0   1   1   1
  .005   .005   .005   .005   .001
   0.2    0.4   0.35    0.4    0.3    0.1   .0025
  0.01   0.02   0.01   0.01   10.0  1000.0
   2.0    1.0    6.0    2.0    2.0
   0.1    0.4    0.4    0.4    0.4
  4.3E3  0.0E00  0.0E00
 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.15 0.97 10.0
 8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3  8.3
     2
     1   15.0    1.50   0.350     0.0     0.0     0.0     0.0
          0.5     0.5 .000001  .00001    0.05    0.05
         0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
          2.5    .350    .150    0.06      1.
          8.3    10.0    60.0     0.0     0.0
     2   30.0    1.50   0.350     0.0     0.0     0.0    0.0
          0.5     0.5 .000001  .00001    0.05    0.05
         0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.000
          2.5    .350    .150    0.06      1.
          8.3    10.0    60.0     0.0     0.0
     1      0
 8.8000  8.8000  8.8000  8.8000  8.8000  8.8000  8.8000  8.8000
 8.8000  8.8000  8.8000  8.8000  8.8000  8.8000  8.8000  8.8000
 8.8000  8.8000
  WATR    MNTH      1    PEST    MNTH      1    CONC     DAY      1
    3    YEAR
  RFLX1   TSER        1.0E05
  THET    TSER      2
  INFL    TSER      2
```

This PRZM input file represents a scenario where biodegradation is used. Aldicarb is applied with application targeted for May 12, 1982. With the FRMFLG option set, a window application date of 10 days has been specified to check for the ideal soil-moisture conditions around the target application date. Solid, liquid, and gas phase degradation rates have been set to zero to observe only the decay resulting from biodegradation.

```
***********************************FLOW*************************************
1 CHEMICAL, 3 MATERIAL, VADOSE ZONE FLOW SIMULATION FOR ZONE 1
61        3         0    1    1    1    1         1         0         0
20        2         1    .01
 1        1         1    1    0    1    2         1         0
                    0.0       1.0       1.0                 1.0
 1                  0.0       1.0
 3
 1        20        1    40.0
 2        20        2    40.0
 3        20        3    40.0
0.00E00 0
 0        1         0.0  0.0E00  0    0                     0         0
7.12E02 .43E00  0.0E00  0.0E00
24.96E00         .43E00  0.0E00  0.0E00
 1.06E02         .41E00  0.0E00  0.0E00
 0.045E00        -1.0E00 0.145E00         2.68E00 0.626E00
 0.078E00        -1.0E00 0.036E00         1.56E00 0.358E00
 0.065E00        -1.0E00 0.075E00         1.89E00 0.470E00
   5  10
YEAR
**********************************TRANSPORT*********************************
1 CHEMICAL, 3 MATERIAL, VADOSE TRANSPORT SIMULATION FOR ZONE 1
61        3         1    1    0    1
 0        1         1    0    0    1    2         1
                    0.0       1.0       1.0                 1.0
 1                  0.0       1.0
 3
 1        20        1    40.0
 2        20        2    40.0
 3        20        3    40.0
0.0E00             1
 0        0         0.0       0.0  0    0         0         0
0.12E02 .43E00
1.480E00           0.0E00
0.12E02 .43E00
1.480E00           0.0E00
0.12E02 .41E00
1.480E00           0.0E00
 1        1.0
 1        0.0            1.0  0.0E00
 1        0.001E00       0.0E00
 2        0.0            1.0  0.0E00
 2        0.005E00       0.0E00
 3        0.0            1.0  0.0E00
 3        0.004E00       0.0E00
 1        1
 5        10
YEAR
```

This VADOFT file represents a 1 chemical simulation with 61 nodes and 60 elements at a depth of 120 cm. Retardation and degradation are simulated.

