SESOIL

A SEASONAL SOIL COMPARTMENT MODEL

by

M. Bonazountas
J. Wagner

1981
First
Version

Arthur D. Little, Inc.
Cambridge, Massachusetts

SESOIL MODEL UPDATES

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"SESOIL"

A SEASONAL SOIL COMPARTMENT MODEL

by

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This Model Version Prepared for

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Office of Toxic Substances
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Task Manager: Annette Nold
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ABSTRACT

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Prepared for U.S. Environmental Protection Agency, Office of Toxic Substances
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SESOIL is a "user-friendly" statistical mathematical model designed for long-term environmental pollutant fate simulations that can describe: water transport (quality/quantity); sediment transport (quality/quantity); pollutant transport/transformation; and soil quantity. Simulations are performed for a user specified soil column (designated as compartment), extending between the ground surface and the lower part of the saturated soil zone of a region. The simulation is based upon a three-cycle rationale, each cycle being associated with a number of processes. The three cycles are the: (1) water cycle which takes account of rainfall, infiltration, exfiltration, surface runoff, evapotranspiration, groundwater runoff, snow pack/melt and interception, (2) sediment cycle which takes account of sediment resuspension (because of wind) and sediment washload (because of rain storms), and (3) pollutant cycle which takes account of convection, diffusion, volatilization, adsorption/desorption, chemical degradation/decay, biological transformation/uptake, hydrolysis, photolysis, oxidation, complexation of metals by organics and nutrient cycles. Model development has been sponsored by the U.S. Environmental Protection Agency and has been validated--as an unsaturated soil zone pollutant transport model--at waste land treatment disposal sites. The entire model development has not yet been accomplished; however, certain model features are operational.

Key words: SESOIL, mathematical modeling, pollution, soil quality, groundwater, pathways, land treatment, waste disposal, multi-media modeling.

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1.0 INTRODUCTION

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1.0 INTRODUCTION

1.1 Preamble Notes

- This modeling effort and its documentation have been accomplished at an expense (professional time, all other expenses) of less than $70,000 and, as such, they should be evaluated or criticized correspondingly.

- This documentation is a preliminary draft and has not been publicly released by the U.S. Environmental Protection Agency; however, it has been circulated to scientists for comments on its technical approach. Since model developers have not published their original work, quotations related to SESOIL or the processes described in this documentation must be referenced (Bonazountas and Wagner 1981) as indicated in the abstract.

- All models are good as long as: (i) users are aware of the assumptions upon which they have been developed; and (ii) they are employed and applied appropriately.

- SESOIL is a "user-friendly" model that can be operated with very few input data, mostly available from government records or other literature (e.g., handbooks). This has been achieved with a sophisticated mathematical description of all SESOIL processes, a task that has exceeded previous similar efforts of the literature. However, "amateur (modelers) can do more harm than city fellers on a farm" (Groundwater 1981); therefore, potential users should be careful when employing this friendly and easy to use package.

- Most environmental models of the literature can be "forced" by their developers to predict almost exactly what their developers desire to predict--via calibration coefficients; this is not a secret among modelers. In that respect, SESOIL is at an advantageous position because no calibration coefficients accompany its theory; however, users should validate model predictions with available data as far as possible. (See also Section 3.4.)

- The authors intend to continue improving SESOIL--both in its newly developed scientific basis and its range of applicability--and to update this documentation as appropriate. In that respect, they: (a) solicit any critical review, and (b) kindly ask users to make sure to have the latest version of the model code.

- SESOIL has been carefully developed and its software has been tested; however, the ultimate responsibility for its use rests with the user, since this is the first version of the model, and developers have not repeatedly applied the model to the real world. However, developers intend to correct any errors which users may report.

- This SESOIL version presents only a subset of all model features. The computer code, therefore, contains control nodes and dummy statements and loops that will facilitate potential future development. It would be inappropriate for a user to modify the code without notifying model developers, because this may result in incorrect calculations.

- Roughly speaking, this version of SESOIL can be employed as: (i) a hydrologic basin model (watershed, unsaturated soil zone, groundwater recharge); and (ii) a pollutant transport model of the unsaturated soil zone, however, interacting (for mass balance purposes) with both the watershed and the groundwater of a soil environment. (See Section 2.0.)

- Strong appreciation is given by model developers to all the people who have supported this effort. (See Section 1.4.)

- Users are advised to read this documentation carefully and, in case of questions, to contact developers. The authors would be happy to provide assistance--as far as possible--to potential users.

1.2 Organization of this Documentation

The main intentions while drafting this documentation have been: simplicity, clarity and expandability; therefore, it has been structured around two major parts containing:

(1) an overall presentation, and
(2) twenty appendices

It is believed that this documentation format allows:

(1) readers to clearly understand both the various scientific areas modeled (described in the appendices) and the SESOIL operations, and

(2) users to efficiently apply SESOIL following knowledge gained after reading the entire documentation.

The overall presentation is covered in three main sections:

- Section 1.0 - Introduction
- Section 2.0 - SESOIL Description
- Section 3.0 - User's Manual

The 20 appendices are self-contained, short documents and give both background information, and mathematics employed for the various areas of science (hydrology, sedimentation, chemistry, other) modeled via SESOIL. Each appendix is designated with two characteristic letters as shown in the Table of Contents of this documentation. References are given in each section or each appendix and are aggregared in Appendix RE.

It is believed that this format permits expansion, improvement and substitution of the background and parts of the theory given in this documentation without affecting the overall model presentation. This loose-leaf binder version also provides the possibility of single-page substitutions in the near future. The latest version of a page is printed with a date next to the page number; if no date is given, the date of the first page of the section of appendix is assumed. The appendix format facilitates reading because the same text is not to be found in two different chapters; it also facilitates users who do not actually care for the background during an application.

A potential user, however, is advised to read all sections of the report, namely, from the Introduction to the last appendix (Appendix MI, Miscellaneous). A user who desires to only use a few aspects of the model operation (e.g., pollutant cycle) would have to refer only to the corresponding appendix (i.e., Appendix PT, Pollutant Transport Cycle). In the computer code, reference is made to the equations of individual appendices.

1.3 Raison d'Être of SESOIL

SESOIL is the acronym for a SEasonal SOIL compartment model, a development motivated by the individual needs of various technical and regulatory offices within the U.S. Environmental Protection Agency. SESOIL was designed to be an integrated package of a "user-friendly" tool for modeling hydrologic, sediment and pollutant cycles in soil "compartments." Many reasons supported this development as described below.

First, in reference to a soil compartment (see cover figure), we have today a variety of excellent watershed simulation (e.g., Johanson et al 1979) models, a variety of unsaturated soil zone numerical (e.g., Adams et al 1976) models, a variety of stochastic soil moisture models, or a number of watershed erosion and sediment transport models (e.g., Leytham et al 1979). However, we do not have an integrated, and developed from "scratch," soil compartment mathematical model, designed for long-term (defined below) environmental process simulations that can describe simultaneously water transport (quantity/quality), sediment transport (quantity/quality), pollutant fate (transport/transformation) and soil quality. SESOIL has been designed to fill this need.

Second, current regulations (e.g., the Resource Conservation Recovery Act) require that decision makers consider the environment as a continuum. Thus, pollutant fate must be modeled in this continuum--encompassing air, soil and water compartments--rather than in single medium. This request brought model users to the dilemma of "which model to interface with what model" in order to create a useful continuous package (Fiksel et al 1981). In many cases, data requirements and time resolutions of the various models were so different, that interfacing requirements necessitated the writing of complicated or lengthy data management computer programs. In addition, separate calibration procedures may have to be followed for different submodels (e.g., watershed submodel, unsaturated soil zone submodel) of one and the same environmental compartment (i.e., soil compartment), resulting in much duplication of effort.

In response to the above regulations, an immediate need for integrated modeling packages has emerged, leading to a boom in environmental modeling and the use of models as decision mechanisms. This immediate necessity has not left enough time to model developers to "sit back" and develop truely "integrated" approaches. The difficulties created by employing and interfacing incompatible submodels is analogous, for example, to the industry where in an attempt to quickly release a new product, manufacturers assemble--not always successfully--a new product with parts desinged for other similar situations. With SESOIL, an attempt is made to better integrate certain model categories and provide an efficient interfacing module between air and water compartmental models of the literature toward a formulation of an environmental continuum.

Third, a characteristic of the existing environmental models is the simulation time step. Most of the watershed soil models consist of a set of equations solved after each storm event. Therefore, hydrology, sedimentation and pollution mass transport at the end of a season (e.g., month, year) is estimated by summing up distribution estimates after each storm event. This necessitates lengthy data inputs of hydrologic records, a fact that makes use of models very time consuming, and may not necessarily lead to more accurate cycle (hydrology, sediment, pollutant) estimates. The SESOIL seasonality provides a different and flexible approach to this issue.

Principally, SESOIL is intended to be a model that:

(1) is seasonal--provision is also made for storm-by-storm simulations;

(2) is independent from the size and the shape of the soil column, i.e., independent from the numerical discretization mathematical problems of some models;

(3) is user-friendly and requires a minimum number of hydrologic and other input data;

(4) can study the hydrologic cycle, the sediment cycle, pollutant fate and soil quality of the compartment in one integrated effort;

(5) is operational at various "levels" depending on users' needs and data availability;

(6) is operational either as a self-standing soil compartment model or as a model to be interfaced with an atmospheric and a fresh water body model toward the formation of a mathematical environmental continuum;

(7) does not require calibration of coefficients that do not describe physical or chemical parameters, yet it might be calibrated via its basic parameters if field data are available;

(8) a user can operate with data obtained from existing data bases (even on-line) or from handbooks;

(9) is expandable in logic and capabilities; and

(10) can be operated at minimum expense (time, cost) and by uses who may or may not exactly follow all the theoretical background of the various processes/subroutines modeled.

The attempt to accomplish the above 10 desires/needs is the "raison d'être" of SESOIL. It is hoped that it will become a valuable tool in environmental quality planning. The fact that SESOIL is user-friendly, comprehensive and inexpensive to run should stimulate users to take advantage of its benefits.

1.4 Acknowledgements

This report has been submitted by Arthur D. Little, Inc., in partial fulfillment of the requirements of EPA Contract No. 68-01-6271. The study was performed for the U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. The authors would like to extend their graditude to all the contributors to this project.

Special thanks are extended to the Arthur D. Little, Inc., staff members who have contributed extensively to this report: Warren Lyman (Appendices HD, CE, CM), Diane Gilbert (Appendices SR, ID), Joo Hooi Ong (Appendix NV), Kate Scow (Appendix DE), Irene Rickabaugh (report coordination), Linda Nazaretian and Emma Wood (general support).

The authors extend their thanks to all scientists within EPA who have assisted them on this and the previous SESOIL contracts.

Dr. Annette Nold of the Office of Toxic Substances (OTS) has been the Project Officer of this first finalized model version (1981). She has assisted the authors in the improvement of the model over the past versions, she has been patient with developmental problems, and she was always ready to compile scientific and other information for us. We have appreciated our collaboration with her.

Dr. William Wood, at the head of OTS Modeling Group, has been the Project Officer and Mrs. Joan Leffler supervised in 1979 the EPA contract which lead to the conceptualization of SESOIL (Aravamudan et al 1979). The authors appreciate both the scientific advice and the support received for the SESOIL concept.

Following its conceptualization in 1979, a model improvement and an application were sponsored in 1980 by the EPA, Monitoring and Data Support Division (MDSD). Mr. Michael Slimak, at the head of MDSM, has been the Project Officer and Mr. John Segna supervised that task. The authors appreciate the overall advice of Mike Slimak, the technical advice of John Segna and the ongoing support received from this office.

The authors would like to extend their appreciation to: Mr. Michael Callahan, head of the Exposure Assessment Branch, EPA/OTS; Dr. James Dragun, EPA/OTS, for his participation in the model development in 1979 and for reviewing the chemistry aspects of the model and insisting on valuable improvements; and Dr. Ronald Kickert, EPA/Corvallis Research Laboratory for requesting detailed information regarding the model and making substantial comments.

The authors express their graditude to Professor Peter S. Eagleson, Massachusetts Institute of Technology, Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics, who has voluntarily reviewed and has made suggestions for the application of his annual water balance theory (Eagleson 1978) in respect to the long-term (averaged) estimates of pollutant concentrations in the unsaturated soil zone of SESOIL.

Appreciation is expressed to Professor George R. Foster, Purdue University, Agricultural Engineers Department, for his generosity in releasing his sedimentation theory (Foster et al 1980) and its computer code to the authors, although integration of his theory (Appendix SW) into the SESOIL framework has not yet been initiated.

Finally, we would like to thank Ms. Gayaneh Contos at Versar, Inc., and Dr. George Harris, at Arthur D. Little, Inc., who have managed this contract with the EPA; Dr. Alfred Wechsler, Dr. Alan Eschenroeder, Dr. Philip Levins; and Dr. Frank Feeley who have supported us in many different ways.

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2.0 THE SESOIL MODEL

2.0 THE "SESOIL" MODEL

This section contains only an executive summary of all appendices presented in this documentation, and as such it does not offer anything new to model readers or users.

The model developers have purposely kept this section brief because;

(1) They feel that users of this first SESOIL version should read/consult--for their own benefit--the entire theory of each major area of science presented in each appendix separately, in order to appreciate both the capabilities of SESOIL and the limitations or assumptions supporting this model version.

(2) SESOIL development has not yet been completed and since the model is limited to simulating the unsaturated soil zone of the soil compartment, the developers do not want to give the impression of having accomplished all their goals.

The executive summary of SESOIL is presented in the following pages. Please contact the authors with any questions regarding this model version and/or questions as to potential (future) capabilities of the model.

"SESOIL"

A SEASONAL SOIL COMPARTMENT MODEL

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GENERAL INFORMATION

SESOIL is a newly developed "user-friendly" mathematical model for long-term environmental pollutant fate simulations that has been designed to describe:

- water transport (quality/quantity),
- sediment transport (quality/quantity),
- pollutant fate (transport/transformation), and
- soil quality

within a user specified soil column (designated as compartment) extending between the ground surface and the lower part of the saturated soil zone of a region. (See figure 2-1.)

SESOIL is designated as "seasonal" because it statistically estimates the pollutant distribution in the soil column after a season (e.g., year, month) "directly." It does not estimate pollutant distribution indirectly (i.e., by summing up pollutant distribution estimates in the soil column after each major storm event) as do existing models described in the literature.

SESOIL has been designed to become, in the long run: (1) a watershed model; (2) an unsaturated soil zone model; and (3) a groundwater model. However, the current SESOIL version can only simulate processes of an unsaturated soil zone of a compartment and can roughly account for certain watershed aspects of the compartment. The groundwater aspects of SESOIL are part of the long-range plans of the developers. As such, SESOIL is designed to simulate point or nonpoint pollution from major land use categories, and soil-column pollution originating on the watershed (future development), in the soil column (presently) and in groundwater (ultimate development).

SESOIL is designed as: (1) a self-standing soil compartment model, and (2) a compartment model to be interfaced with other atmospheric and water body models towards the formation of a mathematical environmental continuum (multi-media environmental modeling). The current version can

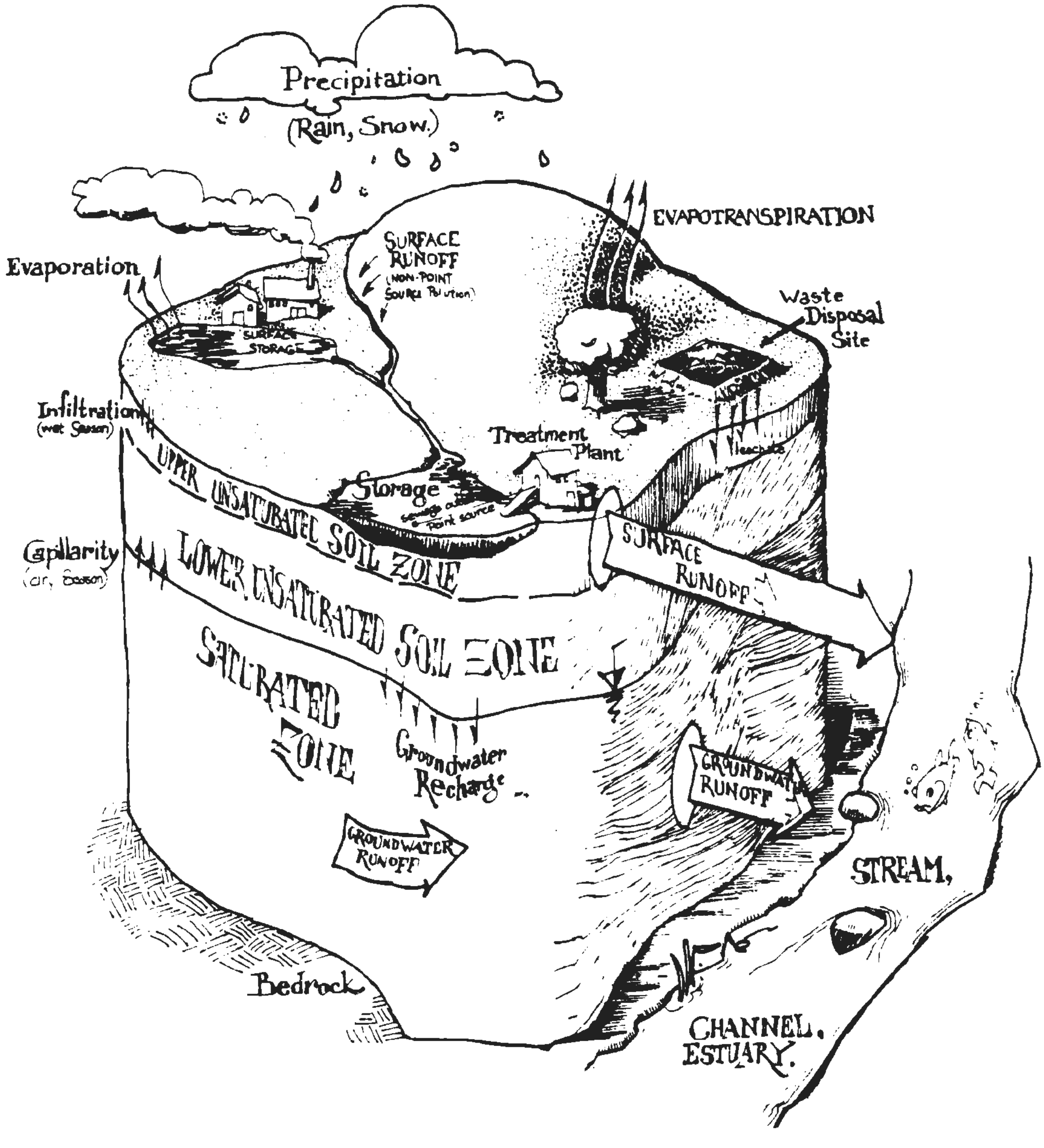

Figure 2-1 SCHEMATIC PRESENTATION OF THE SESOIL COMPARTMENT

be easily interfaced with a groundwater model toward the formulation of an unsaturated/saturated soil compartment model.

SESOIL simulations do not require the extensive and time consuming calibration procedures of other models, although it may be easily calibrated to agree with field records. The model employs theoretically derived equations driven by climatic, soil property, geometric and chemical compound property data. In addition, simulations are performed for the entire compartment (i.e., watershed, unsaturated and saturated soil zones) in one effort in order to circumvent the known calibration difficulties of simulation models. As such, SESOIL may be employed as a precalibration model for other simulation models.

There exist no artifically imposed limitations in: (1) timing and sizing the soil compartment (cell) and (2) the shape of the compartment per se. If the soil column is chosen small enough (i.e., finite approach), SESOIL encompasses the concept of the numerical models (e.g., finite difference/element models); if the soil column is chosen large enough (e.g., a river basin), SESOIL becomes a sophisticated one-compartment model. The unsaturated soil zone of the model can be discretized to account for more than one soil layer in order to best meet simulation needs.

SESOIL is designed to provide great flexibility to the user who can execute various "levels" of model operation, the criterion for a level selection being data availability and study objectives. The major advantage of SESOIL is that it can be executed with easily obtainable input data because this information can be compiled from existing data bases (e.g., NOAA) and known references for the pollutant and soil properties. A data management structure accompanies SESOIL. If the model is not linked to existing data bases, then the number of input data can be less than 50 as contrasted to the other numerical models which may require more than 500, because: (a) the model employs theoretically derived equations which may not require calibration, and (b) the statistical simulation does not take place after each major storm event.

Potential applications of SESOIL include long-term leaching studies from waste disposal sites, acid rain, pesticide and sediment transport on watersheds, contaminant exposure assessments, pre-calibration runs for other simulation models, hydrologic cycles of soil compartments, etc.

This model version has been developed on behalf of the U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C. A model application at industrial land treatment sites has been sponsored for a slightly different model version by the Monitoring and Support Data Division, EPA, Washington, D.C.

SIMULATION CYCLES

The simulation is structured around three cycles, each cycle being associated with a number of processes. These are the:

- Hydrologic cycle which takes account of:
  rainfall, infiltration, soil moisture, surface runoff, exfiltration, evapotranspiration, groundwater runoff, capillary rise, snow pack/melt (not operational in this version) and interception (not operational).

- Sediment cycle which takes account of:
  sediment resuspension (due to wind) and sediment washload (due to rain storms), not operational in this version.

- Pollutant cycle which can take account of:
  advection, diffusion, volatilization, adsorption/desorption, chemical degradation/decay, biological transformation and uptake, hydrolysis, photolysis, oxidation, cation exchange, complexation chemistry (metals by organics) and nutrient cycles (not operational).

The hydrologic cycle controls the sediment cycle, whereas both previous cycles control the pollutant cycle. Cycles, processes, mathematical modeling, application and validation issues are summarized in the following paragraphs.

(1) The hydrologic cycle is based on a statistical dynamic formulation of vertical water budget at a land-atmosphere interface (Eagleson 1978), adapted to account for monthly simulations. Uncertainty of the hydrologic cycle simulation is expressed via probability density functions of the independent climatic variables and yields derived probability distributions of the dependent water balance elements: surface runoff, evapotranspiration, and groundwater runoff. Some details of the hydrologic analysis are (Eagleson 1978):

Seasonal point precipitation is represented by Poisson arrivals of rectangular gamma distributed intensity pulses that have random depth and duration. Infiltration and exfiltration are described by the Philip equation (Philip 1969), which assumes the medium to be effectively semi-infinite, and the internal soil moisture at the beginning of each storm and inter-storm period to be uniform at its long-term space-time average. Gravitation and percolation to groundwater is assumed to be steady throughout the time step of a simulation and at a rate determined by the long-term space-time average seasonal soil moisture. Capillary rise from the water table is assumed to be steady throughout the season and to take place to a dry surface. Soil properties, soil moisture, climate and functional relationships derived by Brooks and Corey (1966) describe the wetting drying soil intrinsic permeability temporal variation.

Seasonal bare soil evaporation and vegetal transpiration are calculated for the interstorm periods as functions of properties of the climate, the storm sequence, the surface, the soil and the average rate of a derived potential evapotranspiration. The work of Penman (1963), Van den Honert (1948), Cowan (1965) is employed (Eagleson 1978). The distribution of surface runoff volume is derived from the distribution of rainstorm intensity and duration and the use of the previously discussed infiltration equation. Specific subroutines of the model have been validated in the literature. The annual dynamic water balance of the model has been validated by Eagleson (Eagleson 1978). The monthly dynamic water balance of the model has been applied; however, it was not validated as a hydrologic routine per se. Validation of the routine was undertaken in connection with pollutant migration in the unsaturated soil zone (Bonazountas and Wagner 1981).

(2) The sediment cycle accounts for both sediment washload due to precipitation and sediment (dust) resuspension due to wind. Two sediment washload routines are accounted by SESOIL: (a) an annual sediment yield equation based on the Universal Soil Loss Equation (USLE) as developed and documented by the U.S. Department of Agriculture (Wischmeier and Smith 1978) and employed by other watershed models of the literature; and (b) a monthly sediment washload routine based on theoretically derived equations and first physical principles (Foster et al 1980).

The theoretical monthly sediment routine can account for: (a) various sizes and shapes of watersheds (e.g., overland flow, channel flow, impoundment, pond); (b) detachment of soil particles, transport and deposition of soil particles, rill and inter-rill erosion on the watershed; (c) sediment characteristics and other fundamental relationships of precipitation energy and erosion sediment transport. The sediment washload model is based on the fundamental theoretical models of Yalin (1963), Foster et al (1980), and Cooley (1980). The sediment routine has not been validated with SESOIL's hydrologic cycle.

The dust resuspension routine estimates the losses from the surface of the SESOIL soil column of any pollutants associated with surface particles. The losses due to physical removal of the particles that have an associated pollutant load are calculated as a function of particle characteristics (chemical composition, diameter, etc.) and weather conditions. Variables such as soil moisture and wind speed are utilized; however, this routine has not been validated yet with SESOIL's hydrologic cycle.

(3) The pollutant cycle accounts for more than 12 chemical processes. (See previous section.) There exists no single equation that can optimally describe each of the pollutant processes under all all conditions, so some alternative simulation options are possible; for example, adsorption is modeled as sorption to soil particles, partitioning to soil organic carbon, or as an ion exchange process simply by varying the input parameters. Another example is volatilization from soil to air that can be modeled with more than one user specified equation (theoretical, experimental).

The pollutant cycle is simulated in more than one soil sub-compartments, each one consisting of three phases: soil-air, soil-moisture and soil-solids. The pollutant cycle routine has been rederived from a pollutant mass balance equation that can be expanded or modified easily in order to account for additional processes and model improvements.

MODEL VALIDATION

A pollutant transport application/validation study was undertaken to assess the long-term predictive pollutant pathway capabilities of SESOIL using field monitoring data and supporting background information already collected as part of another study (monitoring program). The model has been employed as (1) an upper unsaturated soil zone model at two industrial land treatment waste sites, and (2) as an exposure assessment model for fictitious environmental soil compartments. The behavior of two organic pollutants (napthalene, anthracene) and four inorganic pollutants (copper, chromium, nickel, sodium) at two sites was simulated and analyzed. Predicted concentrations and laboratory measured concentrations agreed within expected limits. Calibrated and non-calibrated model runs have been compared (Bonazountas et al 1981).

SESOIL has been also employed as a mathematical tool for exposure assessment studies for predicting the behavior of pollutants in soil compartments, and it proved to be an interesting application for screening, analyzing and prioritizing pollutant behaviors in soil systems (Bonazountas and Wagner 1982).

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3.0 USER'S MANUAL

SECTION 3.0

USER'S MANUAL

FIGURES

TABLES

3.1 INTRODUCTION

3.1.1 General Capabilities

This version of SESOIL can be used as:

(1) a hydrologic cycle model for the watershed and the unsaturated soil zone of the compartment

(2) as a hydrologic and pollutant cycle model for the unsaturated soil zone of the compartment.

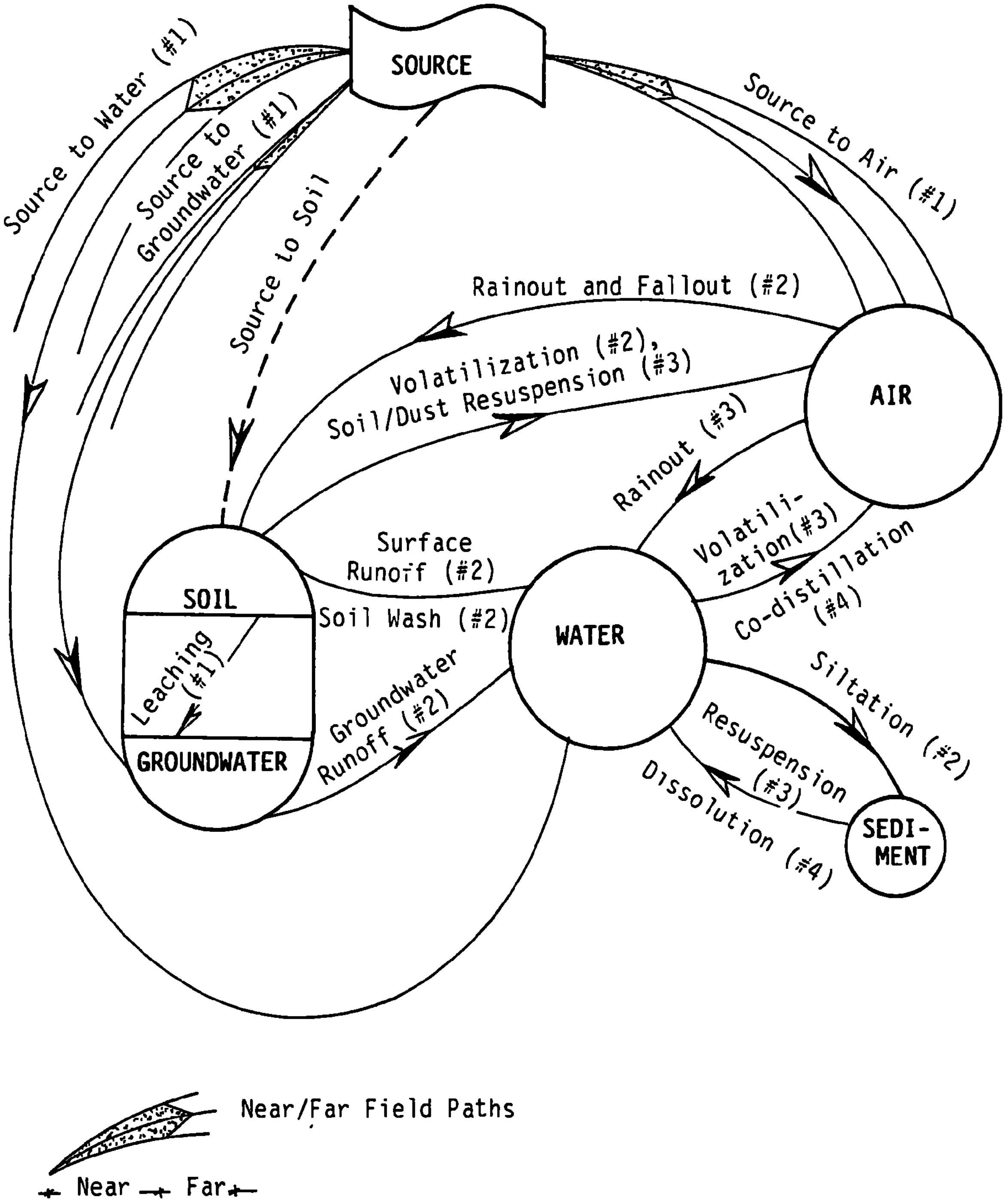
SESOIL is still under development, therefore the following sections only guide a user through details and the input/output data of this version of the model. This section (User's Manual) might be expanded in the future to a self-contained document with guidelines for problem identification, problem structure, optimal compilation of input data, model validation and calibration procedures.

3.1.2 Phenomenology in the Soil Compartment

A soil "compartment" (or cell) is defined as a soil column extending between the ground surface and the bottom of the "upper" saturated soil zone. As such, the soil compartment interacts with the air and the water compartments of an environment as schematically shown in the cover figure of this document (also Figure 2-1). It is evident that the upper saturated soil zone might be underlain by impermeable soil layers and other saturated soil zones (or aquifers); however, these zones are not part of the soil compartment as previously defined.

Physical and chemical processes or phenomena of importance to the quality of a soil compartment are the hydrologic cycle, the sediment cycle, the biologic cycle, and the pollutant cycle. Processes important to each cycle are described in the appendices HY through PT of this documentation.

When released into the environment, pollutants move by a number of fate (transport/transformation) mechanisms. For some pollutants such as phosphorus, ammonia and certain pesticides, surface runoff, soil wash and dust particles might be the primary carriers to the final place of deposition. Other pollutants are directly applied to plants and reach the soil through drift, wash-off or when the plant decays. Many pollutants are transported through the hydrologic cycle or the hydrologic mechanisms of watersheds and have a final destination in the water compartment of an environment. The figure of the next page (Figure 3-1) is a generalized pathway diagram of toxic substances in the environment; from source-to-receiver. The SESOIL model deals with processes interacting and related to the soil compartment of the environment; the "elliptic" subcompartment in this figure.



#1 Direct discharge pathways.

#2-4 Intermedia discharge pathways (primary, secondary, potential).

Degradation of substances can take place in any compartment.

Out-of and into basin transfers are not shown.

Source: Fiksel et al (1981).

FIGURE 3-1: ENVIRONMENTAL PATHWAYS OF TOXIC SUBSTANCES

The manner in which pollutants enter the hydrologic cycle of the compartment depends on the characteristics of the pollutant source, such as location, time and physical or chemical form of pollutant. Gaseous, emulsified and dispersed airborne pollutants enter water by precipitation and/or dry fallout. Soluble pollutants and/or pollutants merely mixed in the water may then enter the soil. Relatively insoluble pollutants discharged to water or soil either are dispersed or are transported by stormwater runoff or are entrained by wind and subsequently redeposited. Pollutants are also adsorbed and desorbed by soil particles and then can be transported by the water cycle in either state.

A major characteristic of a soil compartment -- as contrasted to a water or an air compartment -- is that the temporal physical and the chemical behavior of the compartment is governed by both; out-compartmental forces such as precipitation, air temperature, solar radiation, and in-compartmental forces/features such as soil structure and biology. This characteristic is also one of the main reasons why soil compartmental mathematical modeling is much more complex than water or air modeling.

When dealing with mathematical modeling of pollutant transport in soil compartments, it is a natural way to study pollution migration in the hierarchical order: (1) hydrologic cycle, (2) sediment cycle, which is primarily governed by the first cycle, and (3) pollutant cycle, which is primarily governed by the two previous cycles. It has been, however, a frequent practice to model pollutant migration based upon soil-moisture migration, so that no soil moisture presence results in no pollutant migration. Although the latter is not the case in SESOIL (eg. appendix VO), the logical hierarchy hydrologic cycle, sediment cycle, pollutant cycle has been followed in this modeling effort.

3.1.3 Mathematical Modeling Issues

Environmental mathematical models can be classified in general into: deterministic models which describe the system as cause/effect relationships, and stochastic models which incorporate the concept of risk, probability or other measures of uncertainty. Deterministic and stochastic models may be developed from: observation, semi-empirical approaches, and theoretical approaches. In developing a model, scientists attempt to reach an optimal compromise among the above approaches given the level of detail justified by both the data availability and model objectives.

Deterministic models can be classified into simulation models which employ a well accepted empirical equation, that is forced via calibration coefficients, to describe a system, and analytic models in which the derived equation describes the physics/chemistry of a system. Both the simulation and the analytic models can employ numerical solution procedures for their equations. Although the above terminology is not standard in the literature, it has been used here as a means of outlining some of the concepts of modeling.

This SESOIL version employs the stochastic approach for the hydrologic cycle, and the deterministic approach for the other physical or chemical processes. The sediment cycle of this model will also employ the stochastic approach. Parameters of simulation or empirical models are determined by calibrating the model output against large masses of observational data. This procedure involves curve-fitting and least-squares analyses, and requires extensive field data information. In order to by-pass many calibration difficulties, SESOIL employs primarily theoretically developed stochastic or deterministic routines. Thus, model input variables describe physical or chemical parameters and can be determined or obtained independently either from laboratory analyses, field investigation, handbooks or data bases.

The choice of theoretical stochastic or analytic deterministic models does not imply -- of course -- that these models are always superior to empirical or simulation models. The desire for an alternate approach was of importance, therefore a "modular" structure has been employed for SESOIL, so that a substitution of a particular equation, theory, or subroutine (modules) can be undertaken at any time -- along the course of a model improvement -- and in a straightforward manner. To achieve effectiveness in the modular approach a new, efficient and chemistry strong concept has been employed for the pollutant transport cycle (appendix PT) of SESOIL.

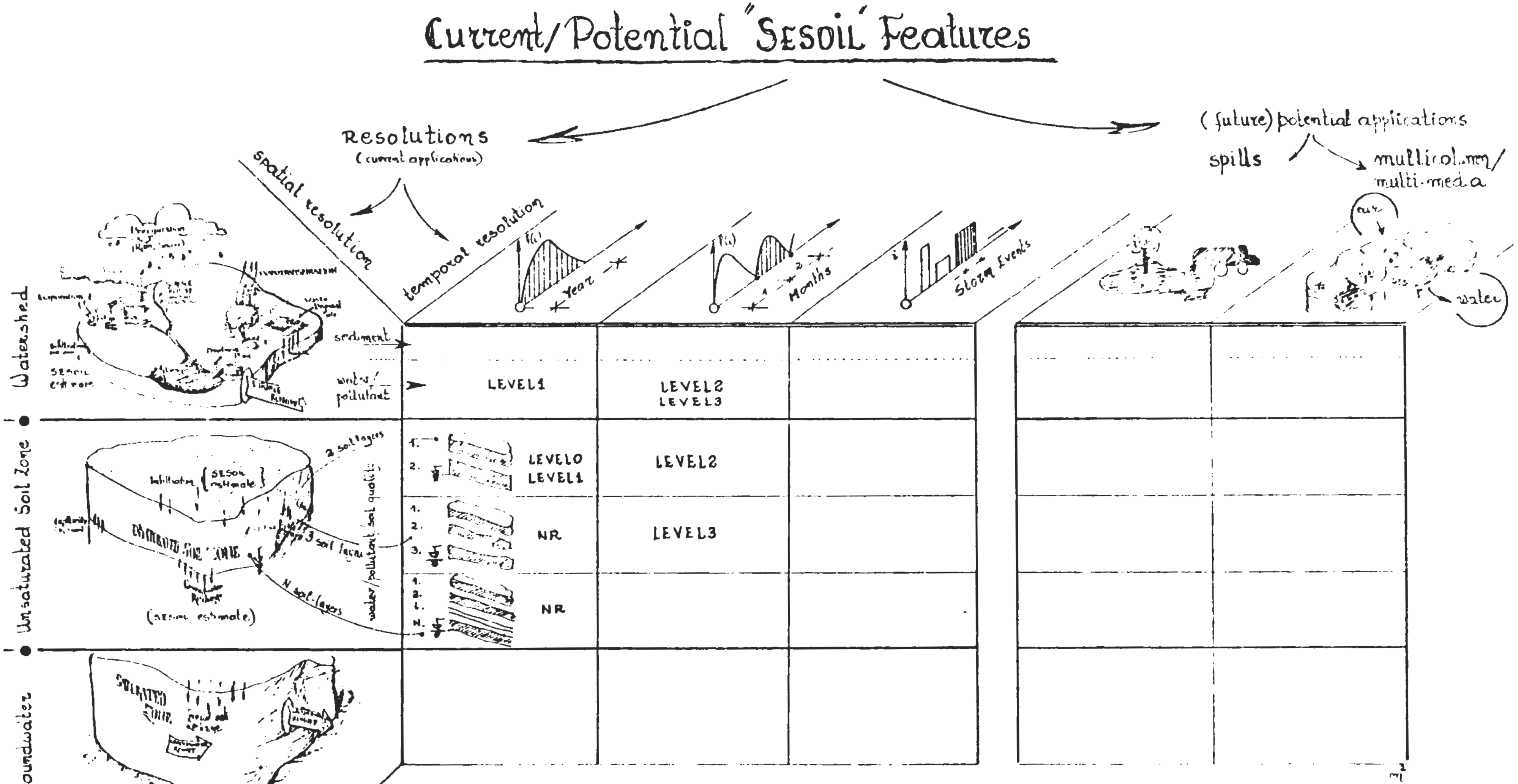
3.1.4 Levels of SESOIL Operations/Capabilities

3.1.4.1 General

Discussions in the following sections are oriented towards the conceptual approaches employed in this methodology and are not intended to fully describe the fundamentals of all the cycles -- hydrologic, sediment, pollutant. For detailed information the reader is referred to the individual appendices.

SESOIL encompasses -- by design -- many features. It can be, for example, a watershed model, an unsaturated soil zone hydrologic model, a sediment transportation model, a soil chemistry model, etc. It can also be operated at annual or monthly time steps, for one-, two-, or three-soil layers. In the future it may be expanded to incorporate the fate of second phase chemicals in the soil column, or nutrient cycles and sedimentation after each storm event. Many SESOIL potential features are schematically presented on the next page (Figure 3-2); however, only a few features are operational at the present time, and these features are focused around the unsaturated soil zone and are offered to users in "integrated" packages designed as "levels" of operation.

In this model version, the four different levels of operation are LEVEL0, LEVEL1, LEVEL2 and LEVEL3. Each level is associated with certain temporal and spatial resolution characteristics, and each has different specific input requirements.



LEVELS OF SESOIL OPERATIONS -- THIS DOCUMENTATION

- Data availability and study objectives determine LEVEL use
- Additional LEVELS available upon request
- NR - Not relevant

CURRENT APPLICATIONS (existing levels)

- Hydrologic cycle partitioning, Pollutant fate, Exposure Assessments, waste sites, etc.

(FUTURE) POTENTIAL APPLICATIONS (to be develop levels)

- Chemical spills, Multi-media modeling, Groundwater mod.

FIGURE 3-2 CURRENT AND POTENTIAL SESOIL RESOLUTIONS, FEATURES, AND CAPABILITIES

3.1.4.2 LEVELO

LEVELO is the simplest operational version of the model and does not require knowledge of the hydrology of the compartment (area modeled). SESOIL is employed as an unsaturated soil zone model interacting hydrologically (for mass balance purposes) with both the watershed and the groundwater table.

This level can be employed for pollutant transport simulations in "fictitious" compartments. The unsaturated soil zone compartment consists of two distinct layers, as shown in Figure 3-3, namely the upper unsaturated soil zone (or watershed zone), and the lower unsaturated soil zone. The saturated soil zone (groundwater) is not part of a level of operation of this model version.

The simulation is performed annually and for only one year. The user has to input: (1) the annual averaged values of rainfall depth, soil moisture (unsaturated soil zones), infiltration and groundwater recharge depths; (2) the total annual pollution load (pollutant mass) to the compartment; (3) chemical/compound related parameters; and (4) soil related parameters. The output from the model is: (1) the pollutant distribution (i.e. concentrations, mass distribution) in the compartment, and (2) the annual pollution contribution (transport) to other environmental compartments by means of surface runoff, volatilization, leaching to groundwater, etc. Additional information for use of this level is provided in section PT-3.2. Details of input data formats are given in section 3-3.2. Details of the output are given in section 3-3.3.

outputs to other compartments

LEVELO should be employed with care and only if "real" climatological and field data are available, because the hydrologic parameters (eg. rainfall vs. soil moisture content) are always correlated, though independency is assumed for these input data.

good

This level has specialized applications, for example: screening of a large numbers of chemicals that have to be compared for their environmental effects when released into non-site specific (fictitious) compartments.

e.g. runoff or volatilization potential

3.1.4.3 LEVEL1

LEVEL1 is philosophically like LEVELO; however, it has been designed for region specific simulations. The simulation is performed annually and for only one year and requires the knowledge of few annual averaged climatic and soil data for the area, in order for the model to estimate the annual hydrologic parameters relating to the compartment which have been a user input to LEVELO.

good

The user has to input: (1) climatic/storm parameters, (2) soil parameters which may vary in the two layers, (3) chemical parameters, and (4) simulation specific parameters. These data are readily available from the literature (eg. NOAA reports, handbooks). The output from the

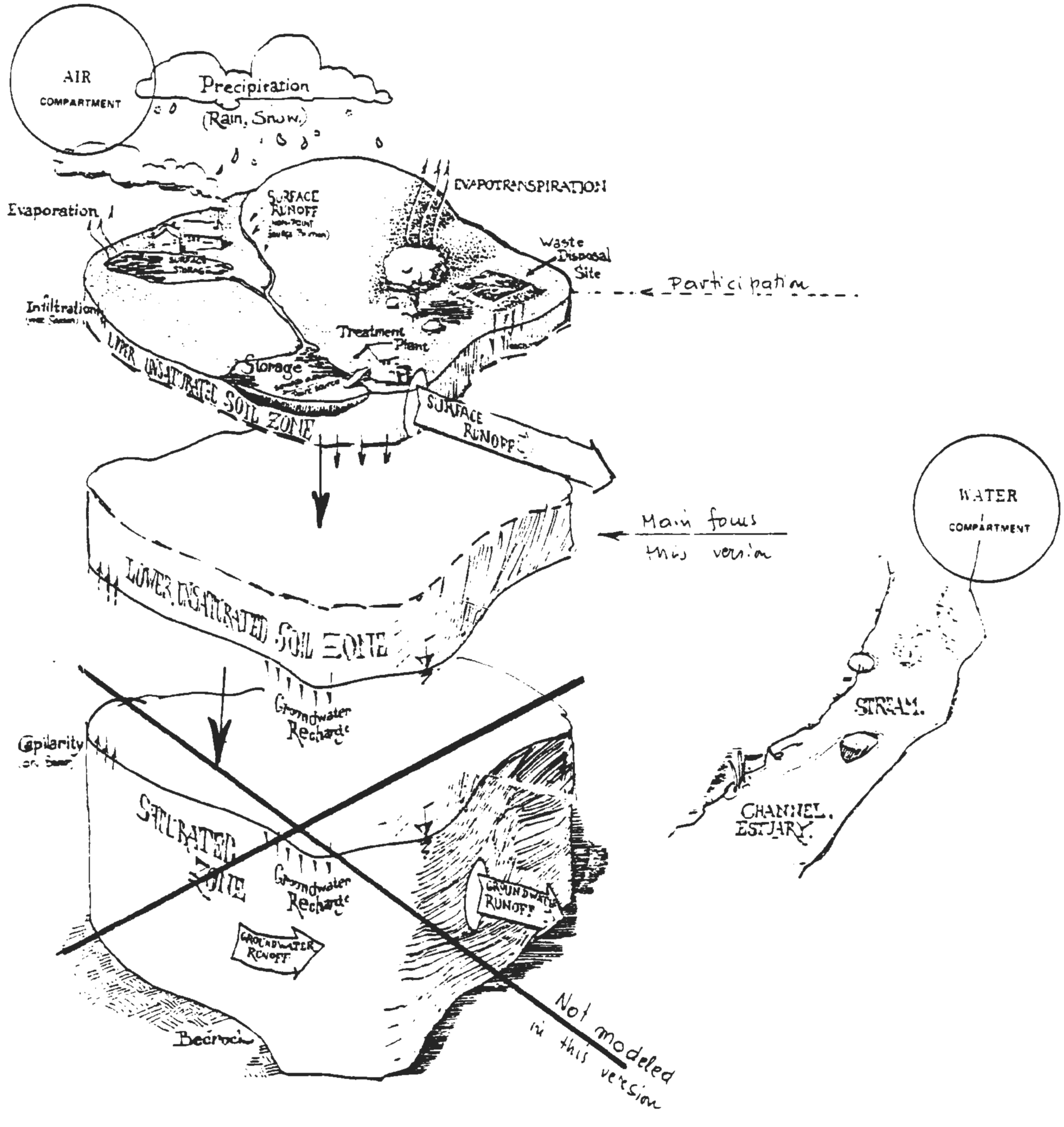


FIGURE 3-3: COMPARTMENT DISAGGREGATION; LEVEL0. LEVEL1, AND LEVEL2 OPERATIONS

model is: (1) the hydrologic cycle components of the annual compartmental water balance, (2) the annual pollution distribution (eg. concentrations, mass to groundwater.)

good

As in LEVEL0 simulations are performed in two unsaturated soil zone layers (Figure 3-3) and are of use for specialized applications. Additional information for this level is provided in section PT-3.2. Details of input/output data formats are given in sections 3-3.2 and 3-3.3.

3.1.4.4 LEVEL2

LEVEL2 resembles LEVEL1 philosophically ~~(Figure 3-3); however~~, operations ~~are performed~~ monthly. ~~Up to 10~~ years can be simulated. In ~~contrast~~ to the input data required by LEVEL1, ~~the user has to~~ know: (1) the monthly distribution of rainfall depths ~~and other~~ climatic parameters ~~in the~~ area, and (2) the monthly distribution of input pollution (pollutant mass) to ~~the compartment~~. Most other input data are similar to LEVEL1. The monthly output from the model resembles the ~~LEVEL1 annual~~ output.

Simulations performed with LEVEL2 may reflect site specificity, both in time (averages over month) and area (reflected in the compartment characteristics). Input data are easily compiled from existing data sources (eg. NOAA, handbook, this documentation); ~~however, for site~~ specific ~~simulations,~~ model output has to be ~~compared~~ to actual field data (for both hydrology and chemistry), and eventua~~lly calibrated~~. Validation of final output is essential.

too bad
forget it

Additional information for this level is provided in section PT-3.3. Details of input/output data formats are given in sections 3-3.0 and 3-3.4.4.

3.1.4.5 LEVEL3

forget it

LEVEL3 resembles LEVEL2 in philosophy (monthly simulations); however, ~~operations~~ are performed in three unsaturated soil zone layers. Therefore, in addition to the input data required by LEVEL2, the user has to input pollutant mass and soil characteristics for an ~~additional layer~~. This fact increases spatial resolution, but also user's required effort. This level has been developed for the needs of this contract and can become a subset of the N-layered monthly SESOIL version (Figure 3-4).

Additional information for this level is provided in section PT-3.3. Details of input/output data formats are given in sections 3-3.2 and 3-3.3.