```
**********************************FLOW*************************************
1 CHEMICAL, 3 MATERIAL, 91 NODES, VADOSE ZONE FLOW SIMULATION FOR ZONE 1
91      3       0   1   1   1   1       1       0       0
20      2       1       .01
 1      1       1   1   0   1   2       1       0
                0.0     1.0     1.0             1.0
 1              0.0     1.0
 3
 1      20      1       40.0
 2      20      2       40.0
 3      50      3       120.0
0.00E00 0
 0      1           0.0 0.0E00  0       0       0       0
7.12E02 .43E00  0.0E00  0.0E00
24.96E00        .43E00  0.0E00  0.0E00
 1.06E02        .41E00  0.0E00  0.0E00
 0.045E00       -1.0E00 0.145E00        2.68E00 0.626E00
 0.078E00       -1.0E00 0.036E00        1.56E00 0.358E00
 0.065E00       -1.0E00 0.075E00        1.89E00 0.470E00
 5      10
YEAR
**********************************TRANSPORT********************************
1 CHEMICAL, 3 MATERIAL, 91 NODES, VADOSE TRANSPORT SIMULATION FOR ZONE 1
91      3       1   1   0   1
 0      1       1   0   0   1   2       1
                0.0     1.0     1.0             1.0
 1              0.0     1.0
 3
 1      20      1   40.0
 2      20      2   40.0
 3      50      3   120.0
0.0E00          1
 0      0           0.0     0.0 0       0       0       0
1.20E00 .43E00
1.000E00        0.0E00
1.20E00 .43E00
1.500E00        0.0E00
1.20E00 .41E00
1.000E00        0.0E00
 1      0.0
 1      0.0             1.0 0.0E00
 1      0.001E00        0.0E00
 2      0.0             1.0 0.0E00
 2      0.005E00        0.0E00
 3      0.0             1.0 0.0E00
 3      0.004E00        0.0E00
 1      1
 5      10
YEAR
```

This VADOFT input file represents 91 nodes and 90 elements at a depth of 200 cm. Dispersion, retardation, and degradation are simulated.

```
***********************************FLOW*************************************
3 CHEMICAL, 2 HORIZON, 1 MATERIAL, VADOSE ZONE FLOW SIMULATION FOR ZONE 1
61      1       1   1   1   1   1       1       0       0
20      2       1       .01
 1      1       1   1   0   1   2       1       0
                0.0     1.0     1.0             1.0
 1              0.0     1.0
 2
 1      20      1       50.0
 2      40      1       80.0
0.00E00 0
 0      1           0.0 0.0E00  0       0       0       0
7.12E02 .43E00  0.0E00  0.0E00
0.045E00        -1.0E00 0.145E00        2.68E00 0.626E00
 5      10
YEAR
**********************************TRANSPORT*********************************
3 CHEMICAL, 2 HORIZON, 1 MATERIAL, VADOSE TRANSPORT SIMULATION FOR ZONE 1
61      1       1   1   0   1
 0      1       1   0   0   1   2       1
                0.0     1.0     1.0             1.0
 1              0.0     1.0
 2
 1      20      1       50.0
 2      40      1       80.0
0.0E00          2       0.0E00  2       0.0E00  2
 0      0           0.0         0.0     0       0       0       0
0.00E00 .43E00
1.000E00        1.000E00    1.000E00    0.0E00  0.0E00  0.0E00
 1              0.1 2   0.1
 1              0.1 2   0.1
 1              0.1 2   0.1
 1              0.0 1.0 0.0E00
 1      0.000E00    0.000E00    0.000E00        0.00E00 0.00E00 0.0E00
 1      1
 5      10
YEAR
```

This VADOFT input file represents 3 chemicals having initial concentrations at the top two nodes. Dispersion, degradation, and dispersion are simulated over 2 horizons with a total depth of 130 cm. 21 nodes are placed at 2.5 cm distances from 20 elements and the remaining 40 nodes are placed at 2 cm distances from the remaining 40 elements.