3.1.4.6 Other Levels

The authors intend to develop additional levels such as:

(1) a storm-by-storm temporal resolution and a N-layered compartment that may handle release of a second phase (insoluble) chemical spill on the soil surface, or

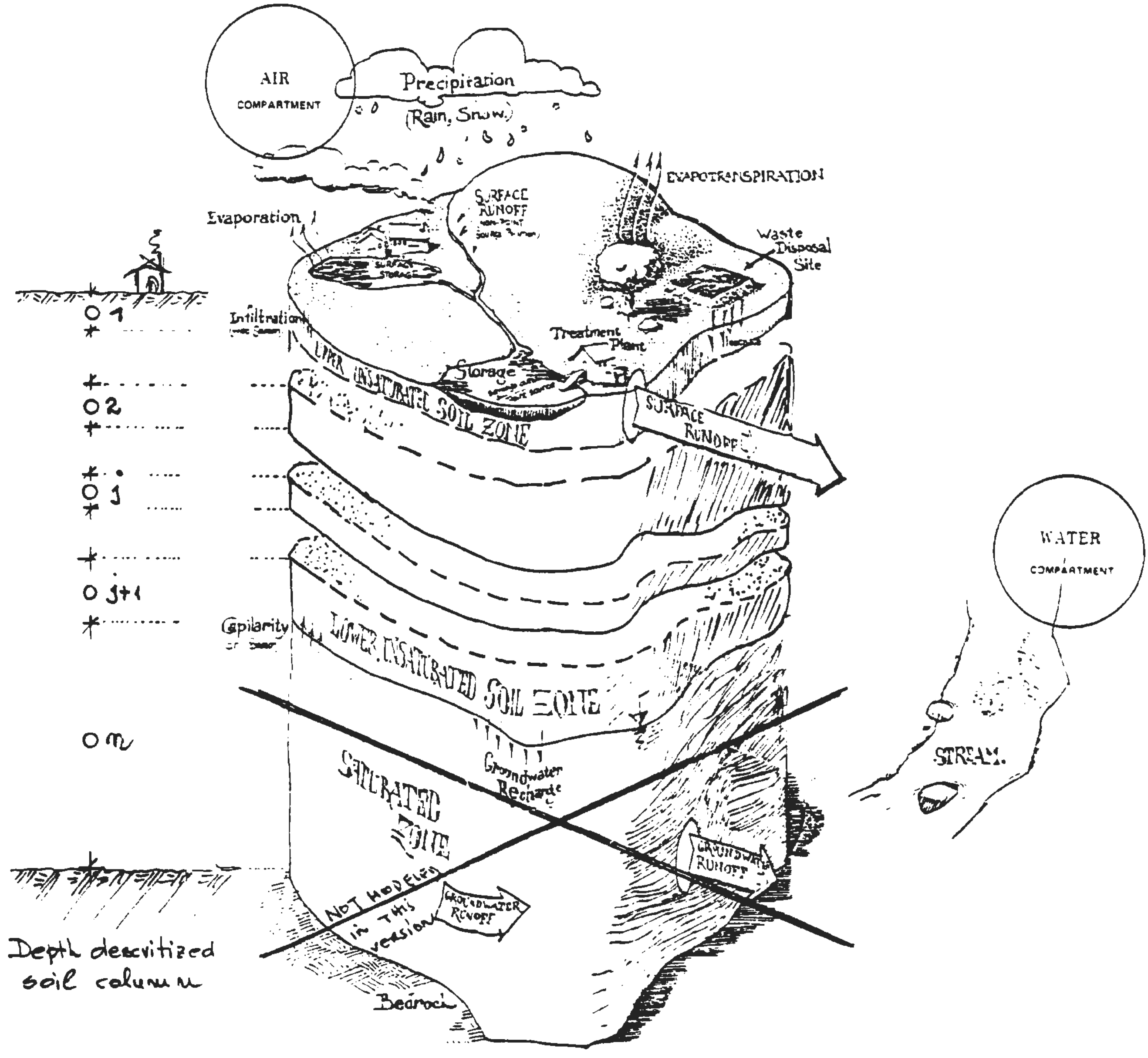


FIGURE 3-4: CONCEPTUAL COMPARTMENT DISCRETIZATION FOR THE LEVEL3 OPERATION

(2) a statistical version to handle pollutant (eg. pesticide) transport on the watershed.

Authors have conceptualized these versions but have not proceeded in ed any real developmental effort. Their main goal will always be a "user friendly" model accepting calibration of parameters describing physical or chemical rate processes (eg. intrinsic permeability of soil, cm^2).

3.1.5 Problem Identification/Level Selection

This section will be expanded in the future to contain information regarding: (1) how to identify a problem suitable for modeling via SESOIL, (2) how to select the compartment's temporal and spatial resolution (i.e., level), and (3) how to proceed with the actual modeling (single medium, multimedia).

3.1.6 Canonical/Scenario's Chemical Fate Modeling

Recent concerns related to environmental quality require a methodology to relate sources and quantities of chemical releases into the environment to the actual amounts of these chemicals to which humans and other biota are exposed. SESOIL is extremely well suited for such environmental exposure studies, which are based on "canonical" environmental compartments and employ typical scenarios (single medium or multimedia). This section will discuss such issues in the future. It has to be emphasized that the selection/compilation of typical/canonical compartments is not an easy issue, and has to involve consideration of statistical techniques (eg. kriging, see section 3.4.3) to optimally/appropriately design the compartments.

3.2 DATA STRUCTURE/MANAGEMENT

3.2.1 General

For a user it is important to understand the model data structure and management, the model execution philosophy of the version accompanying this documentation, and the content of the input data files.

3.2.2 SESOIL Program Structure

A generalized flow chart of SESOIL data files and operation is shown on the next page (Figure 3-5). The executive program of operations, designated as SE81, calls the main program designated as SESOIL, and the latter calls the two basic data subroutines RFILE (read data file), PFILE (print data file), and one of the four operational basic subroutines LEVELO (level "O" operations), LEVEL1, LEVEL2 or LEVEL3. Consequently, each of the basic operational routines calls a number of secondary routines such as HYDROA (annual hydrologic cycle), HYDROM (monthly hydrologic cycle), TRANSA (annual pollutant transport routine), TRANSM (monthly pollutant transport routine; two soil layers) or TRANS3 (three soil layers). Finally, each of the secondary routines calls a variety of functional routines, as presented in appendix FC (FORTRAN Code).

A major emphasis is placed into the data management aspects and the easy input of data. Data are read by the model from 6 data files GE (general), LO (level 0), L1 (level 1), L2, L3 and EXEC (executive operation). In the IBM system data files are accessed via the file name and a "DATA" designation; therefore, reference is made in the following sections to the 5 files GE DATA, LO DATA, L1 DATA, L2 DATA, and EXEC DATA (Figure 3-5), which are all expandable in size.

GE DATA file (see section 3.2.4.1) contains: (1) climatologic data of regions, areas or cities, (2) soil data for various soil types, and (3) chemistry specific data and pollutant parameters.

LO DATA data file (see section 3.2.4.2) contains geometric and simulation related information for the LEVELO applications. L1 DATA contains information (see section 3.2.4.3) for using LEVEL1 of the model, and L2 DATA contains the LEVEL2 information/data (see section 3.2.4.4). Information data or parameters that are used for both LEVEL1 and LEVEL2 operations are given twice (double-input), one in each data file, in order to make each level of operation self-standing and self-contained.

EXEC DATA (see also section 3.2.4.6) contains executive simulation data and information for each actual execution of SESOIL, such as "what level of operation is desired?", "where is the area of simulation?", "what type of a soil or chemical compound is involved?".

Detailed information regarding the "loading" of these files is presented in section 3.2.4 and in appendix DF (Data Files).

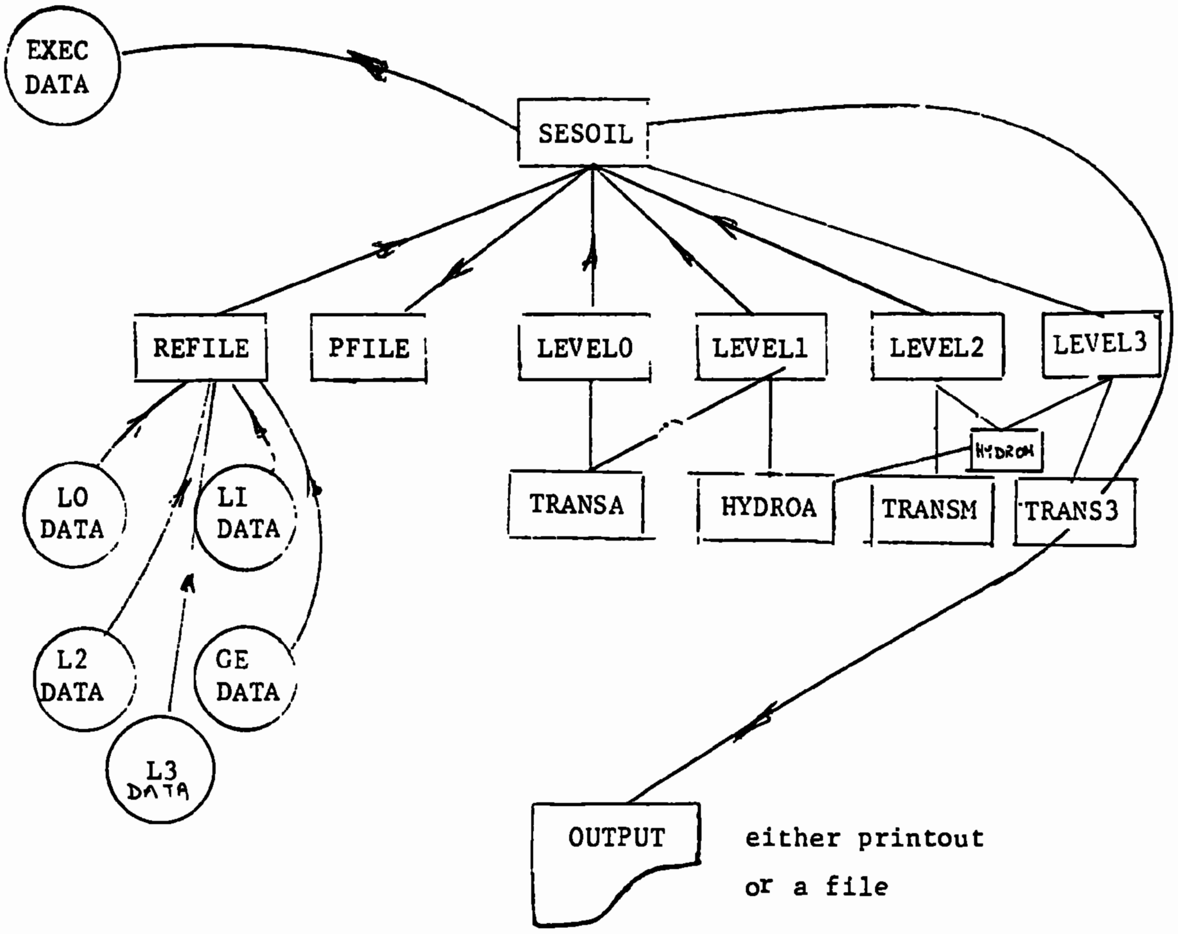


FIGURE 3-5: SCHEMATIC PRESENTATION OF SESOIL OPERATIONS

3.2.3 Model Execution Philosophy

Model execution is accomplished with the following steps:

(1) The SESOIL user selects/decides for a level of operation (i.e. LEVEL#).

(2) The user "edits" his basic data files (section 3.2.3.4) GE DATA, L# DATA and EXEC DATA

- either through an interactive process via a screen terminal (eg. IBM VM-CMS system), or
- by inserting or changing computer cards from his deck.

Editing of the basic data files involves either the input of non-existing values (eg. new climatological data) in the data files, or the updating of the previous information (eg. another region).

Above files have unlimited expansion capabilities so that data from previous simulations may be saved for future comparative runs.

(3) The user asks for program execution via the statement: SE81

3.2.4 Input Data Files

The following 6 sections (3.2.4.1-3.2.4.6) give the information contained in the 6 data files:

GE DATA	File of general information to be employed by all levels of operations
LO DATA	File containing data for LEVELO executions
L1 DATA	File containing data for LEVEL1 executions
L2 DATA	File containing data for LEVEL2 executions
L3 DATA	File containing data for LEVEL3 executions
EXEC DATA	Executive data file of operations

At this point, the reader may find the program/data logic expressed previously to be somewhat confusing; however, this program/data/execution rationale will become clearer after reading the coming sections and paragraphs and the more detailed description of the data files; appendix DF.

3.2.4.1 GE DATA File

3.2.4.1.1 General

This file (Figure 3-6) contains information applicable to all levels of SESOIL operations: LEVEL0, LEVEL1, LEVEL2 and LEVEL3. The file is permanent and self expandable with the insert of new data.

Information contained in the file includes:

(1) Regional Descriptions: climatic, storm data, for areas where the model might be applied,

(2) Soil Classifications: soil, sediment data of typical or specific soil compartments, and

(3) Chemistry Data: related to various pollutants whose fate might be simulated.

Regional Description data are not required for a LEVEL0 operation; however, soil and chemistry data are required.

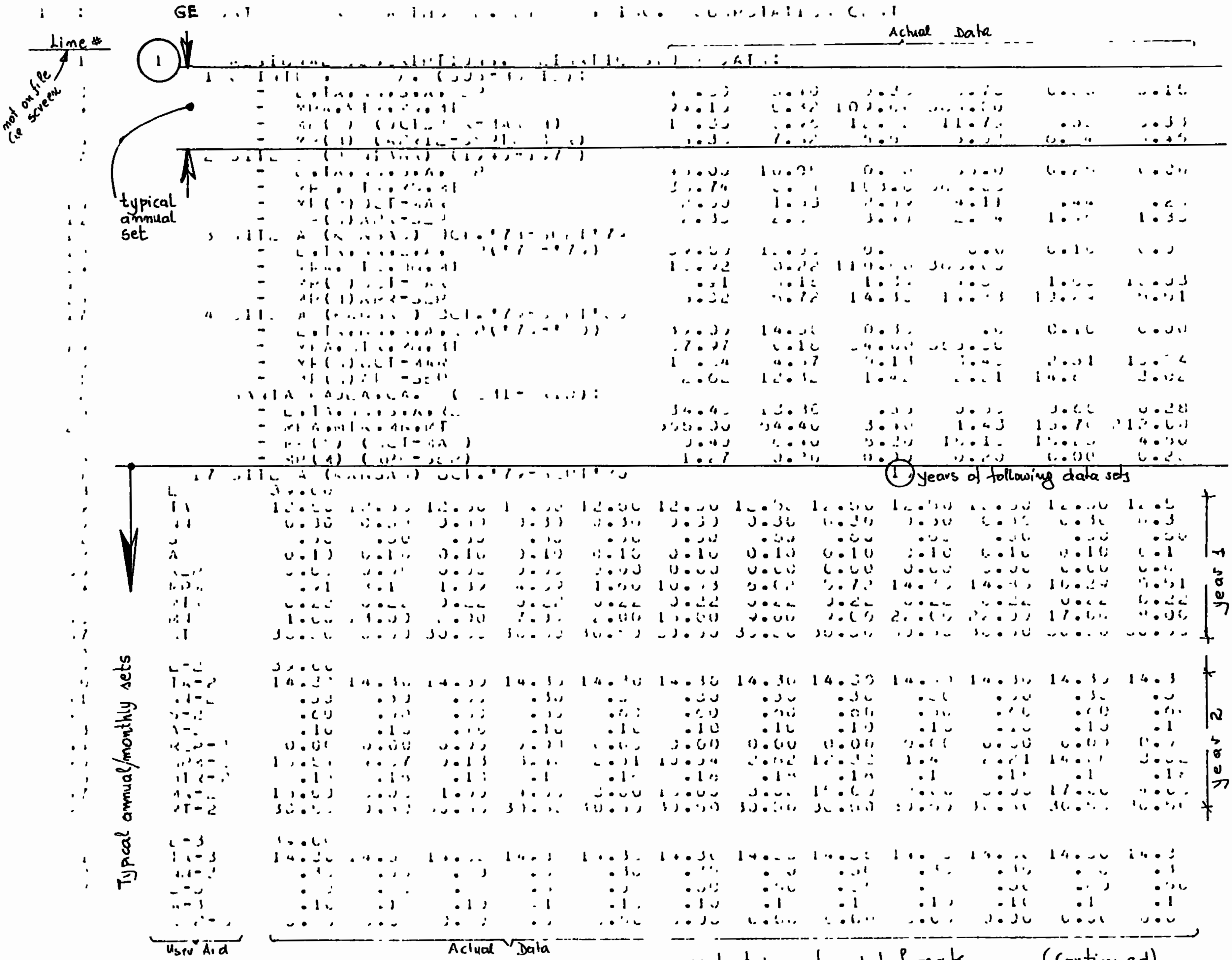
The file is designed to be self explanatory and provision is made for non-readable (by the computer) statements in order to aid the user. The user can input into the file blocks of annual or monthly climatic data in any sequence. The program can "spot" the correct areal climate via a user specified index (eg. "17" SITE A (KANSAS), Figure 3-6). This index does not have to be sequentially numbered. Only the actual input data sets (blocks) have to be correctly given to the file. Most of the other labels and text are designed for the user's aid. However, appropriate labeling and numbering is a good practice.

GE data is the largest file, and as such a new user may find this documentation to be intimidating. However, as the input procedures are easier to do than described, users will find that data input is easy once one becomes familiar with the use of the model.

> Note: The SESOIL data files are formatted and thus it is important that data be entered in the appropriate columns, with decimals if real numbers, right justified if integer etc. The last page of Figure 3-6 presents some sample input data as coded for entry.

The model is delivered with a small input data file, so that section headings and labels of each file -- though described as inputs in the following pages -- do not have to be inserted again by users.

Section 3.2.5 presents a summary of all data entries for all files. Readers familiar with data entries may consult only that section.



see last page for input formats (continued)

FIGURE 3-6 GE DATA file

```
GE
[illegible]
```

Line # not on screen (see last page of table)

FIGURE 3-6 (Cont'd) GE DATA file

FIGURE 3-6 GE DATA File (Continued)

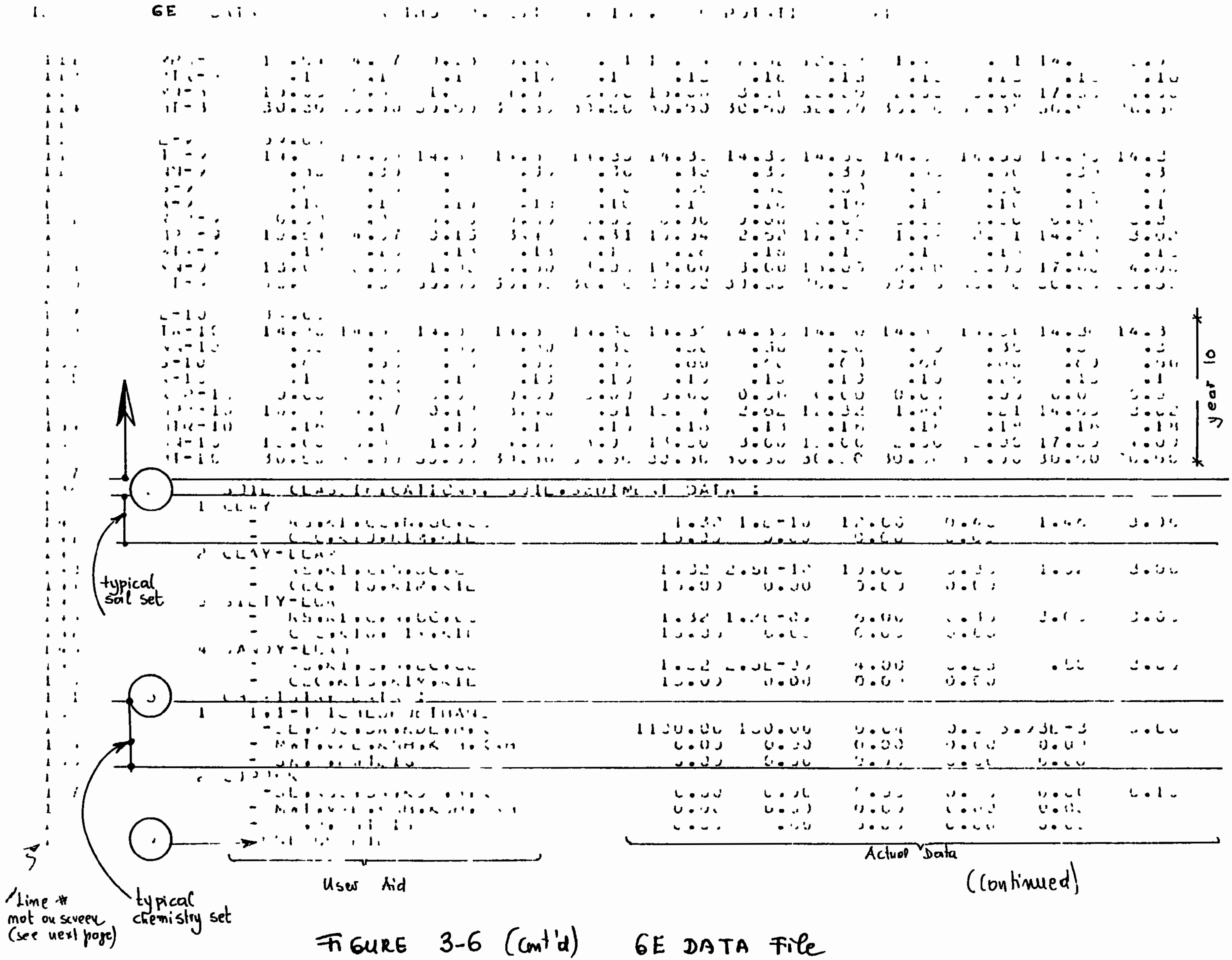


FIGURE 3-6 (Cont'd) 6E DATA File

FIGURE 3-6 (Cont'd) 6E DATA file

IBM

GE DATA file of dEJoic

PROBLEMS: call (617) 8645770

DATE Dec. 15, 81

PAGE 4 FIGURE 3-6

FORTRAN STATEMENT

```
Line
1    (1)      REGIONAL DESCRIPTIONS; CLIMATIC, STORM DATA:
2         1   CLINTON,     MA. (SUB-HUMID):
3              -  L,TA,NN,S,A,REP         42.50    8.40    0.35    0.70    0.30    0.15
4              -  MPA,MTR,MN,MT           94.10    0.32  109.00  365.00
5              -  MP(M) (OCT-MAR)         10.36    8.96   12.52   11.75    8.33    8.33
6              -  MP(M) (APR-SEP)          8.38    7.82    6.60    5.08    6.04    8.46
:         2   SITE B (MONTANA)
:             - - - - - - -
.    * * * * block to be repeated indefinitely.. * * * * *
         see first page of this figure 3-6

27       17   SITE A (KANSAS) OCT.'79-SEPT'80              10
28   L          39.00  39.00  39.00  39.00  39.00  39.00  39.00  39.00  39.00  39.00  39.00  39.00
29   TA         12.50  12.50
30   NN          0.30   0.30
31   S           0.60   0.60
32   A           0.10   0.10
         see 3rd page of this figure 3-6
     (2)      SOIL CLASSIFICATIONS; SOIL, SEDIMENT DATA :
139       1   CLAY
140            -  RS,MA,C,N,OC,CC          1.32   1.E-10   12.00     0.45     1.41     3.00
141            -  CEC,KIU,KIM,KIL         15.00   1.E-10  2.1E-10   2.E-10  3.1E-10  1.3E-10
         file continues

151  (3)      CHEMISTRY DATA
152       1     1,1 TRICHLOROETHANE
153           -SL,KOC,DA,KDE,H,K    1100.00   180.00     0.04     0.003.90E-3       0.00
154           -MWT,VAL,KNH,KBH,KAH     0.00     0.00     0.7E-5   8.00     9.00    10.00
155           -SK,B,MWTLIG             0.20     0.80     4.40     0.00     0.00     0.00
-        see previous page of this figure
-

160  9          END OF FILE
```

FIGURE 3-6 "GE DAT" File (Input Formats ; see table of next page also.

3.2.4.1.2 Data Input

The following data information is entered into the GE file in the following order in the file:

(1) Climatologic Data

  (1.1) Annual

  (1.2) Monthly

(2) Soil Data

(3) Chemistry Data

(4) End of File

Note: Annual and monthly data sets can be interspersed.

In this documentation the following symbols are used:

***** indicates repetition of data lines, or data sets
!!!!! indicates important comments
"..." indicates an emphasis in the word or sentence in quotation

Input parameters for each line, data format, units, and sample input for each line follow.

The line numbers used below (refer to Figure 3-6) are employed for demonstration purposes only and do not appear in the data file.

(1) Climatologic Data

Line 1 FORMAT(I1,5X,12A4)

contains the heading

1 REGIONAL DESCRIPTIONS; CLIMATIC STORM DATA;

The index "1" must appear in the first column (#1, see circled number Figure 3-6) of this statement, because it controls the reading of the climatic data.

The user is not concerned with such an entry, since it is delivered with the SESOIL-code.

!!!!!! Following the above statement, either annual or monthly, climatic sets can be given to the file.

(1.1) Annual Climatic Data Inserts

Only one year of data is contained in an annual data set (lines 2-6) below, since the annual data are used for LEVELS 0 and 1 which run for one year only.

Line 2 FORMAT(2X,I3,1X,12A4)

contains the heading of an area where the model may be applied

1 CLINTON, MA (SUB-HUMID)

The above is not an executable statement. The number "1" before the area has to appear in the statement.

Line 3 FORMAT(38,6F7.2)

contains the numerical data sets of

- either

L	[°N]	latitude of the area (eg. 42.50)
TA	[°C]	temperature of area at surface (eg. 8.40)
NN	[fraction]	fraction of sky covered by clouds (eg. 0.35)
S	[fraction]	relative humidity of the area (eg. 0.70)
A	[-]	shortwave albedo of the surface (eg. 0.30)

- or

REP	[cm/day]	evapotranspiration rate of the area (eg. 0.15)

- or

"both" above sets if the user desires so; however, the program will assume the evapotranspiration rates in the area as "known" and will "not" estimate it from the first data set L, TA, NN, S, A.

Note:

- Above data is stored in array CLIMA1(6); see appendix DF

- Only the temperature is required for a LEVELO model execution; however:
- If line 2 above is inserted, then this data (line 3) must be given even with 0.00 values.

Line 4 FORMAT(38X,4F7.2)

contains the numerical values of:

MPA[cm]	annual depth of rain (eg. 94.10)
MTR[day]	annual mean storm duration (eg. 0.32)
MN[-]	number of storm events per year (eg. 109.00)
MT[days]	mean length of rainy season (eg. 365.00)

Note:

- Above data is stored in the array spaces CLIMA1(6); see appendix DF, figure DF-2.
- This data is not required for a LEVELO execution.
- If line 2 is inserted, then this data (line 4) must be given, even with 0.00 values.

Line 5 FORMAT(38X,6F7.2)

contains the numerical values of:

MPM[cm]	mean monthly (M) depth of rain of the first six months of the year (October through March) starting with the month of October (M=1); eg. 10.36, 8.96, etc.

Note:

- Above data is stored in the array spaces CLIMA3(1-6).
- This data set is not required for the LEVELO and LEVEL1 executions; however:
- If line 2 is inserted, then this data set (line 5) must be given, even with 0.00 values (required by LEVELO and LEVEL1).

Line 6 FORMAT(38X,6F7.2)

contains the numerical value of:

MPM[cm] mean monthly (M) depth of rain of the remaining six months of the year (April through September) starting with the month of April (M=7); eg. 8.38, 7.82, etc.

Note:

- Above data is stored in the array spaces CLIMA3(7-12).
- This data set is not required for the LEVEL0 and LEVEL1 executions; however:
- If line 4 is inserted, then this data set must be given, even with 0.00 values (for LEVEL0).

!!!!! Data in lines 5 and 6 are not used in this form and are usually centered as zero. These lines have been left in this version for future use, and to be compatible with previous versions.

***** Above data entries (lines 2-6) can be repeated as necessary for multiple sites in this permanent and expandable data file (eg. 2 SITE B (MONTANA),..., etc).

(1.2) Monthly Climatic Data Inputs

Note: It is not necessary to input annual climatic data sets before monthly sets; the two types of data sets may be interspersed.

The line numbers used are from Figure 3-6. In the actual file these line numbers may change, although their contents will not. The line numbers are for reference only, they are not used by the code.

Line 27 FORMAT(2X,I3,1X,12A4,I5)

contains the heading of an area/region where the model may be applied

```
17 SITE A (KANSAS) Oct. '79-Sept '80     10
```

This is not an executable statement. However, the numbers "17" and "10" have to appear in the statement and at the correct place in the file. The "17" is the index of the site. The "10" is the index of how many years of data follow this first statement of SITE A (KANSAS) Oct. '79-Sept. '80 (i.e. 10 years).

Following the above statement numerical input data for the climatic parameters for each month and year can be inserted.

Line 28 FORMAT(8X,1F6.2)

This line contains the numerical value of:

L[°N] latitude of area (eg. 39.00)

Lines 29 to 38 FORMAT(8X,12F6.2) for each line

These lines contain the monthly values of the parameter, starting with the October value in column 1 and ending with the following September value in column 12.

29	TA[°C]	temperature of the area (eg. 12.80)
30	NN[fraction]	fraction of sky covered by clouds (eg. 0.30)
31	S[fraction]	relative humidity of area (eg. 0.60)
32	A[-]	shortwave albedo of the surface (eg. 0.10)
33	REP[cm/day]	daily evapotranspiration <u>or</u> 0.0 (see Line 3)
34	MPM[cm]	monthly precipitation (eg. 0.91)
35	MTR[days]	mean time of rain (eg. 0.22)
36	MN[#]	mean number of storm events (eg. 1.00)
37	MT[days]	mean length of rain season (i.e. days in a month). If it rains almost every 3-4 days in a week during the entire month, then MT=365/12=30.50 (eg. 30.50).

38 --- This is an empty line for visual purposes. It indicates end of year.

***** Above lines (28-38) can be repeated for the same area for up to 10 years (by indexing; eg. "10");ie L is given 10-times.

***** The above data set (lines 27-38) can be repeated for any number of areas (by indexing; eg. "17").

Above data is stored in arrays CLIMM1(6,12,10) and CLIMM2(6,12,10); see appendix DF, figure DF-2.

(2) Soil Data Inserts

Following the climatological input entries, the soil data must be given. In Figure 3-6 climatological entries end in line 137. For this documentation, soil data entry starts therefore with line 138 (circled "2"). Note: Lines 137 and 138 are not the real line #s. They only correspond to Figure 3-6.

Line 138 FORMAT(I1,5X,12A4)

This line contains the indexed alphanumeric statement

2 SOIL CLASSIFICATIONS; SOIL, SEDIMENT DATA:

The index "2" has to appear in the first column of the statement. Following this statement, numerical input data for the various soil types are given.

Line 139 FORMAT(2X,I3,1X,12A4)

contains the description of the indexed soil type whose data follow; eg.

1 CLAY

Note:

- The index should always appear (eg. "1")
- This type of data is required by all levels of operation (LEVELO - LEVEL3); therefore, at least one soil-type data set has to be given to activate the program.
- The alphanumeric title is stored in the array spaces TITLES (5,12); see appendix DF.

Line 140 FORMAT(38X,6F7.2)

contains the numerical values of:

RS[g/cm^2]	soil density (eg. 1.32)
K1[cm^2]	soil intrinsic permeability (eg. 1.00 X 10^{-10})
C[-]	soil disconnectedness index (see appendix HY) (eg. 12.00)
N[-]	effective soil porosity (eg. 0.45)
OC[%oc]	organic content of soil (eg. 1.46)
CC[%cc]	clay content of soil (eg. 3.0)

Note:

- Above values are stored in the array spaces SOIL1(6)
- If line 140 is inserted in this file, then this line must be given, even with 0.00 values.

Line 141 FORMAT(38X,4F7.2)

contains the numerical values of:

CEC[me/100 g soil]	soil cation exchange capacity (eg. 15.00)
K1U[cm^2]	intrinsic permeabilities of upper soil layer
K1M[cm^2]	intrinsic permeabilities of middle soil layer
K1L[cm^2]	intrinsic permeabilities of lower soil layer

Note:

- K1U, K1M, K1L are used for LEVEL3; therefore, they do not have to be inserted for other levels. If both K1 and the set of K1U, K1M and K1L are given, the program will ignore the later values and will use the value of K1 for all layers.
- This data is stored in array SOIL2(6); see appendix DF, figure DF-3
- If line 140 is inserted in this file, then this line must be input (even with 0.00 values.

***** Lines 139-141 can be inserted for an "unlimited" number of soils. As such they create the soil-part of the GE DATA base. Note: "indexing" (eg. "1" CLAY) is necessary.

!!!!! Assume that the soil entries have reached line 150, figure 3-6, 3rd page. Chemistry data inputs will follow in line 151.

(3) Chemistry Data Inserts

Following the soil entries, the chemistry data must be given. In Figure 3-6 soil entries end with line 150. For this documentation chemistry data entry starts with line 151.

Line 151 FORMAT(I1,3X,12A4)

contains the headings of the next category of input data.

3 CHEMISTRY DATA:

Following this statement, chemical descriptions and numerical input data are given. The "3" has to appear in the first column of this line.

Line 152 FORMAT(2X,I3,1X,12A4)

contains the name of the compound whose data follow (lines 153-155), eg.

1 1,1-TRICHLOROETHANE

Note:

- The index of the compound (eg. "1") should always appear in this statement.
- This type of input is required for all levels of operation, LEVEL0-LEVEL3; therefore, at least one chemical data set should be given into the GE DATA base (even with 0.0 values).
- The name of the chemical is stored in the spaces of the alphanumeric array TITLE(5,12).

Line 153 FORMAT(38X,6F7.2)

contains the index and the name of the chemical compound and numerical values of parameters associated with it. These parameters are:

SL[ug/mL]	compound solubility in water (eg. 1100)
KOC[(ug/goc)/(ug/mL)]	adsorption coefficient of the compound on organic carbon (eg. 180.00)
DA[cm^2/sec]	diffusion coefficient in air (eg. 0.04)
KDE[day^{-1}]	biodegradation rate of the compound (eg. 0.00)

H[m^3·atm/°K·mol]	Henry's law constant (eg. 3.93E-3)
K[(ug/g)/(ug/mL)]	averaged adsorption coefficient for the compound on the soil (eg. 0.0)

Note:

- Above data are stored in the array CHEM(18).
- If K is given (different from 0.0) then the program uses as an adsorption coefficient this K, otherwise it uses the KOC.

Line 154 FORMAT(38X,5F7.2)

This line contains the numerical values of:

MWT[g/mol]	molecular weight of compound
VAL[-]	valence of compound
KNH[day^{-1}]	neutral hydrolysis constant
KBH[L/mol·day]	base hydrolysis constant
KAH[L/mol·day]	acid hydrolysis constant

All above entries in Figure 3-6 are 0.0.
This data is stored in array CHEM1(18); see appendix DF, figure DF-3

Line 155 FORMAT(38X,3F7.2)

This line contains the numerical value of:

SK[-]	stability constant of compound-ligand complex
B[#]	number of moles of ligand per mole of compound complexed
MWTLIG[g/mol]	molecular weight of ligand

Above entries in Figure 3-6 have 0.0 values.
This data is stored in array CHEM1(18).

***** Lines 152-155 can be repeated for an "unlimited" number of chemicals. Indexing (eg. "1") is essential. For example, lines 156-159 contain "2"; COPPER values.

(4) End of File

Following creation of the chemistry section of the GE DATA file, we designate the "End of File" with (Figure 3-6, 3rd page).

Line 160	FORMAT(I1,5X,12A4)
(End of File)	9 END FILE
	This is the last line of the GE DATA file, and should be identified by the number 9 in the first column (#1, Figure 3-6, 4th page).

A summary of all previously discussed data entries is given in one table in section 3.2.5 (Table 3-1).

3.2.4.2 LO DATA File

3.2.4.2.1 General

This file (Figure 3-7) contains information applicable to the LEVELO operations. This file is used in conjunction with the GE DATA file and contains:

(1) Geometric and other parameters related to a region

(2) Information relating components of the hydrologic cycle of the area and pollutant transport of the LEVELO simulation.

(3) Pollutant (and other chemical) loadings.

Because the LO DATA file is used in conjunction with the GE file, it is assumed that the user is familiar with the presentation of the input data of the previous section 3.2.4.1 (GE DATA File), and therefore input data descriptions are only briefly presented. A reminder: the SESOIL code is delivered with a basic data base that facilitates additional data entry in terms of format.

As was done for the GE DATA file, a summary of all inputs of the LO DATA file is presented in section 3.2.5 of the user's manual. Users familiar with the input data concepts of SESOIL may consult only the summary section.

3.2.4.2.2 Data Input

Spacing and format of data are shown in the 2nd page of Figure 3-7. The content of each line is described below. For clarity, input data to this file are described with reference to the figure; line 1 below does not have to be the first line in the file.

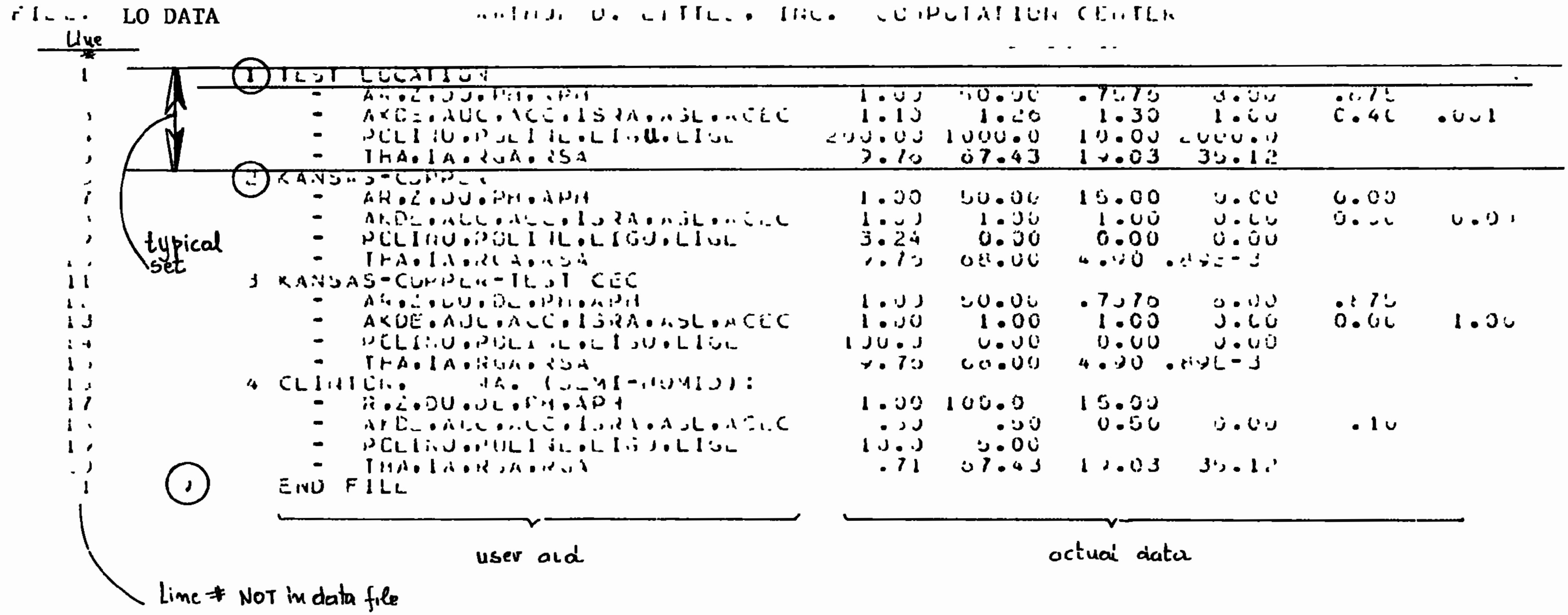
Line 1 FORMAT(2X,I3,1X,12A4)

contains the heading of the first region of the file, eg.

1 TEST LOCATION

Note:

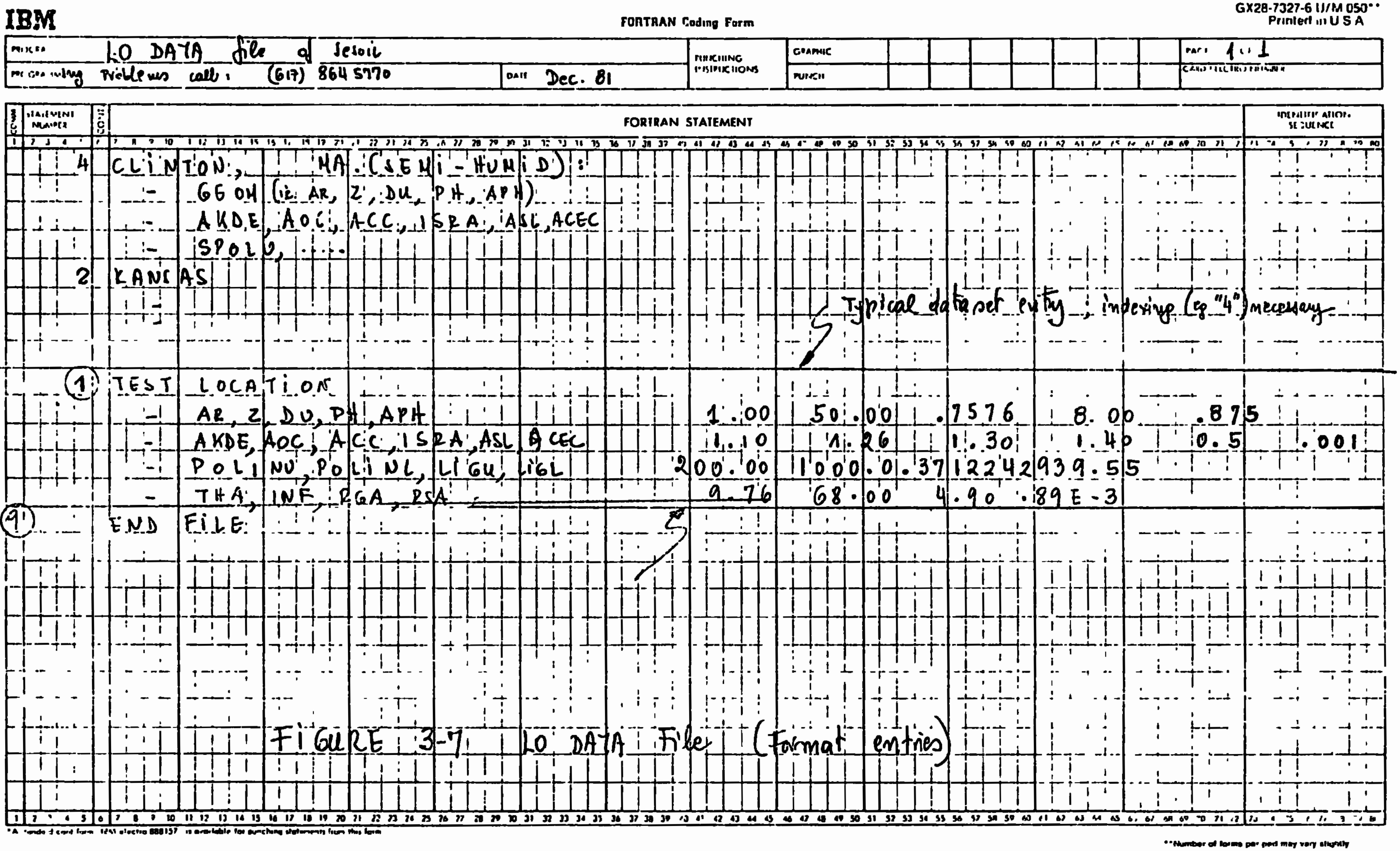
- The index of the region (eg. "1") must appear.
- The title is stored in the first line of the array TITLES(5,12); see appendix DF.



```
FILE: LO DATA                  ARTHUR D. LITTLE, INC.   COMPUTATION CENTER
 Line
  #
  1        1 TEST LOCATION
  2          -   AR,Z,DU,PH,APH                        1.00   50.00   .7575    3.00     .075
  3          -   ARDE,AUC,ACC,ISRA,ASL,ACEC            1.10    1.26    1.30    1.00     0.40   .001
  4          -   PCLINU,PCLIIL,LIGU,LIGL             200.00  1000.0   10.00  2000.0
  5          -   THA,IA,RGA,RSA                        9.76   67.43   19.03   35.12
  6        2 KANSAS-COPPER
  7          -   AR,Z,DU,PH,APH                        1.00   50.00   15.00    0.00     0.00
  8          -   ARDE,ACC,ACC,ISRA,ASL,ACEC            1.00    1.00    1.00    0.00     0.00   0.01
  9          -   PCLINU,PCLIIL,LIGU,LIGL               3.24    0.00    0.00    0.00
 10          -   THA,IA,RCA,RSA                        9.75   68.00    4.90  .895-3
 11        3 KANSAS-COPPER-TEST CEC
 12          -   AR,Z,DU,DL,PH,APH                     1.00   50.00   .7575    3.00     .075
 13          -   ARDE,AUC,ACC,ISRA,ASL,ACEC            1.00    1.00    1.00    3.00     0.00   1.00
 14          -   PCLINU,PCLIIL,LIGU,LIGL              100.0    0.00    0.00    0.00
 15          -   THA,IA,RGA,RSA                        9.75   60.00    4.90  .89E-3
 16        4 CLINICAL   [illegible] (SEMI-HUMID):
 17          -   R,Z,DU,DL,PH,APH                      1.00   100.0   15.00
 18          -   ARDE,ACC,ACC,ISRA,ASL,ACEC             .50     .50    0.50    0.00      .10
 19          -   PCLINU,PULIIL,LIGU,LIGL               10.0    5.00
 20          -   THA,IA,RGA,RSA                         .71   67.43   19.03   35.12
 21        5 END FILE
```

See next page for spacing format

FIGURE 3-7 LO DATA file



IBM FORTRAN Coding Form

GX28-7327-6 U/M 050**
Printed in U S A

PROGRAM: LO DATA file of Sesoil
PROGRAMMING: Problems call: (617) 864 5770
DATE: Dec. 81
PUNCHING INSTRUCTIONS — GRAPHIC — PUNCH
PAGE 1 OF 1
CARD ELECTRO NUMBER

```
STATEMENT
NUMBER    FORTRAN STATEMENT
    4     CLINTON,       MA.(SEMI-HUMID):
       -     GG OH (ie: AR, Z, DU, PH, APH)
       -     AKDE, AOC, ACC, ISRA, ASL, ACEC
       -     SPOLG, ....
    2     KANSAS
       -

   (1)    TEST  LOCATION
       -     AR, Z, DU, PH, APH                 1.00   50.00   .7576    8.00   .875
       -     AKDE, AOC, ACC, ISRA, ASL, ACEC    1.10    1.26   1.30     1.40   0.5    .001
       -     POLINU, POLINL, LIGU, LIGL       200.00  1000.0.37122422939.55
       -     THA, INF, RGA, RSA                 9.76   68.00   4.90  .89E-3
(9)       END   FILE
```

Typical dataset entry; indexing (eg "4") necessary

FIGURE 3-7 LO DATA File (Format entries)

*A standard card form, IBM electro 888157, is available for punching statements from this form

**Number of forms per pad may vary slightly

Line 2 FORMAT(38X,5F7.2)

contains the numerical data of:

AR[cm^2]	surface area of the compartment (eg. 1.00)
Z[m]	depth to groundwater table for this application (eg. 50.00 meters)
DU[cm]	depth of upper unsaturated soil zone for this application (eg. 0.7576 centimeters)
PH[-]	pH of the upper unsaturated soil zone (eg. 8.00)
APH[-]	ratio of pH lower/upper unsaturated soil zone (eg. 0.875)

Note:

- Above data is stored in the array spaces GEOM(20); see appendix DF.

Line 3 FORMAT(38X,6F7.2)

contains the numerical data of:

AKDE[-]	ratio: biodegradation rate of compound in lower soil zone to upper unsaturated soil zone (eg. 1.10)
AOC[-]	ratio: organic carbon content in soil in lower soil zone to upper unsaturated soil zone (eg. 1.26)
ACC[-]	ratio: clay content in soil in lower soil zone to upper unsaturated soil zone (eg. 1.30)
ISRA[-]	index of surface runoff participation in pollutant transport ISRA = 0 no participation ISRA $\neq$ 0, any participation ISRA = 1 pollutant in surface runoff
ASL[-]	ratio of pollutant concentration in rain to maximum solubility in water (eg. 0.40)
ACEC [-]	ratio of CEC, lower/upper soil zone (eg. 0.001)

Note:

- Above data is stored in array spaces of GEOM(20).

Line 4 FORMAT(38X,4F7.2)

contains the numerical data:

POLINU[ug/cm^2]	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the upper zone (eg. 200.00)
POLINL[ug/cm^2]	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the lower zone (eg. 1000.0)
LIGU[ug/cm^2]	ligand input mass to upper zone (ug/cm^2) (eg. 10.00)
LIGL[ug/cm^2]	ligand input mass to lower zone (ug/cm^2) (eg. 2000.0)

Note:

- This data is stored in array LOAD(6); see appendix DF.

Line 5 FORMAT(38X,4F7.2)

contains the numerical data:

THA[-]	soil moisture content (%) (eg. 9.76)
IA[cm]	infiltration (eg. 67.43)
RGA[cm]	groundwater recharge (eg. 19.03)
RSA[cm]	surface runoff (eg. 35.12)

Note:

- Above data is stored in array RUNLO(6); see appendix DF.

***** Lines 1-5 can be repeated for an unlimited number of entries by "indexing" each time the new region (eg. "4" TEST LOCATION)

Line 21 FORMAT(I1,5X,12A4)
(End File)

This is the last statement of the LO DATA file, given as

9 END FILE

3.2.4.3 L1 DATA File

3.2.4.3.1 General

This file (Figure 3-8) contains information required to perform a LEVEL1 simulation. This file is used in conjunction with the GE DATA file, and may contain information existing in other files (eg. GE DATA), in order to make this level of operation a self-contained section for the user. As such, L1 DATA contains:

(1) Geometric and other parameters related to a region.

(2) Pollutant (and other chemical) loadings.

It has been assumed again that the user is familiar at this point with the data entry presentation of the previous section; therefore, only brief statements are given below.

3.2.4.3.2 Data Input

Spacing (format) of data and parameter descriptions (Figure 3-8) is described below. For clarity, input data to this file is described with reference to the figure. Line 1 below does not have to be necessarily the first line of the file.

Line 1 FORMAT(2X,I3,1X,12A4)

contains the heading:

1 CLINTON, MASS

Note:

- The index (eg. "1") must appear.
- The title is stored in alphanumeric array spaces TITLES(5,12); see appendix DF.

Line 2 FORMAT(38X,5F7.2)

contains the numerical data of:

AR[cm^2]	surface area of the compartment (eg. 1.00 cm^2)
Z[m]	depth to groundwater table for this application (eg. 100.00 meters)
DU[cm]	depth of upper unsaturated soil zone for this application (eg. 15.00 centimeters)

```
FILE:   L1 DATA               ARTHUR D. LITTLE, INC.  COMPUTATION CENTER

  1      ① CLINTON,     MA. (COT-HUMID):
  2          -   AR,Z,DU,PH,APH                    1.00  100.0   15.00   3.00    .075
  3          -   ARDL,ADC,ACC,IGRA,ASL,ACC          .10    .10    0.10   1.00    0.40    0.01
  4          -   POLINO,POLINL,LIGO,LIGL           10.0    5.00   10.00  20.00
  5      ② KANSAS-CORPS
  6          -   AR,Z,DU,PH,APH                    1.00   50.0   15.00   7.00    1.00
  7          -   ARDL,ADC,ACC,IGRA,ASL,ACC         0.60    1.00   0.00   0.00    0.00
  8          -   POLINO,POLINL,LIGO,LIGL           3.24    0.00   0.05   0.00
  9        3 KANSAS-CORPS-TEST CDC
 10          -   AR,Z,DU,PH,APH                    1.00   50.00   .7576  8.00    .075
 11          -   ARDL,ADC,ACC,IGRA,ASL,ACC         1.00    1.00   1.00   0.10    0.00    1.00
 12          -   POLINO,POLINL,LIGO,LIGL          100.0    0.00  10.00 5000.0
 13        4 TEST LOCATION.
 14          -   AR,Z,DU,PH,APH                   10.00   50.00   .7576  0.00    .075
 15          -   ARDL,ADC,ACC,IGRA,ASL,ACC         1.10    1.20   1.30   1.40    0.5     .001
 16          -   POLINO,POLINL,LIGO,ALIGL        200.00  1000.0   5.00   0.00
 17    ⑤     END OF FILE
```

typical set

This Line # not In file

Figure 3-8. L1 DATA FILE

PH[-]	pH of the upper soil zone (eg. 8.00)
APH[-]	ratio of pH, lower/upper soil zone (eg. 0.875)

Note:

- This data is stored in spaces of array GEOM(20); see appendix DF.

Line 3 FORMAT(38X,6F7.2)

contains the numerical data of:

AKDE[-]	ratio: biodegradation rate of compound in lower soil zone to upper unsaturated soil zone (eg. 0.10)
AOC[-]	ratio: organic carbon content of soil in lower soil zone to upper unsaturated soil zone (eg. 0.10)
ACC[-]	ratio: clay content of soil in lower soil zone to upper unsaturated soil zone (eg. 0.10)
ISRA[-]	index for pollutant participation in surface runoff ISRA = 0.00; no surface runoff participation ISRA ≠ 0.00; any participation (eg. 1.4) ISRA = 1.00; surface runoff participation
ASL[-]	ratio of pollutant concentration in rain to maximum pollutant solubility in water
ACEC[-]	ratio: lower/upper cation exchange capacity of soil (eg. 0.01)

Note:

- Above data is stored in the array spaces GEOM(20)

Line 4 FORMAT(38X,4F7.2)

contains the numerical data of:

POLINU[ug/cm^2]	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the upper zone (eg. 10.00)
POLINL[ug/cm^2]	total pollution load (mass) per unit area (cm^2) per year, entering the compartment in the lower zone (eg. 5.00)

LIGU[ug/cm^2]	pollutant input mass per unit are in upper zone (eg. 10)
LIGL[ug/cm^2]	pollutant input mass per unit are in lower zone (eg. 20)

Note:

- This data is stored in array LOAD(6); see appendix DF.

***** Lines 1-4 can be inserted for an unlimited number of data sets. Area has to be indexed (eg. "1" CLINTON, MA).

Line 17 (End of File) FORMAT(I1,5X,12A4)

This is the last statement of this file, given as

9 END OF FILE

A summary of all data entries is presented in Table 3-3 of section 3.2.5.

3.2.4.4 L2 DATA File

3.2.4.4.1 General

This monthly data file (Figure 3-9) contains information required to perform a LEVEL2 simulation. This file is used in conjunction with the GE DATA file. L2 DATA contains:

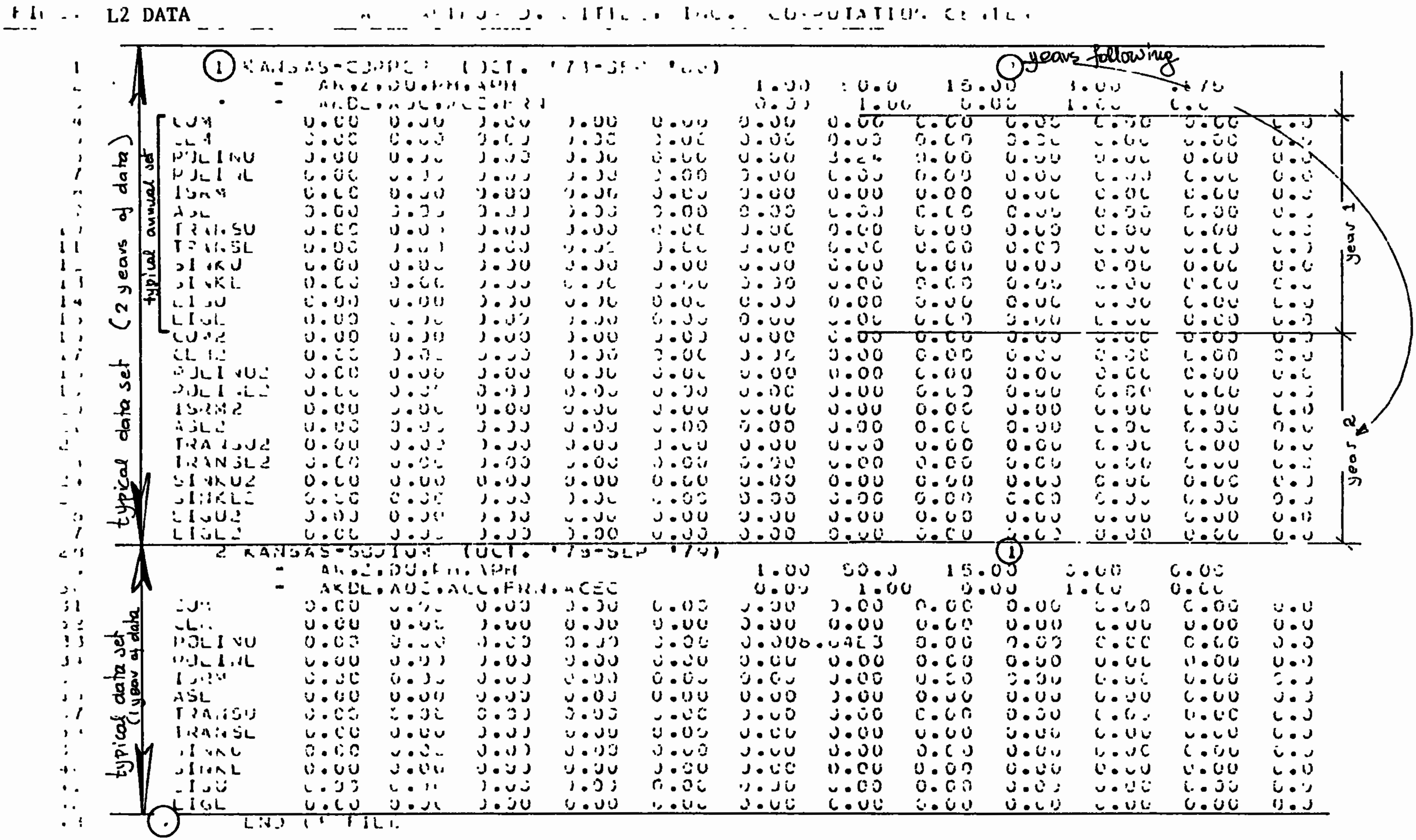
(1) Soil quality and soil moisture quality data (input) for the months of a year, and

(2) Pollutant input/transformation data for each month of a year.

In the following sections it is assumed that the user is familiar with data entries in the previous files, GE DATA, LO DATA, L1 DATA; therefore, data entries are described only briefly.

3.2.4.4.2 Data Input

Spacing and format of data are shown in Figure 3-9 and is described below. For clarity, data input is described by means of an example; line 1 does not need to be the first line of the file.



```
FILE .. L2 DATA          ARTHUR D. LITTLE, INC.  COMPUTATION CENTER

        1 KANSAS-CORPCP  (OCT. '7[illegible]-SEP '[illegible])
              -   AK.2.DU.PH.APH                       1.00    50.0    15.00    3.00   .175
              -   AKDL.AOC.ACC.FRN                     0.00    1.00     0.00    1.00    0.0
  COM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  CLM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  POLINU    0.00   0.00   0.00   0.00   0.00   0.00   0.24   0.00   0.00   0.00   0.00   0.0
  POLINL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ISRM      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ASL       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSU    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKU     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKL     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGU      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGL      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  COM2      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  CLM2      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  POLINU2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  POLINL2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ISRM2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ASL2      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSU2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSL2   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKU2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKL2    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGU2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGL2     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
        2 KANSAS-SOUTOR  (OCT. '78-SEP '79)
              -   AK.2.DU.PH.APH                       1.00    50.0    15.00    3.00    0.00
              -   AKDL.AOC.ACC.FRN.ACEC                0.00    1.00     0.00    1.00    0.00
  COM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  CLM       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  POLINU    0.00   0.00   0.00   0.00   0.00   0.006.0413   0.00   0.00   0.00   0.00   0.0
  POLINL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ISRM      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  ASL       0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSU    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  TRANSL    0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKU     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  SINKL     0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGU      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
  LIGL      0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.00   0.0
        END OF FILE
```

FIGURE 3-9 L2 DATA file

Line 1 FORMAT(2X,I3,1X,12A4,I5)

contains the heading related to the region/application for which data follow, eg.

```
1  KANSAS-COPPER (OCT '78-SEP '80)      2
```

Note:

- the index "1" of the region (or description) must be given
- "2" represents the number of years for which a simulation will be performed (2=IYRS). This number may be 1-10.
- the title is stored in the alphanumeric array TITLES(5,12); see appendix DF.

Line 2 FORMAT(38X,5F7.2)

contains the numerical geometric and other data of:

AR[cm^2]	surface area of the compartment (eg. 1.00)
Z[m]	depth to groundwater table for this application (eg. 100.00 meters)
DU[cm]	depth of upper unsaturated soil zone for this application (eg. 15.00 centimeters)
PH[-]	pH of upper soil zone layer(eg. 8.00)
APH[-]	ratio of pH for lower/upper soil layer(eg. 0.875)

Note:

- This data is stored in the array spaces GEOM(20); see appendix DF.

Line 3 FORMAT(38X,5F7.2)

contains the numerical data of:

AKDE[-]	ratio: biodegradation rate of compound in lower soil zone to upper unsaturated soil zone (eg. 0.00)
AOC[-]	ratio: organic carbon content of soil in lower soil zone to upper unsaturated soil zone (eg. 1.00)

ACC[-]	ratio: clay content of soil in lower soil zone to upper unsaturated soil zone (eg. 0.00)
FRN[-]	Freundlich equation exponent (eg. 1.00)
ACEC[-]	ratio: lower/upper soil zone cation exchange capacity (eg. 0.00)

Note:

- Above data are stored in the array GEOM(20); Appendix DF

Line 4 FORMAT(8X,12F6.2)

contains the numerical data:

CUM(Oct-Sept)[ug/mL] concentration of pollutant in soil moisture of upper zone. If an application is to start with an already polluted column, this concentration should be entered in the month before any loading is specified.

Note:

- These data are stored in the 1st line of the array RUNM1(10,12); see appendix DF.

Line 5 FORMAT(8X,12F6.2)

contains the numerical data:

CLM(Oct-Sept)[ug/mL] concentration of pollutant in soil moisture of lower zone. If an application is to start with an already polluted column, this concentration should be entered in the month before any loading is specified.

Note:

- These data are stored in the 2nd line of the array RUNM1(10,12); see appendix DF.

Line 6 FORMAT(8X,12F6.2)

contains the numerical data:

POLINU(Oct-Sept)[ug/cm^2]; monthly pollution load
(mass) per unit area (cm^2) entering
the upper soil zone.

Note:

- These data are stored in the 4th line of the array RUNM1(10,12); see appendix DF.

Line 7 FORMAT(8X,12F6.2)

contains the numerical data:

POLINL(Oct-Sept)[ug/cm^2]; monthly pollution load
(mass) per unit area (cm^2) entering
the lower soil zone.

Note:

- These data are stored in the 6th line of the array RUNM1(10,12); see appendix DF.

Line 8 FORMAT(8X,12F6.2)

contains the numerical data:

ISRM(Oct-Sept)[ug/cm^2]; monthly index for
pollutant appearance in surface runoff.

ISRM=0	no surface runoff participation
ISRM$\neq$0	any runoff participation
ISRM=1	pollutant in surface runoff

Note:

- These data are stored in the 7th line of the array RUNM1(10,12); see appendix DF.

Line 9 FORMAT(8X,12F6.2)

contains the numerical data:

ASL(Oct-Sept)[-] monthly ratio: concentration of
pollutant in rain to maximum solubility
in water.

Note:

- These data are stored in the 1st line of the array RUNM2(10,12); see appendix DF.

Line 10 FORMAT(8X,12F6.2)

contains the numerical data:

TRANSU(Oct-Sept)[ug/cm^2] monthly amount of pollutant transformed (chemically, biologically or other) in upper soil zone, and not accounted by individually existing model processes.

Note:

- These data are stored in the 2nd line of the array RUNM2(10,12); see appendix DF.

Line 11 FORMAT(8X,12F6.2)

contains the numerical data:

TRANSL(Oct-Sept)[ug/cm^2] monthly amount of pollutant transformed (chemically, biologically or other) in lower soil zone, and not accounted individually.

Note:

- These data are stored in the 4th line of the array RUNM2(10,12); see appendix DF.

Line 12 FORMAT(8X,12F6.2)

contains the numerical data:

SINKU(Oct-Sept)[ug/cm^2] monthly amount of pollutant "lost" by processes not directly described by the model (eg. plant uptake) in the upper soil zone.

Note:

- These data are stored in the 5th line of the array RUNM2(10,12); see appendix DF.

Line 13 FORMAT(8X,12F6.2)

contains the numerical data:

SINKL(Oct-Sept)[ug/cm^2] monthly amount of pollutant "lost" by processess not directly described by the model in the lower soil zone.

Note:

- These data are stored in the 7th line of the array RUNM2(10,12); see appendix DF.

Line 14 FORMAT(8X,12F6.2)

contains the numerical data:

LIGU(Oct-Sept)[ug/cm^2] ligand mass input to the upper soil zone

Note:

- These data is stored in the 8th line of the array RUNM2(10,12); see appendix DF.

Line 15 FORMAT(8X,12F6.2)

contains the numerical data:

LIGL(Oct-Sept)[ug/cm^2] ligand mass input to the lower soil zone

Note:

- These data is stored in the 10th line of the array RUNM2(10,12); see appendix DF.

***** Lines 4-15 can be repeated up to 10 times (10 years) for multi-annual applications of the same site. The number of sets of lines 4-15 should be specified as IYRS in line 1 (eg. IYRS=2).

Lines 1-15 can be repeated for an unlimited number of site-applications by "indexing" (eg. 2 KANSAS, SODIUM) the region/application).

Line 43 (End of file) FORMAT(I1,5X,12A4)

This is the last statement of this file (line 43, figure 3-9)

9 END OF FILE

The previous information is summarized also in Table 3-4 of section 3.2.5.

3.2.4.5 L3 DATA File

This monthly data file contains (Figure 3-10) information required to perform a LEVEL3 application. This file is used in conjunction with the GE DATA file. This file is in structure almost identical to L2 DATA with the exception of additional entries for the third (middle) soil layer.

A user who desires to employ both levels 2 and 3 should load both files, or should load file L3 DATA, copy it into L2 DATA, and consequently eliminate from the L2 DATA the lines he doesn't need for the level 2 simulation.

Because data files L2 and L3 are almost identical, only a file output is presented in this section (Figure 3-10). The user is referred to section 3.2.4.5 for the units of the input parameters or to section 3.2.5 where input information for all files is summarized.

3.2.4.6 EXEC DATA File

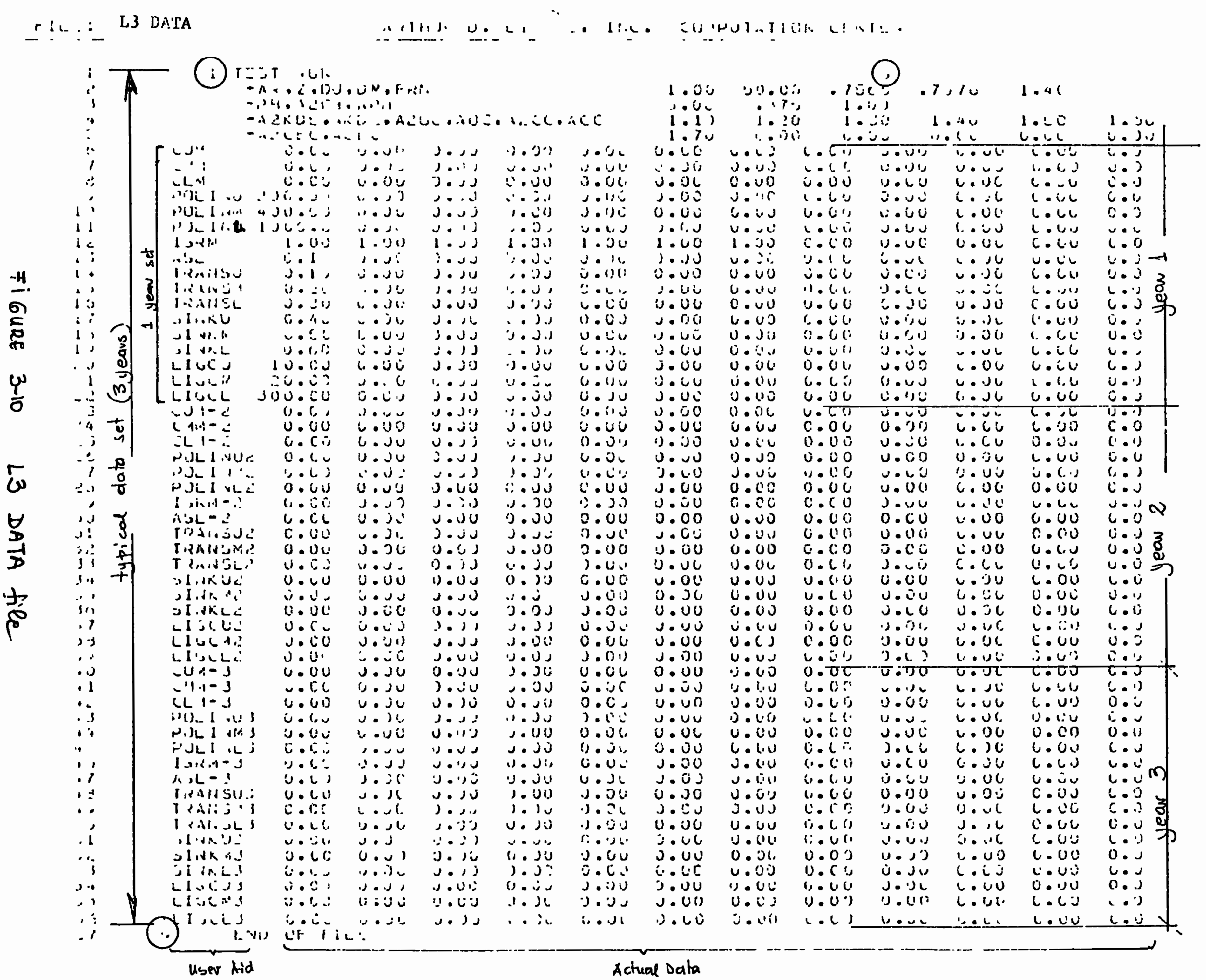
This file is used with all levels of operation and controls the execution of the program, as well as the reading of the various data files. As such, EXEC DATA is employed in conjunction with one or more of the previously described data files.

Each line of the EXEC DATA file corresponds to one run of SESOIL. An unlimited number of runs can be specified. Each line of the file contains 8 integer (control) numbers (Fiugre 3-11). Format and description of these parameters are as follows:

Line 1 FORMAT(8I5)

controls the control variables:

JRUN[-]	incremental number of the run (i.e. 1,2,...)
LEVEL[-]	SESOIL level of operation (i.e. 0-3)
JRE[-]	index of area of application (eg. 17, i.e. CLINTON, MASS from data file EXEC DATA)
JSO[-]	soil type (eg. 8, i.e. CLAY-LOAM)
JCH[-]	chemical compound (eg. 20, i.e. TCE)
JNUT[-]	nutrient cycle participation (for later use, enter as 0 now)
JAPPL[-]	application area (eg. 21, i.e. CLINTON, MASS '79-'80)
JYRS[-]	number of years to be simulated (eg. 1)



```
FILE: L3 DATA                    ARTHUR D. LITTLE, INC.  COMPUTATION CENTER

         1 TEST RUN
             =AK,Z,DU,DM,FRM                           1.00    50.00    .7500    .7370    1.40
             =PH,V2T,...                               5.00     .475    1.00
             =A2KOL,AKOL,A2OL,AOL,A2CC,ACC             1.10     1.20    1.30     1.40     1.50     1.60
             =A2CFC,ACFC                               1.70     0.00    0.00     0.00     0.00     0.00
       COM          0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CMM          0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CLM          0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINO     200.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINM     400.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINL    1000.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       ISRM         1.00    1.00    1.00    1.00    1.00    1.00    1.00    0.00    0.00    0.00    0.00    0.0
       ASL          0.1     0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSO       0.10    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSM       0.20    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSL       0.30    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKO        0.40    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKM        0.50    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKL        0.60    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCO       10.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCM       20.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCL      300.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CO1-2        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CM1-2        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CL1-2        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINO2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINM2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINL2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       ISRM-2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       ASL-2        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSO2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSM2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSL2      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKO2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKM2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKL2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCO2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCM2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCL2       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CO1-3        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CM1-3        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       CL1-3        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINO3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINM3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       POLINL3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       ISRM-3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       ASL-3        0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSO3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSM3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       TRANSL3      0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKO3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKM3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       SINKL3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCO3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCM3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
       LIGCL3       0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.00    0.0
             END OF FILE
```

Figure 3-10 L3 DATA file

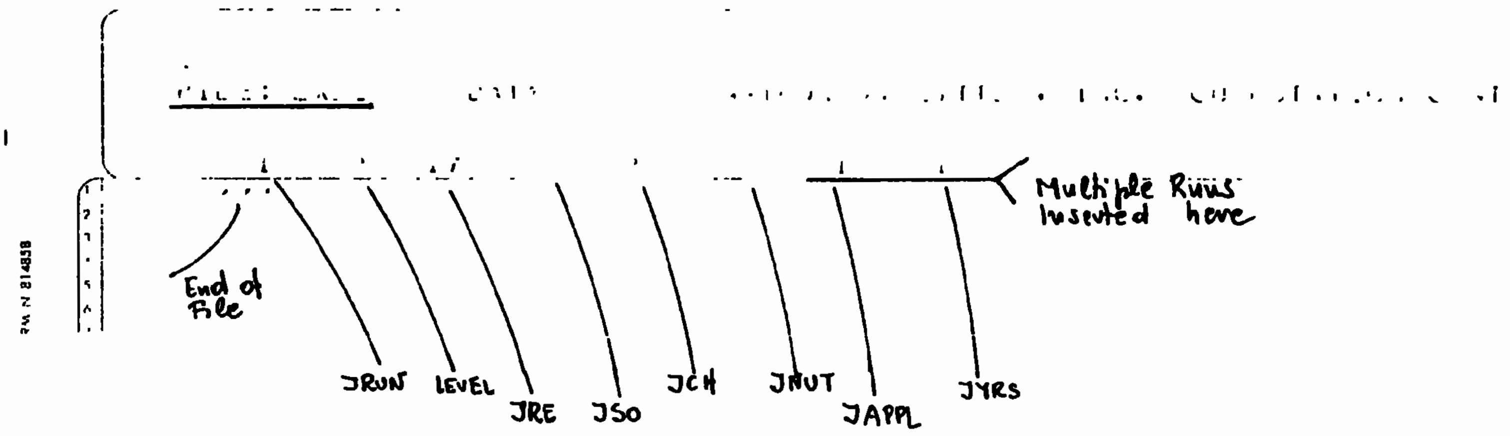


FIGURE 3-11 EXEC DATA File (Expandable & Permanent)

***** Multiple runs are specified with multiple run/line entries.

END OF FILE The number 999 [FORMAT(I5)] indicates end of file.

3.2.5 Summary of Data Input

Table 3-1 summarizes all input data of the GE DATA file.

Table 3-2 summarizes all input data of the L0 DATA file.

Table 3-3 summarizes all input data of the L1 DATA file.

Table 3-4 summarizes all input data of the L2 DATA file.

Table 3-5 summarizes all input data of the L3 DATA file.

Note: Only 1 region, 1 soil type, 1 chemical and 1 application area are shown in the following tables. Following his familiarization with SESOIL, the user may consider consulting only the following tables to load data.

TABLE 3-1

GE DATA FILE

Line				Input Parameter/Variable	FORTRAN Format
Section 3.2.4.1.2					
1			①	Regional Data	I1,5X,12A4
2	Annual Data		1	Regional Title	2X,I3,1X,12A4
3				L TA NN S A (REP)[1]	38X,6F7.2
4				MPA MTR MN MT	38X,4F7.2
5				MPM(OCT) . . . . . . MPM(MAR)	38X,6F7.2
6				MPM(APR) . . . . . . MPM(SEP)	38X,6F7.2
27	Monthly Data		2	Regional Title (IYRS)	2X,I3,1X,12A4,I5
28		IYRS (Sets)		L	8X,1F6.2
29				TA(OCT) . . . . . . TA(SEP)	8X,12F6.2
30				NN(OCT) . . . . . . NN(SEP)	8X,12F6.2
31				S(OCT) . . . . S(SEP)	8X,12F6.2
32				A(OCT) . . . . A(SEP)	8X,12F6.2
33				REP(OCT)[1] . . . . . REP(SEP)	8X,12F6.2
34				MPM(OCT) . . . . . MPM(SEP)	8X,12F6.2
35				MTR(OCT) . . . . . MTR(SEP)	8X,12F6.2
36				MN(OCT) . . . . . . MN(SEP)	8X,12F6.2
37				MT(OCT) . . . . . . MT(SEP)	8X,12F6.2
38				Empty Line	. . . . . .[1]
138			②	Soil Data	I1,5X,12A4
139			1	Soil Title	2X,I3,1X,12A4
140				RS K1 C N OC CC	38X,6F7.2
141				CEC K1U K1M K1L	38X,4F7.2
151			③	Chemical Data	I1,5X,12A4
152			1	Chemical Title	2X,I3,1X,12A4
153				SL KOC DA KDE H K	38X,6F7.2
154				MWT VAL KNH KBH KAH	38X,5F7.2
155				SK B MWTLIG	38X,3F7.2
160			⑨	End of File	I1,5X,12A4

[1] see section 3.2.4.1.2.

TABLE 3-2

LO DATA file

Line Section 3.2.4.2.2		Input Parameter/Variable	FORTRAN Format
1	Area Set	① Application Area / Title	2X,I3,1X,12A4
2		AR Z DU PH APH	38X,5F7.2
3		AKDE AOC ACC ISRA ASL ACEC	38X,6F7.2
4		POLINU POLINL LIGU LIGL	38X,4F7.2
5		THA INF RGA RSA	38X,4F7.2
21		⑨ End of File	I1,5X,12A4

TABLE 3-3

L1 DATA file

Line Section 3.2.4.2.2		Input Parameter/Variable	FORTRAN Format
1	Area set	① Application Area / Title	2X,I3,1X,12A4
2		AR Z DU PH APH	38X,5F7.2
3		AKDE AOC ACC ISRA ASL ACEC	38X,6F7.2
4		POLINU POLINL LIGU LIGL	38X,4F7.2
17		⑨ End of File	I1,5X,12A4

TABLE 3-4

L2 DATA file

Line				Input Parameter/Variable	FORTRAN Format
Section 3.2.4.4.2					
1	Area Set		①	Application Area / Title IYRS	2X,I3,1X,12A4,I5
2				AR Z DU PH APH	38X,5F7.2
3				AKDE AOC ACC FRN ACEC	38X,5F7.2
4		IYRS (sets)		CUM(OCT) . . . . CUM(SEP)	8X,12F6.2
5				CLM(OCT) . . . . CLM(SEP)	8X,12F6.2
6				POLINU(OCT) . . .POLINU(SEP)	8X,12F6.2
7				POLINL(OCT) . . .POLINL(SEP)	8X,12F6.2
8				ISRM(OCT . . . . ISRM(SEP)	8X,12F6.2
9				ASL(OCT) . . . . ASL(SEP)	8X,12F6.2
10				TRANSU(OCT) . . .TRANSU(SEP)	8X,12F6.2
11				TRANSL(OCT) . . .TRANSL(SEP)	8X,12F6.2
12				SINKU(OCT) . . . SINKU(SEP)	8X,12F6.2
13				SINKL(OCT) . . . SINKL(SEP)	8X,12F6.2
14				LIGU(OCT) . . . LIGU(SEP)	8X,12F6.2
15				LIGL(OCT) . . . LIGL(SEP)	8X,12F6.2
43			⑨	End of File	I1,5X,12A4

TABLE 3-5

L3 DATA file

Line Figure 3-10			Input Parameter/Variable	FORTRAN Format
1	Area Set	①	Application Area/Title IYRS	2X,I3,1X,12A4,I5
2			AR Z DU DM FRN	38X,5F7.2
3			PH A2PH APH	38,3F7.2
4			A2KDE AKDE A2OC AOC A2CC ACC	38X,6F7.2
5			A2CEC ACEC	38X,2F7.2
6		IYRS(sets)	CUM	8X,12F6.2
7			CMM	"
8			CLM	"
9			POLINU	"
10			POLINM	"
11			POLINL	"
12			ISRM	"
3			ASL	"
14			TRANSU	"
15			TRANSM	"
16			TRANSL	"
17			SINKU	"
18			SINKM	"
19			SINKL	"
20			LIGCU	"
21			LIGCM	"
22			LIGCL	"
57		⑨	End of File	I1,5X,12A4

3.3 MODEL EXECUTION

3.3.1 Data Requirements

Input of data to the model consists of "adding to" and "editing" the various data files previously described. The following data files and corresponding lines (blocks of data) have to be included for a simulation run (see Tables 3-1 through 3-5).

LEVEL0 Operations

- GE DATA

  Lines 1, 138, 151, 160 -- Titles
  Lines 2, 3(only TA), and 4, 5, 6 with 0.00 -- Climate
  Lines 139, 140, 141 -- Soil
  Lines 152-155 (B=1) -- Chemistry

- LO DATA

  at least 1 set (5 lines)

- EXEC DATA

  at least 1 line

LEVEL1 Operations

- GE DATA

  Lines 1,138, 151, 160 -- Titles
  Lines 2, 3, 4, and 5, 6(with 0.0) -- Climate
  Lines 139, 140, 141 -- Soil
  Lines 152-155 (B=1) -- Chemistry

- L1 DATA

  at least 1 set (4 lines)

- EXEC DATA

  at least 1 line

LEVEL2 Operations

- GE DATA

  Lines 1, 27, 138, 151, 160 -- Titles
  and
  Lines 28-38 -- Climate
  Lines 139, 140, 141 -- Soil
  Lines 152-155 -- Chemistry

- L2 DATA

  at least 1 set (15 lines)

- EXEC DATA at least 1 line

LEVEL3 Operations

- GE DATA

  as in LEVEL2 operations

- L3 DATA

  at least one set (22 lines)

- EXEC DATA

  at least one line

3.3.2 Execution Statement

The user has to give the statement SE81, via a terminal or a card to start the model execution.

3.3.3 Examples of Execution (Output)

The output is intended to be self explanatory and presently it provides information on

(1) all simulation input data (application, climatic, chemical, soil, other) employed in a particular run/execution

(2) the hydrologic cycle components (estimated or assumed in LEVELO), and the monthly or annual pollutant cycle in two or three zones of the compartment, depending upon the level of operation

(3) pollutant concentrations (in soil-moisture, soil-air and adsorbed on soil) in the various soil zones modeled

(4) pollutant masses in the various phases and zones within the soil compartment and released to air and groundwater

(5) averaged and/or totaled behavior of above cycles over a year of monthly simulations via LEVEL2 or LEVEL3.

The SESOIL code is released (upon request) with four pre-programmed runs (see editing of data file EXEC). The user can give the statement SE81 and receive an output for levels 0,1,2 and 3. Periodically developers undertake aesthetic improvements of the output. If necessary they will notify receivers of their tape, and/or provide updated model versions.

A typical input/output is presented in appendix AP (Applications)

3.4 MODEL "VALIDATION"

3.4.1 General

Model output validation is essential to any modeling effort. However, model "validation" is a very broad term and may include model verification, application, calibration, validation and frequently sensitivity and model capabilities. The definition of these terms and the procedures needed to accomplish these objectives is discussed in this section.

Model verification is defined as "the action during which model computer code is run to extremes and model equations are applied to boundary conditions to assure proper code operation" under all potential climatic, soil and other input parameters. Such an action has been undertaken by the developer (see also section 1.1) and users should not be extremely concerned with it. Therefore, only the remaining issues are discussed below.

3.4.2 Model Application

Once a verified model has been obtained, data have to be compiled and input to the model for the "first" application (i.e. model application). Input data can be compiled from:

- site specific investigations and analyses (eg. leaching rates of pollutants, soil permeability);
- national data bases (eg. climatological data from the NOAA); and
- other sources (eg. diffusion rate of pollutants from handbooks).

Compilation of input data for site specific computer runs are model specific, geohydrology and chemistry specific. Some data categories are pollutant source data, climatological data, geographic data, particulate transport data and biological data. Table 3-6 presents some parameters associated with each category.

TABLE 3-6

SOIL MODELING MAJOR INPUT PARAMETER CATEGORIES

CLIMATE:

- Evapotranspiration
- Temperature
- Latitude
- Sunlight
- Plant Cover
- Humidity
- Cloud Cover
- Wind Precipitation

SOIL:

- Porosity
- Density
- Hydraulic Conductivity
- Permeability
- Adsorption Capacity
- Organic Carbon Content
- Clay Content

GEOGRAPHY:

- Slope
- Surface Storage
- Terrain
- Area Coordinates

SOURCES:

- Leaching Rates
- Release Mechanisms
- Patterns of Operation (continuous, batch)
- Locations

Compilation of input data can be relatively straightforward for SESOIL, since SESOIL employs parameters with a physical/chemical meaning. However, time and spatial resolution input data are user-decision input parameters and have to be determined with a previous understanding of the hydrogeology, soil and pollutant characteristics.

Expected outputs from the SESOIL model are:

- temporal and spatial pollutant concentration distributions in soil-air, soil-moisture;
- temporal and spatial pollutant concentration distributions on soil particles; and
- leachate (pollutant mass) migration from the unsaturated soil zone to groundwater.

However, the first application of SESOIL can not be expected to match monitoring records. The common procedure prior to seeking "final" model output is the performance of a number of model runs associated with model applications, model calibrations and a final model validation. This is an iterative operational procedure as discussed in the following sections.

3.4.3 Model Calibration

The calibration, or identification, of a model is the process in which the various model parameters (and that may also include its geometry, inputs, etc.) are redetermined -- although knowledge of them is available from the application stage -- or verified (if such information is available).

The calibration is based on data obtained from observation of the behavior of the simulated "regime" (eg. water balance of basin) in the past. Such data usually include:

- soil moisture, soil infiltration or percolation rates; and
- water levels at gaging station of the basin.

As discussed in Appendix PT, unsaturated models are mathematically structured by:

- developing a flow (moisture movement) submodel;
- developing a quality (pollutant transport) submodel; and
- interfacing the above two submodels.

Calibration procedure, in the context of SESOIL, applies to the flow model part of a code and, therefore, is *defined* as "the effort (parameter estimation) towards a historical matching of the climate, soil and water balance of a basin."

The calibration procedure is often referred to as the "inverse problem." Methods of solving this problem are discussed in the literature. Table 3-7 lists a number of current research efforts that are oriented towards calibrating mainly groundwater models. The same techniques might be applied for unsaturated soil zone models, although unsaturated soil zone modeling is complicated and no single mathematical method can optimally be applied. The following general discussion presents the concept of calibration as applicable to the SESOIL model.

When performing simulations, two different systems are being compared: (1) soil column and (2) the (conceptual) model. Data are taken from the first system, say, on basin annual yield (Eagleson 1978), in order to calibrate the latter. Roughly speaking, the calibration procedure for the model consists of finding a parameter set (intrinsic permeability, porosity) that minimizes deviations between observed and calculated values of annual yields. Least square's deviation is one of the methods employed in the literature. Other methods are linear programming, quadratic programming, and dynamic optimization. The least square's criterion may be written as:

$$\text{Minimize} \quad \sum_{i=1}^{n} \left[Y^{(x,y,t)}_{\text{observed}} - Y^{(x,y,t)}_{\text{calculated}} \right]^2_i$$

where i = 1, . . . n, and n is the number of observed yield values.

The statistical analysis of parameter estimates and model predictions are very promising areas of current research. The mathematics involved, unfortunately, tend to be rather advanced and may be beyond the scope or needs of this modeling effort. Many of the parameter estimation techniques require both initial estimates of the soil cell parameters and their statistical properties. This has stimulated an interest in obtaining the statistical properties directly from field data. One of the more promising procedures is "kriging," which is a stochastic interpolation technique (Delhomme 1979), the developers are planning to use.

Calibration is not a single process, neither is it a process that can be designed step by step *a priori*. As more data become available, the calibration process should be repeated leading to improved model parameters. A schematic of the proposed calibration procedure is shown in Figure 3-12.

Table 3-7

References of Current Research in Calibration/Validation Procedures for Soil/Groundwater Models

Aguado, E.; N. Sitar; and I. Remson (1977). Sensitivity Analysis in Aquifer Studies. Journal of Geophysical Research, Vol. 13, No. 4, p. 733.

Bachmat, Y. and A. Dax (1979). An Iterative Method for Calibrating a Multicell Aquifer Model. Water Resources Research.

Brakensiek, D.L. and C.A. Onstad (1977). Parameter Estimation of the Green and Ampt Infiltration Equation. Water Resources Research, Vol. 13, No. 6, p. 1009.

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Dettinger, M.D. and J.L. Wilson (1981). First Order Analysis of Uncertainty in Numerical Models of Groundwater Flow. 1. Mathematical Development. Water Resources Research, Vol. 17, No. 1, pp. 149-161.

Gambolati, G. and G. Volpi (1979). A Conceptual Deterministic Analysis of the Kriging Technique in Hydrology. Water Resources Research, Vol. 15, No. 3, pp. 625-629.

Haverkamp, R. and M. Vauclin (1979). A Note on Estimating Finite Difference Interblock Hydraulic Conductivity Values for Transient Unsaturated Flow Problems. Water Resources Research, Vol. 15, No. 1, p. 181.

Table 3-7 (continued)

Hayhoe, H.N. (1978). Study of the Relative Efficiency of Finite Difference and Galerkin Techniques for Modeling Soil-Water Transfer. Water Resources Research, Vol. 14, No. 1, p. 97.

Hefez, E.; U. Shamir; and J. Bear (1975). Identifying the Parameters of an Aquifer Cell Model. Water Resources Research, Vol. 11, No. 6, p. 993.

Kohberger, R.C.; D. Scavia; and J.W. Wilkinson (1978). A Method for Parameter Sensitivity Analysis in Differencial Equation Models. Water Resources Research, Vol. 14, No. 1, p. 25.

McElwee, C.D. and M.A. Yukler (1978). Sensitivity of Groundwater Models with Respect to Variations in Transmissivity and Storage. Water Resources Research, Vol. 14, No. 3, pp. 451-459.

Murty, V.V.N. and V.H. Scott (1977). Determination of Transport Model Parameters in Groundwater Aquifers. Water Resources Research, Vol. 13, No. 6, p. 941.

Navarro, A. (1977). A Modified Optimization Method of Estimating Aquifer Parameters. Water Resources Research, Vol. 13, No. 6, p. 935.

Nutbrown, D.A. (1975). Identification of Parameters in a Linear Equation of Groundwater Flow. Water Resources Research, Vol. 11, No. 4, p. 581.

Sagar, B.; S. Yakowitz; and L. Duckstein (1975). A Direct Method for the Identification of the Parameters of Dynamic Nonhomogeneous Aquifers. Water Resources Research, Vol. 11, No. 4, p. 563.

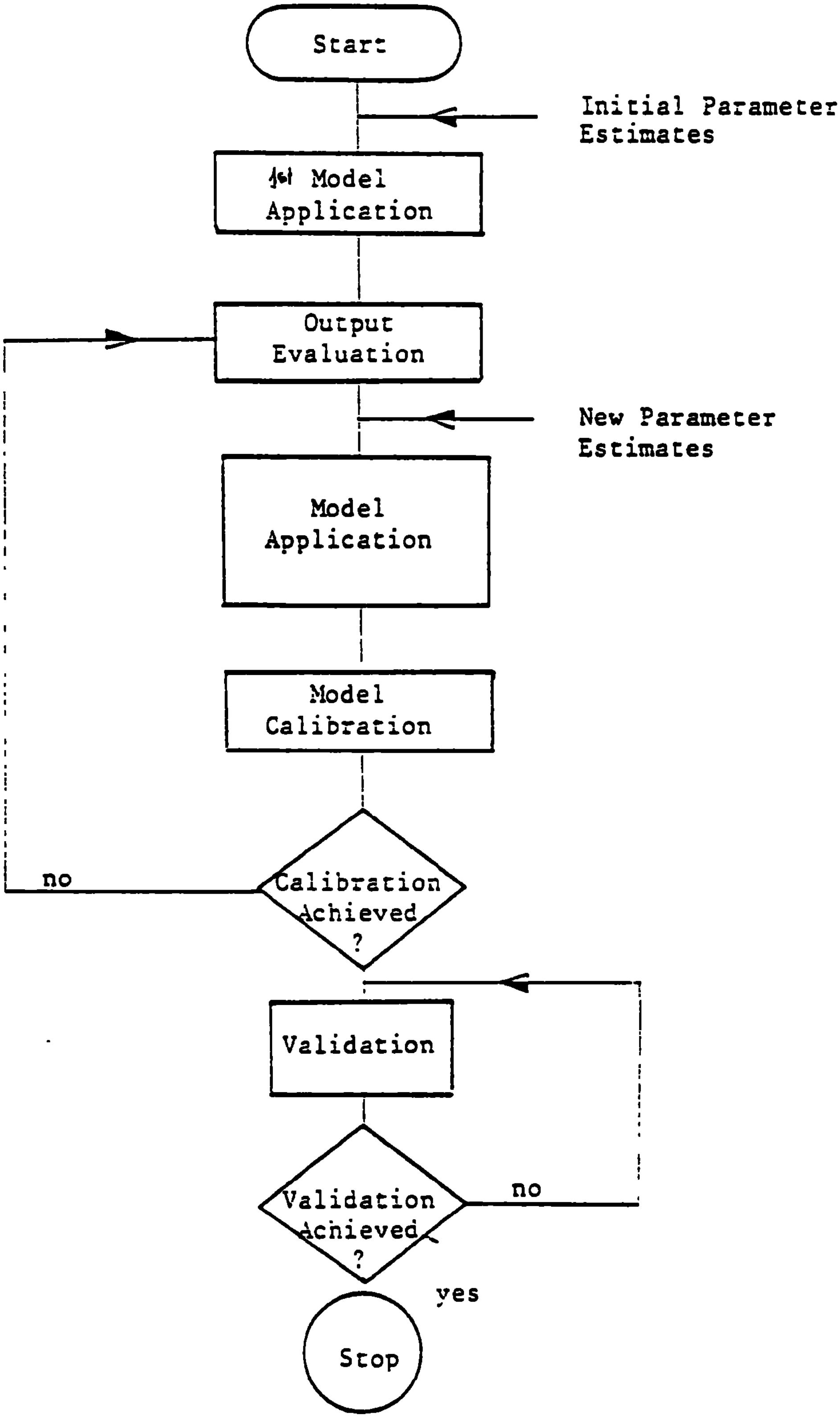

Figure 3-12 SCHEMATIC OF MODEL APPLICATION/CALIBRATION/VALIDATION

Calibration of unsaturated soil zone models can be uncertain and difficult because climate, soil moisture, soil infiltration and percolation are strongly interrelated parameters that can be difficult and/or expensive to measure in the field. Therefore, calibration of unsaturated soil zone models is frequently associated with a model validation (described in the next section).

For the available version of SESOIL that employs Eagleson's (1978) annual water balance theory (as expanded to monthly simulations and with moisture transfer budget in the course of the months), authors recommend model calibration by varying the intrinsic permeability (k), the pore disconnectedness index (c) and the porosity (n) of the soil; all input parameters to the model (see appendix ID, section 3.0).

The outlining of steps for the calibration procedure of SESOIL is a feasible task; however such a task would require a thoughtful elaboration of this issue by the authors prior to outlining it in this document.

3.4.4 Model Validation

Frequently, the definitions of calibration and validation are synonymously employed in the literature because of the large number of nonvalidated but calibrated groundwater models and the limited number of noncalibrated but validated unsaturated soil zone models. For SESOIL , model validation is defined as "the process which analyzes the validity of final model output." In SESOIL, the validity of the predicted pollutant concentrations would be compared to available knowledge of measured pollutant concentrations from monitoring data (field sampling).

A disagreement in absolute levels of concentration (predicted versus measured) does not necessarily indicate that either method of obtaining data (modeling, field sampling) is incorrect or that either data set needs revision. Field sampling approaches and modeling approaches rely on two different perspectives of the same situation.

Field data give concentrations at points in time and space, models predict "average" concentrations for a particular assumed set of conditions. Thus, field and model results may differ and still both be correct. Some possible reasons for a discrepancy are:

- The field sample was taken from a spot with atypical concentrations (eg. a water sample may be close to an unidentified confounding source, and so give abnormally high readings).

- The sample was taken under a typical conditions (eg. on the one day/month that it rained); model results were calculated for average conditions, which may rarely occur (eg. at the "average" soil moisture content which occurred only for a short period).

- The sample contained interactive compounds (eg. a water sample contained some sodium that may have resulted in increased soil permeabilities).

- The extraction procedure for the sample was under or over efficient (eg. it not only extracted all organic pollutants from a soil sample but also dissolved the soil).

Mathematically, the available model validation procedures and techniques are similar to those presented in the previous section. Following a validation procedure with good field data, "no better model predictions" can be made. This will be the "best possible" output.

For SESOIL, the approach -- at the present time -- would be to:

- apply simplified mathematical techniques (as described above for calibration);

- exercise the professional experience, gained from original model application work to refine the results; and

- document the validation logic for the SESOIL level employed.

A schematic figure of the previously discussed processes is shown in Figure 3-12.

3.4.5 Model Sensitivity Analysis

It is frequently worthwhile to perform sensitivity analyses to determine the effect on the predicted concentrations caused by a change in the input parameters. These sensitivity analyses are particularly important when data gaps or uncertain input values exist. It may also be useful to rerun SESOIL to estimate the impact of various site management or design strategies on pollutant distribution and concentrations in the environment. Two main techniques are widely used to perform sensitivity analyses:

- model simulations; and

- analytic techniques.

Model simulations are performed by running and rerunning the model, simultaneously varying the value of one or more parameters following a "scenario" logic. Model concentration predictions may be compared to monitoring data as described in the previous section.

Analytic techniques of linear systems theory (Dooge 1973) and optimization theory (Haimes 1977) may correlate sensitivity of model input (eg. leaching quantity) to model output (eg. soil concentrations) "without" performing multiple model reruns (simulations). An example is given below for an analytic technique (Fiksel et al 1981).

Assume a SESOIL column receiving pollutant input quantifies I in all layers (cells). Assume SESOIL accounting for a linear Freundlich adsorption coefficient and assume that average predicted adsorbed concentrations in the N cells are the c(N). Then the following matrix, linear response function F(N) can be written:

$$\underline{I(N)} = \underline{F(N)} \cdot \underline{c(N)}$$

where F(N) a low triangular (f,0) matrix:

$$\underline{F}(N) = \left| \; f \diagdown^{\,0} \; \right|$$

From the first relation, we have:

$$\underline{F}(N) = \underline{I}(N) \cdot \underline{c}(N)^{-1}$$

from which all elements N of F can be estimated. Given a possible linearity of c versus I, we are at a position now to vary input sources of the model and estimate concentration "without" having to run and rerun SESOIL. This approach has not been exercised by the developers; however, they may consider it in the future for certain processes and parameters.

3.4.6 Model Limitation

Any mathematical model is "as good as its weakest link"; therefore, limitations of the model are correlated with the limitations of each of the routines and processes coded (see also section 1.1). In general, limitations can be due to:

- data availability,
- inoptimal single medium model application to a particular site,
- omission of important chemistry reactions, and

- lack of appropriate model validation opportunity

Data availability refers to environmental data (eg. climatic, soil, water resource), source data (eg. pollutant leaching from the site), chemistry data (eg. chemical properties of pollutants) and monitoring data (eg. ambient concentrations). It is not appropriate, for example, to drive any soil model without a proper set of weather records and then attempt to validate the model output with available monitoring data.

Omitting certain important pathways or chemistry reactions or processes (eg. volatilization) because of lack of data can become an issue of concern. Such pathways should be evaluated outside the model or, at certain times, another modeled via SESOIL as far as possible. A model sensitivity analysis of omitted (or to be omitted) processes is essential.

3.4.7 Discussion

During the SESOIL development a number of verifications, calibration, validation and sensitivity steps have been performed to one degree or another.

The model code has been verified by extensive testing and under extreme conditions of input data. Each level of operation has been run multiple times and the results have been compared and rectified with sample hand calculations and by other models.

On an earlier contract to the EPA, SESOIL has been applied to two actual land treatment sites at which considerable monitoring data were available. Good agreement was obtained between monitoring data and model results. This study provided to model developer the only validation of SESOIL. These sites were also used for a sample calibration effort where the soil parameters of intrinsic permeability and adsorption coefficients (K, K_{oc}) were calibrated/validated to field records (Bonazountas et al 1981).

One short study for metals has been performed (Bonazountas et al 1981) and another short study for halogenated solvents is underway (Wagner & Bonazountas 1982), both aimed to evaluate the overall fate of pollutants in the soil compartment, including losses to the air and to groundwater. In both studies, canonical/scenario environments were designed by combining a range of climates, soils and pollutants, in order to trace sensitivity of various parameters upon the long-term overall pollutant fate.

In the future model developers hope to extend these efforts, particularly to include increased calibrations and validations with actual field data, an essential task for model improvement and validity.

3.5 References

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HY - hydrologic cycle

APPENDIX HY

HYDROLOGIC CYCLE

To the Reader/User:

Information contained in this appendix is not well documented at all, for reasons explained below, and authors fully recognize this fact.

For the authors -- although the hydrologic cycle governs the model operations -- the full and accurate hydrologic cycle "documentation" has not been of primary importance because:

- Hydrologic cycle development of SESOIL has not been accomplished yet.
- The hydrocycle of SESOIL is primarily based on Eagleson's annual "Climate, Soil, and Vegetation" theory, which is excellently documented in the literature (Eagleson 1978; other publications). Therefore, the author would have spent appreciable effort in representing Eagleson's work.
- Budget constraints of this contract (see section 1.1) led the authors to prioritize documentation of chemistry related and other issues of SESOIL, i.e. original information generated for SESOIL.
- This SESOIL documentation is not to be released in the public domain, therefore, a tentative draft regarding the hydrologic cycle would be sufficient for a reader/user to understand the basic "concept" adapted for the hydrologic cycle; i.e. Eagleson's theory adaptation.
- The hydrologic cycle documentation is of secondary importance to a reader or a user, contrasted to the documentation of other processes, because of the simplicity of input data (and here lies the sophistication and elegancy of Eagleson's theory) required to drive this part (hydrology) of SESOIL.

However: Eagleson's annual theory has been adapted to SESOIL needs by

- expanding the work into monthly hydrocycles,

- accounting of moisture storage transfer from month-to-month in the entire compartment,
- not fully employing the vegetational aspects of the basic theory, because the watershed aspects of SESOIL have not been developed yet,
- accounting for zero rain (depth, number of storm events, etc)
- accounting for a "smooth" heterogeneity along the soil column (soil type stratification)
- omitting vegetational and soil surface moisture retention for reasons related to SESOIL needs under the current contract (i.e. a model for overall fate of pollutants) at non-vegetated areas rather than a model for basin-specific pollutant transport on the watershed.
- presenting (model output) only expected values of the statistical distributions of the hydrologic processes model.

The above adaptation issues are not always clearly documented in this appendix. The authors are aware of the deficiencies of this document that was drafted in 1980 (see page HY-1) when SESOIL was conceptualized; however, they intend to improve it when possible.

The SESOIL authors appreciate that Eagleson's work might have been frequently misquoted, paraphrased and mis-duplicated. The issue is not so much of credit given to Eagleson by citing his work, but rather it is one of possible misunderstanding and misuse of his theory. Therefore, readers or users are advised to consult Eagleson's original theory.

CONCEPTUAL DRAFT

(see section 1.1)

APPENDIX HY

HYDROLOGIC CYCLE

1.0 INTRODUCTION

1.1 General

The hydrology of the soil compartment can be:

(1) Assumed annually known (LEVEL0),
(2) Simulated annually (LEVEL1), or
(3) Simulated monthly (LEVEL2, LEVEL3).

Simulations* (LEVEL1, LEVEL2, LEVEL3) are performed via two hydrologic cycle subroutines, designed as HYDROA (Annually) and HYDROM (Monthly), the latter being an extention of the first.

1.2 Hydrologic Processes Involved

The two hydrologic subroutines (HYDROA and HYDROM) simulate the atmosphere, surface and subsurface hydrologic processes shown in Figure HY-1. The hydrologic processes are the main governing factors of pollutant movement in the soil compartment.

Precipitation encompasses rainfall and snow. Snowpack and snowmelt affect pollutant movement first by reducing erosion and secondly by causing less polluted runoff than the corresponding rain runoff.

Infiltration is the movement of water through the soil surface into the soil column. Infiltration rates are variable and change with the moisture content of the soil profile. During a storm event, the rate of infiltration decreases as the soil voids become filled. Usually more than half of the water which infiltrates is retained in the soil until it is returned to the atmosphere by evapotranspiration. Some infiltrated water may move laterally through the upper soil through the stream channel as interflow, and some may enter temporary storages and be later discharged into the stream channel as base or groundwater flow. The infiltration capacity is a function of the plant cover and of variable hydrogeologic characteristics, primarily soil moisture content.

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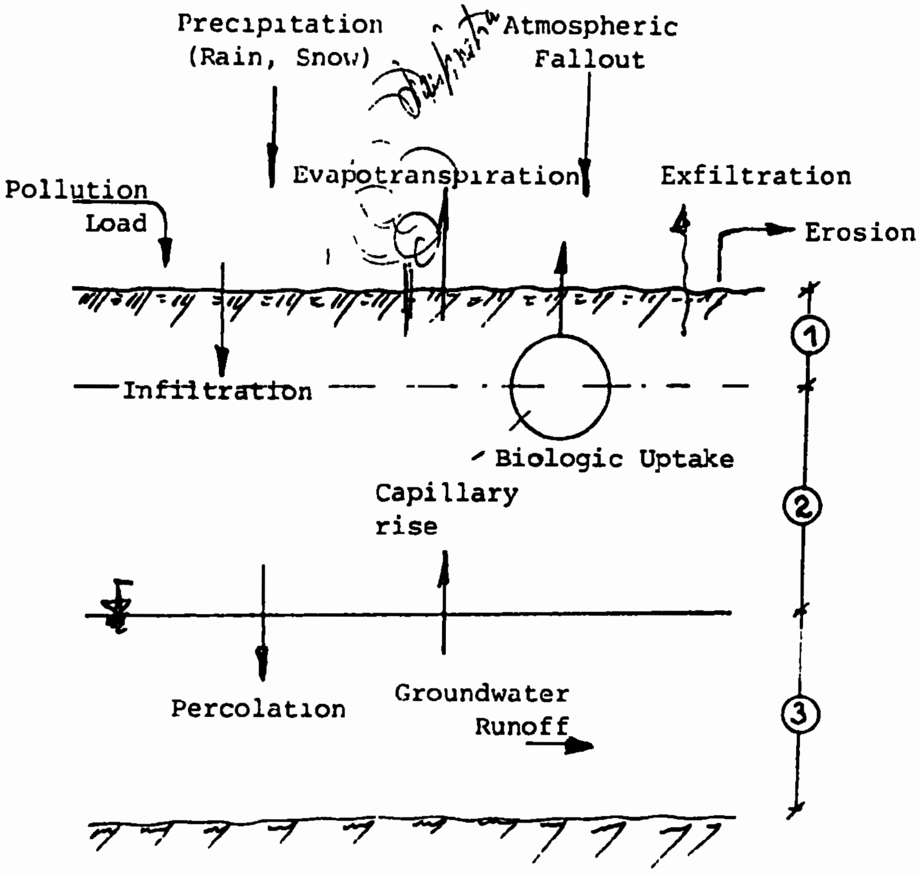
*In this appendix the word simulation is equivalent to modeling.



① Upper Unsaturated Soil Zone

② Lower Unsaturated Soil Zone

③ Saturated Soil Zone

Figure HY-1

Atmosphere, Land, Surface, Subsurface,

Biotic and Pollutant/Processes

Evapotranspiration is the transfer of water from land, vegetative cover and water bodies to the atmosphere. The term involves two distinct processes, exfiltration and transpiration. The volume of water leaving the watershed through evapotranspiration is greater than the total contribution to the base streamflow of most systems. All surfaces that are exposed to precipitation are considered to have a potential for evapotranspiration. Transpiration is a function of a vapor pressure gradient between air and leaf cells and occurs when leaf pores are stimulated by light. Deeply rooted plants continue to transpire even in periods of infrequent rainfall.

Interception is the amount of precipitation remaining on leaves, branches, and stems. This volume may or may not return to the atmosphere through transpiration. Intercepted water quantities during a single storm are relatively minor. However, they can have a significant effect on long term surface runoff volumes. Interception is a function of the type and extent of vegetation, land and meteorologic characteristics of the area (wind, temperature, solar radiation, precipitation, etc.)

Percolation results in groundwater runoff. Percolation rates depend mainly upon the infiltration rate, the moisture storage in the unsaturated soil zone and the depth to groundwater. During dry seasons percolation may become negative (upward) due to capilarity.

1.3 Modeling Background

Previous efforts to model combined hydrologic, soil and vegetational systems of an area have been in two noteworthy directions (Eagleson, 1979; p. 924):

(1) Empirical studies that provide validated interrelationships among the principle variables but that, due to their weak physical basis, lack both the generality and the parametric incorporation of climate, soil and vegetal properties that are necessary for general insight into soil processes. Prominent among these studies are the works of Lettan (1973) and Thornthwaite (1948); and

(2) Numerical studies--that utilize detailed formulations of the physics at the microprocess scale but that, due to their complexity, impose infeasible validation data requirements and impede the generation of overall behavioral insight. Prominent among these studies are the works of Adams and Jurisa (1976), Donigian, et al (1977), and Novotny, et al (1978).

It is beyond the scope of this study to review the literature and describe the physics and mathematics of the previous studies. SESOIL does not employ either an empirical or a numerical hydrologic routine; instead it employs the statistical analytic "annual water balance" model of Eagleson (1978), which couples atmosphere, soil and vegetation systems. In SESOIL, however, Eagleson's model is modified to perform both annual and monthly simulations. The scientific background of the annual model has been presented and discussed in various journals since 1978. Therefore, this appendix (HY) is intended to presently only an "extracted" outline of the model as previously given in Eagleson's publications. The following paragraphs intend only to inform the reader about the nature of the hydrologic routine employed and <u>not</u> to give a thorough background of it. To maintain a consistent approach, Eagleson's notation is followed. Readers interested in the derivation of the annual equations presented in the following sections, are referred to the original publications.

The work of Eagleson presents a "generalized" annual water balance model based upon simplified physics of the component proceses. The model is detailed enough to capture the "essential" system dynamics yet simple enough to permit analytical (as opposed to numerical) solution. It produces valuable insights into the role of soil moisture in environmental compartments, of which moisture is one of the most important factors governing pollutant transport and decay in the soil cell. Eagleson's model has a unique statistical approach in coupling systems and represents the state of the art in environmental modeling. The model is easy to use because of the limited number of input parameters required. The latter is fully justified by the sophisticated mathematical approach developed by Eagleson.

Section 2.0 of this appendix provides the hydrologic cycle background for the LEVELO model operation, dealing with "known" hydrologic components of the soil compartment. The following two main sections (Sections 3.0 and 4.0) outline the theoretical background for the "annual" hydrologic cycle subroutine (HYDROA) and the "Monthly" hydrologic cycle subroutine (HYDROM), the latter being developed based upon the theory of the first.

2.0 LEVELO - ANNUALLY "KNOWN" HYDROLOGIC COMPONENTS

2.1 Input Data

The following parameters must be known (input) for the LEVELO operation of SESOIL.

I_A = annual infiltration; (cm)

R_{sA} = annual surface runoff; (cm)

R_{gA} = annual groundwater runoff; (cm)

Θ = mean annual soil moisture content; (mL/mL)

2.2 Discussion on Soil Water Models

Recent developments of soil water models based on column mass balance provide an alternative to directly or indirectly measuring soil moisture in the field. Figure HY-1 is a schematic diagram of the physical system and the driving forces that must be considered in modeling the system.

Based upon conservation of mass, the soil moisture in the system at any time can be determined using the relationship:

$$P_A = E_{TA} + \Delta s_o + R_{gA} + R_{sA} \qquad \text{(HY-0)}$$

where:

P_A = total annual precipitation

R_{sA} = total annual surface runoff

E_{TA} = total annual evapotranspiration

Δs_o = $s_o(t)-s_o(t-1)$; annual change in the soil moisture storage.

R_{gA} = total annual groundwater runoff

Four of the above variables are user supplied input, the fifth is estimated. A standard practice in annual soil water budget modeling is to estimate Δs_o from the above equation, using site-specific estimates of the other parameters. Consequently $s_o = s_o(t)$ is estimated from the relationship $s_o(t) = \Delta s_o - s_o(t-1)$, given the historical moisture storage $s_o(t-1)$.

Various references (e.g., National Water Atlas, Gerapty & Miller, Inc.) can be consulted for the annual averages of P_A, E_{TA}, R_{GA} and R_{SA}, for various locations in the U.S.

3.0 LEVEL1 - ANNUALLY "ESTIMATED" HYDROLOGIC CYCLE

3.1 General

The theory for the "annual" hydrologic cycle routine is presented by Peter S. Eagleson, in Water Resources Research (WRR), Volume 14, October 1978, Number 5, pages 705 through 776 and in a number of other publications. In this report, reference is mainly made to the above publication by indicating the page number and the equation number of the equations employed.

3.2 Definitions

It is the writer's feeling that the reader of this documentation and of Eagleson's publications might be confused with the definitions: annual, seasonal, monthly, long-term, etc., unless they are thoroughly acquainted with the theoretical background of the hydrologic cycles presented in this documentation. Therefore, it is worthwhile to clarify at this point the following expressions applicable to both the "annual" (Section 3.0) and the "monthly" (Section 4.0) hydrologic cycle routines.

(1) For the "annual" hydrologic cycle routine the "simulation period" or simulation time (or time step) equals a period of "one year" (i.e. 12 months). Within this year we have a rainy "season" which can be shorter or equal to one year (12 months) depending on the climate of the area.

(2) For the "monthly" hydrologic cycle routine, the "simulation period" or simulation time equals a period of "one month". Within this month we have a rainy "season" which can be shorter or equal to one month (1 month) depending on the climate of the area.

Eagleson employs both expressions "annual/seasonal" while presenting his "annual" water balance theory [e.g.,WRR,p.749,eq.(1)]. This is fully justified from his perspective, however, to avoid confusion (e.g. seasonal for annual vs. seasonal for monthly simulation) in the following section we will standardize our definitions as discussed above, and will explicitly define the terms.

3.3 Annual Mathematical Analysis

3.3.1 Assumption

The principal assumptions made are [Eagleson, 1977]:

(1) No consideration of heavy snow or ice precipitation

(2) Consideration of vegetation only as it affects surface albedo and roughness

(3) One-dimensional analysis, involving vertical processes only

(4) All processes are stationary in their long-term (annual/seasonal) average

(5) First-order analysis, namely, long-term averaged behavior, is used to represent relationships between seasonal averages.

3.3.2 Theoretical Overall Approach

3.3.2.1 The Water Balance Equation

The analysis of subroutine HYDROA is based upon:

(1) The volumetric water balance equation per unit area of the soil column over time [WRR,p.706,eq.(1)]:

$$\int_0^t [i(t)-e_T(t)-v_s(t)]dt = \int_0^t [r_s(t)+r_g(t)]dt = \int_0^t y(t)dt \qquad \text{(HY-1)}$$

where:

t = time

s = soil moisture concentration

$i(t)$ = precipitation

$e_T(t)$ = potential evapotranspiration rate

$v_s(t)$ = rate of moisture storage in soil, vegetation, snow, ice, lakes, etc.

$r_s(t)$ = surface runoff rate

$r_g(t)$ = groundwater runoff rate

$y(t)$ = yield rate

(2) The surface infiltration conservation equation over time [WRR,p.706,eq.(3)]:

$$\int_0^t i(t)dt - \int_0^t v_{ss}(t)dt - \int_0^t f_i(t)dt = \int_0^t r_s(t)dt \qquad \text{(HY-2)}$$

where:

v_{ss} = rate of capture of precipitation in surface storage (i.e., on the soil and vegetal surface)

$f_i(t)$ = infiltration rate

Assuming all evapotranspiration comes from soil moisture and considering only systems which are steady-state in long-term average, Eagleson [WRR,p.706,eq.(2)] developed the water balance equation:

$$E[P_A] - E[E_{TA}] = E[R_{sA}] + E[R_{gA}] = E[Y_A] \qquad \text{(HY-3)}$$

where:

$E[x]$ = $m_{[x]}$, expected value or mean of a variable x

P_A = annual precipitation; (depth, cm)

R_{sA} = annual surface runoff; (depth, cm)

R_{gA} = annual groundwater runoff; (depth, cm)

E_{TA} = annual total evaporation; (depth, cm)

Y_A = annual yield; (depth, cm)

Rearranging the above equation and by omitting the E[ ] designations [WRR,p.707,eq.(4)]:

$$\underbrace{I_A(P_A)}_{\text{Infiltration}} = \overbrace{P_A}^{\text{Precipitation}} - \overbrace{R_{sA}(P_A)}^{\substack{\text{Surface}\\ \text{Runoff}}} \tag{HY-4}$$

$$= \underbrace{E_{TA}(P_A)}_{\text{Evapotranspiration}} + \underbrace{R_{gA}(P_A)}_{\substack{\text{Groundwater}\\ \text{Runoff}\\ \text{(Recharge}\\ \text{and Loss)}}}$$

The following sections present a summary of the mathematical expressions developed by Eagleson for the various terms of the above equation. This equation is designated later on as "soil moisture (s_o)" equation because factors become soil-moisture dependent. It must also be noted that the above equation involves the implicit assumption of constant water storage over the given water season. This is only an approximation of reality; it is closest in nature to an arid, seasonal climate with ephemeral streams because the end-of-year moisture storage is there only at its annual minimum, and therefore very small.

Significant snowfall may have large interception losses, theoretically invalidating the above. However, the authors believe that the employment of Eagleson's model -- a discussion for snow pack/melt and interception is made in a later section -- is strongly desired because of its advantages in its formulation that is based on a relatively few physical parameters and very few input data.

3.3.2.2 Precipitation

The storm sequence is represented in the model by Poisson arrivals of rectangular pulses, as shown in Figure HY-2.

The cumulative distributive function for normalized annual point precipitation is [WRR,p.715,eq.(36)]:

$$\mathrm{Prob}\left[\frac{P_A}{m_{PA}} < z\right] = e^{-\omega m_\tau}\left\{1+\sum_{\nu=1}^{\infty}\frac{(\omega m_\tau)^\nu}{\nu!}P[\nu\kappa,\omega m_\tau \kappa z]\right\} \qquad \text{(HY-5)}$$

where:

P_A = total seasonal precipitation (cm)

m_{PA} = average seasonal precipitation (cm)

ω = storm arrival rate (days^{-1})

m_τ = average length of rainy season (days)

κ = shape parameter of Gamma distribution of storm depth (h)

ν = number of storms

P[ ] = Pearson's incomplete Gamma function

z = p/m_{PA}

p = value of annual rainfall (taken on by the random variables p_A).

The Gamma distribution of storm depth is given by [WRR,p.714,eq.(15)]:

$$f_H(h) = G(\kappa,\lambda) = \frac{\lambda(\lambda h)^{\kappa-1} e^{-\lambda h}}{\Gamma(\kappa)} \qquad \text{(HY-6)}$$

with mean [WRR,p.714,eq.(16)]:

$$m_H = \kappa/\lambda = m_{PA}/\omega\cdot m_\tau \qquad \text{(HY-7)}$$

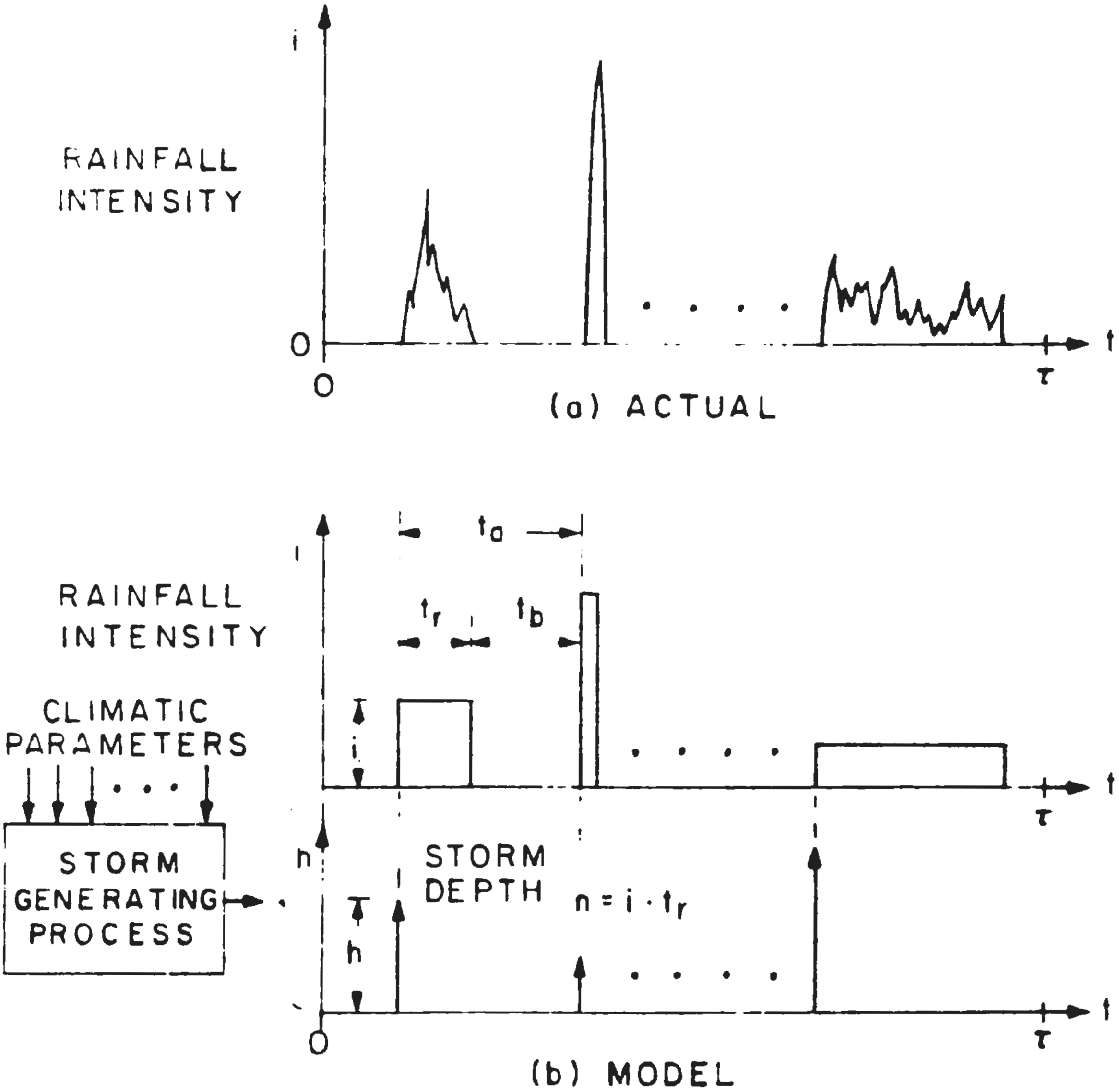


Figure HY-2

Precipitation Event Model

Source: [WRR,p.707,Figure 5]

and variance [WRR,p.714,eq.(17)]:

$$\sigma_H^2 = \kappa/(\lambda)^2 \qquad \text{(HY-8)}$$

in which:

h = storm depth (cm)

λ = parameter of Gamma distribution of storm depths, equal to κ/m_H (cm^{-1})

Equation HY-6 is shown to accurately reproduce the observed annual precipitation probability relationship in applications to both humid and arid-seasonal climates using only a few years (e.g., five) of storm data.

3.3.2.3 Soil Infiltration

The following assumptions were made for deriving statistical equations for capillary rise from the water table (dry seasons), infiltration, exfiltration (i.e., desorption against gravity), and percolation to groundwater table [P.Eagleson, 1977]:

1. Homogeneous soil
2. No vegetation, snow or ice presence
3. Movement of water vapor negligible
4. Soil column is effectively semi-infinite concerning surface processes of infiltration and exfiltration (i.e., the water table or other boundary is deeper than the penetration depth of the surface processes)
5. Soil moisture is spatially uniform at the beginning of each storm and interstorm period with a value s_o, given by the long-term temporal and spatial average
6. Infiltration processes (infiltration, exfiltration, gravitational percolation and capillary rise) are considered as separable superimposable processes
7. Infiltration is described by the Phillip equation.

The derived soil moisture velocity equations are:

Capillary Rise from the Water Table [WRR,p.728,eq.(59)]:

$$w = \left[\frac{mc + 1/2}{mc-1}\right] K(1) \left[\frac{\Psi(1)}{Z}\right]^{mc} \qquad \text{(HY-9)}$$

$$\Psi(1) = \frac{\sigma_w}{\gamma_w}\left[\frac{n}{k(1)\phi(c)}\right]^{1/2} \qquad \text{(HY-10)}$$

in which:

w = apparent velocity of capillary rise; (cm/sec)

m = pore size distribution index; (-)

n = effective medium porosity; (cm^3/cm^3)

c = pore disconnectedness index; (-)

$K(1)$ = saturated effective hydraulic conductivity (cm/sec),

$$\equiv \frac{\gamma_w \cdot k(1)}{\mu_w}$$

$k(1)$ = spatial average effective soil permeability at saturation; (cm^2)

$\Psi(1)$ = saturated matrix potential; (cm)

Z = depth to groundwater table; (cm)

σ_w = surface tension of pore liquid; (dynes/cm)

ϕ = pore shape parameter; (-)

γ_w = specific weight of liquid; ($dynes/cm^3$)

μ_w = dynamic viscosity of pore fluid; (poises)

Infiltration [WRR,p.726,eq.(42);p.723,eq.(16)]:

$$f_i(t,s_o) = (1-s_o)\left[\frac{5nK(1)\Psi(1)\phi_i(d,s_o)}{3\pi mt}\right]^{1/2} + \frac{1}{2}K(1)[1 + s_o^{c}]-w \qquad \text{(HY-11)}$$

$$\phi_i = 10^{(0.66 + 0.55/m + 0.14/m^2)} \qquad \text{(HY-12)}$$

where:

f_i = apparent infiltration velocity; (cm/sec)

n = soil effective porosity; (-)

ϕ_i = infiltration diffusivity function; (-)

d = $c - 1 - (1/m)$; [WRR,p.723,eq.(12)]

Exfiltration [WRR,p.727,eq.(44)], simplified for no vegetation:

$$f_e(t,s_o) = s_o^{1+d/2}\left[\frac{nK(1)\Psi(1)\phi_e(d)}{\pi mt}\right]^{1/2} + w \qquad \text{(HY-13)}$$

where:

f_e = apparent exfiltration velocity; (cm/sec)

ϕ_e = dimensionless exfiltration diffusivity; (-)

Percolation to Water Table [WRR,p.729,eq.(62)]:

$$v(s_o) = K(1)s_o^{\,c} - w \qquad \text{(HY-14)}$$

where:

v = apparent percolation velocity (cm/sec)

3.3.2.4 Annual Infiltration and Surface Runoff

The principal assumptions made are [Eagleson, 1977]:

1. No evaporation from surface storage at any time
2. No infiltration from surface storage following cessation of precipitation
3. No surface inflows from outside region
4. Soil moisture is uniform at s_o at the beginning of each storm
5. Precipitation intensity, i, and duration, t_r, are statistically independent.

The probability density function of storm surface runoff is determined and gives the:

Frequency of Flood Volume [WRR,p.746,eq.(72)]:

$$\frac{1}{T_E} = 2m_\nu z^{1/2} e^{-G-2\sigma} K_1(2z^{1/2})\ \Gamma(\sigma + 1)/\sigma^\sigma \qquad \text{(HY-15)}$$

Annual Average Surface Runoff, $E[R_{sA}]$; [WRR,p.746,eq.(68)]:

$$\frac{E[R_{sA}]}{m_{PA}} = e^{-G-2\sigma}\ \Gamma(\sigma + 1)/\sigma^\sigma \qquad \text{(HY-16)}$$

in which [WRR,p.746,eq.(69)]:

T_E = recurrence interval of flood of depth, R_{sj}

$z = R_{sj}/m_H$

$$\sigma = \left[\frac{5n\eta^2 K(1)\Psi(1)(1-s_o)^2 \phi_i(d,s_o)}{6\pi\delta m}\right]^{1/3} \qquad \text{(HY-17)}$$

and [WRR,p.746,eq.(70)]:

$$G = \frac{\alpha K(1)}{2} [1 + s_o^{\ c}] - \alpha w \qquad \text{(HY-18)}$$

where:

η^{-1} = mean storm depth, m_H ; (cm)

δ^{-1} = mean storm duration, m_{tr} ; (sec)

and

α^{-1} = mean storm intensity = m_H/m_{tr}; (cm/sec)

For representative soil properties Equation HY-16 illustrates the range of observed surface runoff values. A graphical presentation of the surface runoff function is shown in Figure HY-3.

Net Infiltration

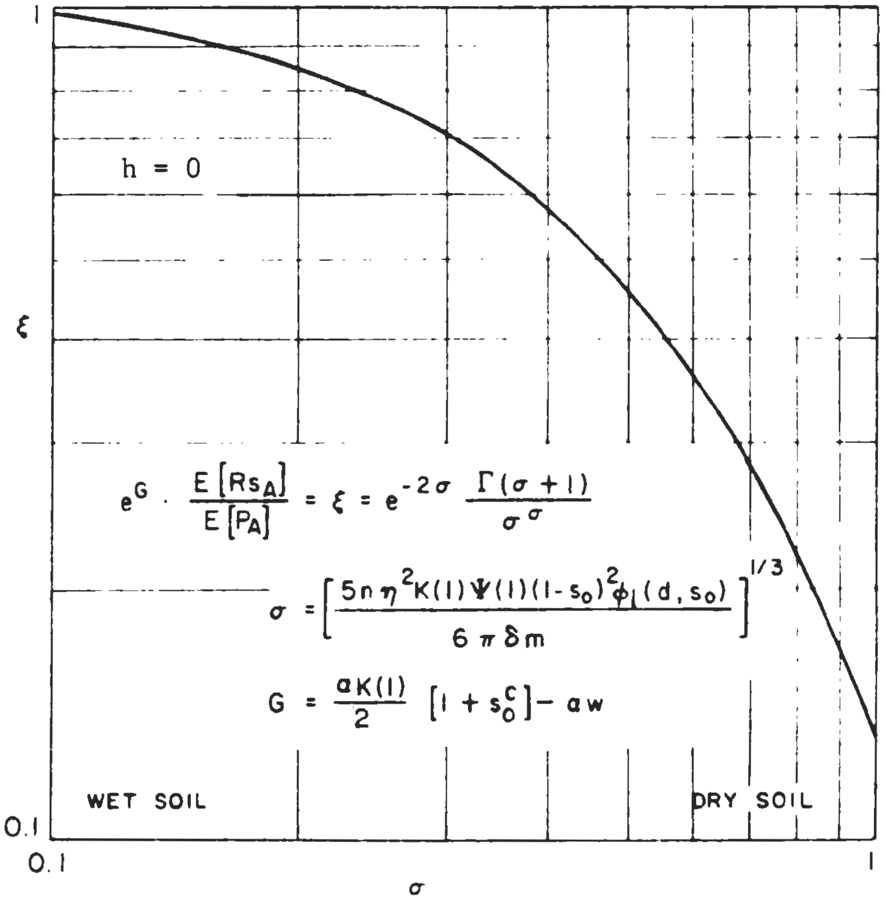
Based upon Equation HY-16 and because [WRR,p.747,eq.(74)]:

$$E[I_A] = m_{PA} - E[R_{sA}] \qquad \text{(HY-19)}$$

the expected seasonal net infiltration as a function of precipitation equals [above equation and WRR,p.746,eq.(68)]:

$$\frac{E[I_A]}{E[P_A]} = 1-e^{-G-2\sigma}\ \Gamma(\sigma + 1)/\sigma^{\sigma} = 1-\xi \qquad \text{(HY-20)}$$

This also represents the fraction of all storms which do not produce surface runoff.



Source: [WRR,p.746, Figure 6]

Figure HY-3

Surface Runoff Function [Eagleson, 1979]

3.3.2.5 Potential Evaportranspiration

The "potential" evapotranspiration of an area can be estimated based on the following assumptions [Eagleson, 1977]:

(1) The energy balance equation may be time averaged by replacing variables by their time averages

(2) The average rates of energy advection and storage are zero

(3) Difference between surface and atmospheric temperatures may be neglected in estimating net outgoing longwave radiation.

The modified Penman energy balance equation can be used to estimate the average rate of potential evapotranspiration.

$$\bar{e}_p = \frac{\bar{q}_i(1 - A) - \bar{q}_b + H}{\rho_e L_e(1 + \gamma/\Delta)} \qquad \text{(HY-21)}$$

in which:

$\bar{q}_i$ = average rate of insolation (ly/min)

$\bar{q}_b$ = average rate of net outgoing longwave radiation (ly/min)

H = average sensible heat flux residual (ly/min)

A = shortwave albedo of surface

ρ_e = mass density of evaporating water (g/cm^3)

L_e = latent heat of vaporization (cal/g)

γ/Δ = atmospheric parameter (a function of temperature)

Empirical values of $\bar{q}_i$, $\bar{q}_b$ and H are presented by Eagleson (1977) in a form suitable for practical use. (Table HY-1). The potential evapotranspiration can be <u>either</u> an input variable to SESOIL <u>or</u> can be estimated using the above equation.

TABLE HY-1

Observed Values of Annual Potential Evapotranspiration

		Observed							Calculated
Location	Ref.	E_p in/yr	ϕ[1] °N	A[2]	$\bar{T}_a$[3] °C	N[4]	$\bar{S}$[5]	u_2[5] m/sec	$\bar{r}_a \times 10$ min/cm
Mesilla, N.M.	50	34.0	32.27	0.26	14.6	0.18	0.53	4.2	5.5
Pecos, N.M.	50	35.3	35.57	0.26	13.8	0.18	0.45	4.1	4.4
Sangamon R., Ill.	50	29.2	40.02	0.26	11.5	0.34	0.70	3.8	4.2
Green R., Ky.	50	31.4	37.90	0.26	13.1	0.46	0.73	3.0	6.4
Tallapoosa R, Ga.	50	33.0	32.50	0.26	15.4	0.36	0.77	2.3	8.7
Mad R., Ohio	50	25.8	40.00	0.26	10.8	0.40	0.72	3.0	8.6
Skunk R., Iowa	50	27.0	40.70	0.26	9.4	0.34	0.70	4.0	4.3
W.Fork,White R.,Mo.	50	31.0	37.00	0.26	13.4	0.33	0.72	4.0	4.6
N. Platte R., Neb.	50	23.8	42.00	0.26	9.0	0.30	0.60	4.2	7.0
Black R., Wis.	50	22.2	43.93	0.26	8.0	0.40	0.74	3.5	7.9
Cyprus Crk., Tex.	50	36.2	32.00	0.26	17.9	0.20	0.75	5.0	3.5
Wagon Wheel Gap,Col.	50	15.6	37.77	0.40	5.3	0.25	0.60	3.8	7.2
Merrimac R., Ma.	50	21.5	43.20	0.30	7.6	0.47	0.78	2.5	7.0
West R., Vt.	50	21.5	42.98	0.30	7.6	0.47	0.78	2.5	7.0
*Lake Cochituate,Ma.	50	23.2	42.50	0.30	10.7	0.33	0.70	4.9	3.7
Swift R., Ma.	50	23.1	42.50	0.26	8.4	0.33	0.70	3.9	5.9
*Phoenix, Ariz.	45	71.6	33.43	0.05	21.3	0.20	0.43	2.7	4.8
*Davis, Cal.	45	50.0	38.37	0.05	15.7	0.30	0.52	3.9	5.2
*Fresno, Cal.	45	60.0	36.77	0.05	16.8	0.25	0.43	2.8	3.4
*Grand Junction,Col	45	35.6	39.12	0.05	11.5	0.30	0.34	3.4	5.0
*Boise, Idaho	45	33.4	43.57	0.05	10.5	0.35	0.37	3.8	3.7
*Dodge City, Kans.	45	62.6	37.77	0.05	12.7	0.27	0.50	6.0	1.8
*Glascow, Mon.	45	38.0	48.22	0.05	5.3	0.25	0.54	4.8	3.0
*Great Falls, Mon	45	35.0	47.48	0.05	7.2	0.25	0.50	5.9	3.9
*Ely, Nev.	45	46.0	39.28	0.05	6.7	0.28	0.36	4.7	5.4
*Bismarck, N.Dak.	45	34.1	48.77	0.05	5.2	0.30	0.63	4.4	3.2
*Stillwater, Ok.	45	57.0	36.13	0.05	15.6	0.35	0.50	5.5	1.8
*Astoria, Ore.	45	20.0	46.15	0.05	10.3	0.50	0.80	4.0	-
*Medford, Ore.	45	32.0	42.37	0.05	11.7	0.50	0.66	2.2	-
*Rapid City, S.D.	45	40.6	44.03	0.05	8.1	0.35	0.56	4.6	3.7
*Brownsville, Tex.	45	58.0	25.90	0.05	23.2	0.40	0.77	5.2	3.9
*Fort Worth, Tex.	45	57.2	32.82	0.05	18.6	0.40	0.63	4.8	4.6
*Midland, Tex.	45	71.3	31.93	0.05	17.7	0.25	0.50	4.5	2.0
*Spokane, Wash.	45	38.4	47.62	0.05	8.5	0.40	0.42	3.9	4.5
*Lander, Wyo.	45	35.0	42.80	0.05	6.9	0.25	0.42	3.2	14.3

* Water surface

[1] Estimated from [illegible]

[2] A = 0.26 chosen for vegetal surfaces (slightly greater for seasonal snow or ice)
A = 0.05 chosen for water surfaces

[3] Average annual value taken from National Weather Service Climatological Summary at nearest station

[4] From Climatological Summary at nearest station

[5] Average from Climatological Summary at nearest station

Source: P. Eagleson (1977)

3.3.2.6 Annual Evapotranspiration

The previous background and the following assumptions lead to the estimation of the "expected annual" evapotranspiration $E[E_{TA}]$:

(1) No evaporation except from water which has first infiltrated

(2) No effect of vegetation in bringing soil moisture to surface

(3) Soil moisture is uniform at s_o at the beginning of each interstorm period

(4) Variance of average annual rate of potential evapotranspiration is negligible

(5) $\bar{e}_p >> w$.

The annual average evapotranspiration $E[E_{TA}]$ is given by [WRR,p.736, eq.(45)]:

$$\frac{E[E_{TA}]}{m_{PA}} = J(E) = 1 - [1 + 2^{1/2}E]e^{-E} + (2E)^{1/2}\,\Gamma[\tfrac{3}{2},E] \qquad \text{(HY-22)}$$

in which [WRR,p.762,eq.(70),(71)]:

$$E = \frac{2\beta nK(1)\Psi(1)\phi_e(d)}{\pi m(\bar{e}_p - w)^2}\; s_o^{d+2} \qquad \text{(HY-23)}$$

where:

β^{-1} = mean time between storms, m_{tb}, (sec)

E = exfiltration parameter

3.3.2.7 Groundwater Runoff

The annual groundwater runoff is defined as the "net" groundwater recharge from the unsaturated soil zone, namely the percolation flow reduced by the capillary rise flow.

The following assumptions are associated with the potential seasonal groundwater runoff estimate:

(1) Percolation to water table is steady throughout the wet season at value determined by the average soil moisture, s_o, and is zero during the dry season

(2) Capillary rise from the water table is steady throughout the entire year at the rate given by a dry surface

(3) Water table elevation, $z = Z$, is constant.

The annual non-dimensional average groundwater runoff, $E[R_{gA}]$ is given by [WRR,p.751,eq.(20)]:

$$\frac{E[R_{gA}]}{m_{PA}} = \frac{m_\tau K(1)}{m_{PA}} s_o^c - \frac{Tw}{m_{PA}} \qquad \text{(HY-24)}$$

Assuming that no groundwater storage occurs within a season, the total groundwater runoff will recharge adjacent surface waters.

3.3.2.8 Annual Hydrologic Water Balance

The annual water budget (HY-4) is given by:

$$E[I_A(s_o)] = E[E_{TA}(s_o)] + E[R_{gA}(s_o)] \qquad \text{(HY-25)}$$

Equations HY-20, HY-22 and HY-24 contribute to the first-order dimensionless water budget equation [WRR,p.766,eq.(6)]:

$$\overbrace{[\underbrace{1}_{\text{Precip.}}\ \underbrace{-\ e^{-G-2\sigma}\,\Gamma(\sigma+1)\sigma^{-\sigma}]}_{\text{Surface Runoff}}}^{\text{Infiltration}} = \underbrace{\frac{E_{PA}}{P_A}\ J(E)}_{\text{Evapotranspiration}} + \underbrace{\overset{\text{Groundwater:}}{\overbrace{\frac{m_\tau K(1)}{P_A}\ s_o^{\,c}}^{\text{Recharge}} - \overbrace{\frac{Tw}{P_A}}^{\text{Loss}}}}_{\text{Groundwater Runoff}} \qquad \text{(HY-26)}$$

A graphic presentation of function J(E), equation HY-22, is shown in Figure HY-4 [WRR,p.737, Figure 5].

The above equation is used to define the dependent variable, s_o, which can be used, in turn, to define the separate terms of the water budget in terms of the independent climate and soil variables and paraparameters.

The annual water yield, Y_A, is determined in this way as

$$Y_A(P_A) = R_{sA}(s_o(P_A)) + R_{gA}(s_o(P_A)) = g(P_A) \qquad \text{(HY-27)}$$

and is used to transform the CDF of annual precipitation $[Y_A(P_A)]$ into the CDF of annual yield according to

$$\text{Prob}\left[\frac{Y_A}{m_{PA}} < z\right] = e^{-\omega m_\tau}\left\{1+\sum_{\nu=1}^{\infty}\frac{(\omega m_\tau)^\nu}{\nu!}\,P[\nu\kappa,\omega m_\tau g^{-1}(z)]\right\} \qquad \text{(HY-28)}$$

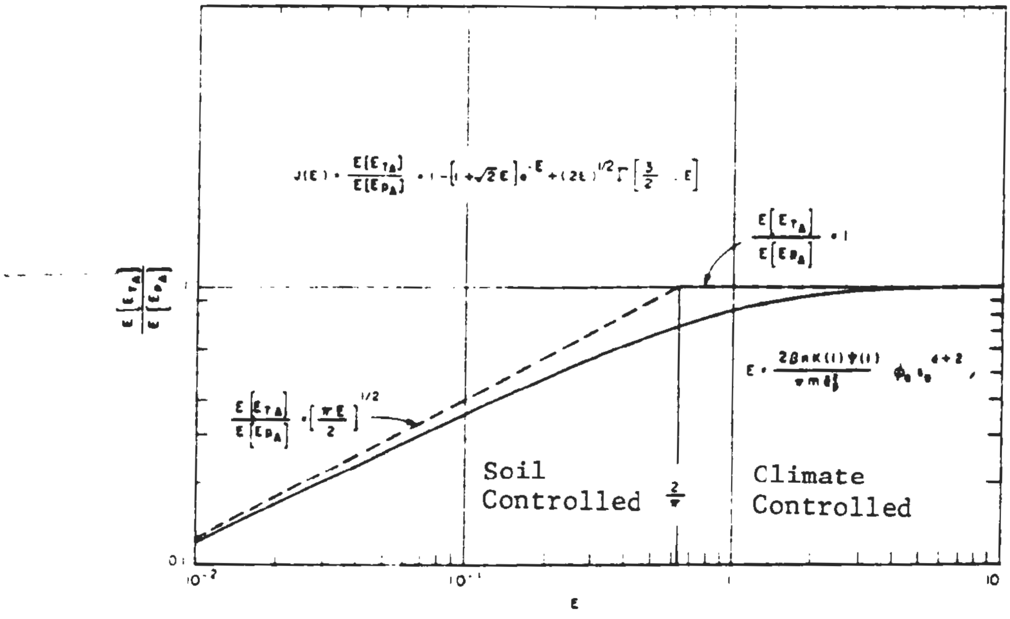


Figure HY-4

Base Soil Evaporation Function ($w/\bar{e}_p << 1$)

Source: Eagleson (1978); WRR, p.737, Figure 5

3.3.2.9 Depth Dependent Infiltration

In the previous sections the infiltration (I) is defined as the total depth of rainfall infiltrating the ground surface (see Figure HY-4.1). Consequently the groundwater runoff (R_g) is defined as the excess of water in the soil column percolating the ground, namely reaching the saturated soil zone.

SESOIL is designed to estimate pollution distribution in the upper, middle and lower unsaturated soil zone of the compartment. It is, therefore, required to have a seasonal averaged estimate of the infiltration at a depth z of the soil column as shown in Figure HY-4.1. This estimate (I_z) is required for both the annual and the monthly simulations of the pollutant transport.

Based upon the geometry of the soil compartment we may make the assumption that the annual (A) -- section 3.3 of this appendix -- and monthly (M) -- section 3.4 of this appendix -- variations are given by:

$$I_z(A,M) = R_g(A,M) + d_l \cdot \tan\alpha =$$

$$= R_g(A,M) + \frac{d_l}{d_u + d_l}\,[I(A,M) - R_g(A,M)] \qquad \text{(HY-28.1)}$$

where d_u and d_l the depths of the upper and the lower unsaturated soil zones respectively. The I_z values estimated by the above equation are employed by the pollutant transport routines, Appendix PT, equations PT-6, PT-13, PT-28 and PT-31.

The layered averaged intrinsic permeability of the compartment is approximated to

$$k_z = (d_u + d_M + d_L)/(d_u/k_u + d_M/k_M + d_L/k_L) \qquad \text{(HY-28.2)}$$

and each infiltrating quantity (depth) is given by

$$I(A,M) = I_z(A,M) \qquad \text{(HY-28.2)}$$

where

$$\overline{k_1} = k_1,\ \overline{k_2} = (d_u + d_M)/(d_u/k_u + d_M/k_M),\ \overline{k_3} = k_z \qquad \text{(HY-28.2)}$$

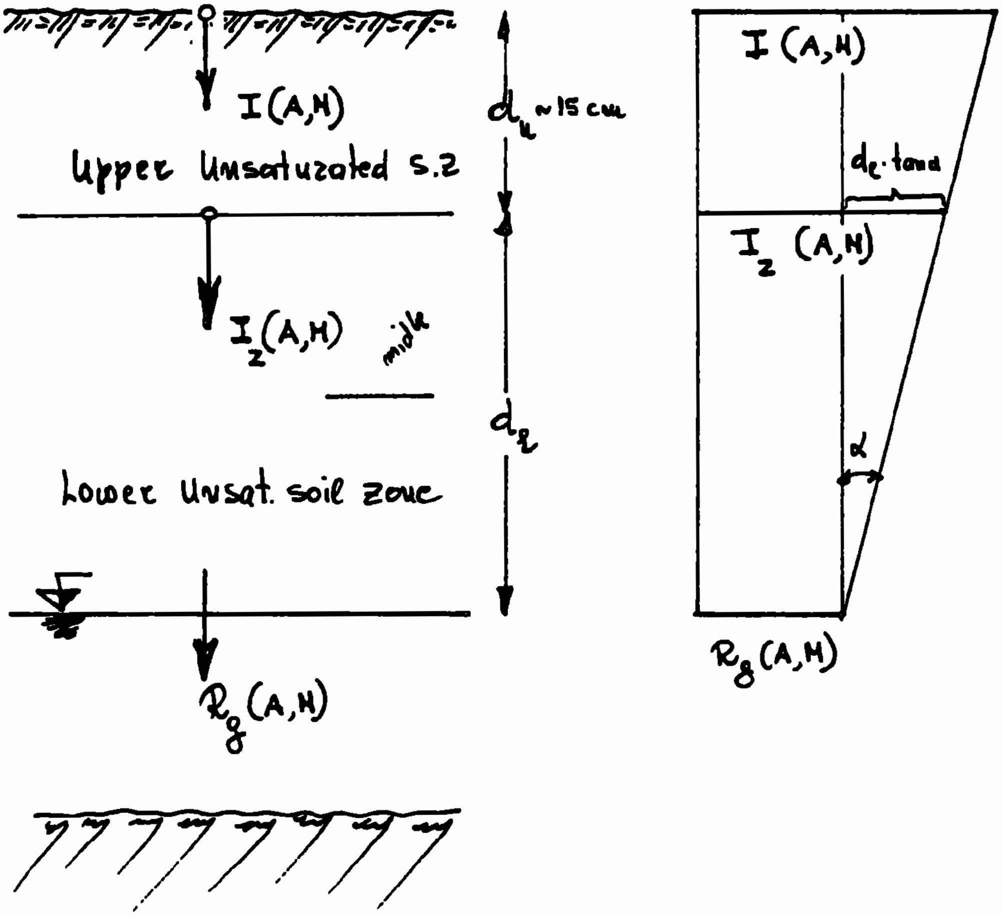


Figure HY-4.1

Depth Dependent Infiltration in the Soil Column

3.4 Model Variables/Parameters

The full set of twenty (20) parameters and variables governing the previous equations are:

m_{PA} = mean annual precipitation; (cm)

$E[E_{PA}]$ = mean annual potential evapotranspiration; (cm)

$\bar{e}_p$ = mean annual rate of potential evapotranspiration; (cm)

m_{tr} = δ^{-1} = mean storm duration; (days)

m_{tb} = β^{-1} = mean time between storms; (days)

m_H = η^{-1} = mean storm depth; (cm)

m_i = α^{-1} = mean storm average intensity; (cm/sec)

m_τ = mean length of rainy season; (days)

T = duration of capillary rise from watertable ; (days)

k(1) = spatial average effective soil permeability at saturation; (cm^2)

$\bar{T}_a$ = normal annual temperature of surface soil moisturn; (°C)

c = soil conductivity index; (-)

m = soil matrix potential index ; (-)

d = soil diffusivity index; (-)

n = effective soil porosity; (cm^3/cm^3)

$\Psi(1)$ = spatial average soil matrix potential at saturation; (cm)

Z = depth to watertable; (cm)

ϕ_e = exfiltration diffusivity function: (-)

ϕ_i = infiltration diffusivity function; (-)

s_o = spatial and temporal average soil moisture within the soil boundary layer; (-)

Introducing a twenty-first parameter,

m_ν = mean number of storms per season, (#)

we have ten supplementary relations in addition to the water budget equation (HY-26):

$m_H = m_{PA}/m_\nu$ (definition)

$m_\tau = m_\nu(m_{tb} + m_{tr})$, $m_\nu \geq 1$ (definition)

$m_i = m_H/m_{tr}$ (assuming independence of i and tr)

$E[E_{PA}] = m_\nu m_{tb}\bar{e}_p$ (definition)

$d = (c + 1)/2$ (semi-empirical) (HY-29)

$m = 2/(c-3)$ (semi-empirical)

T = one year (definition)

$\Psi(1) = \Psi(n, k(1), \bar{T}_a)$; [WRR,p.724,eq.(17)]

$\phi_i = \phi_i(d, s_o)$ (Figure HY-5)

$\phi_e = \phi_e(d)$ (Figure HY-6)

To solve the water budget relation for the dependent variable, s_o, we must therefore specify the values of ten parameters (i.e., 21 variables minus 11 equations). Thus:

(1) INPUT parameters to the model are:

Soil system:

$$k(1),\ c,\ n,\ \bar{T}_a,\ \text{and}\ Z \qquad \text{(HY-30)}$$

Climate System: Five independent parameters may be chosen from the set of six:

$$m_{PA},\ \bar{e}_p,\ m_H,\ m_{tr},\ m_\nu,\ m_\tau \qquad \text{(HY-31)}$$

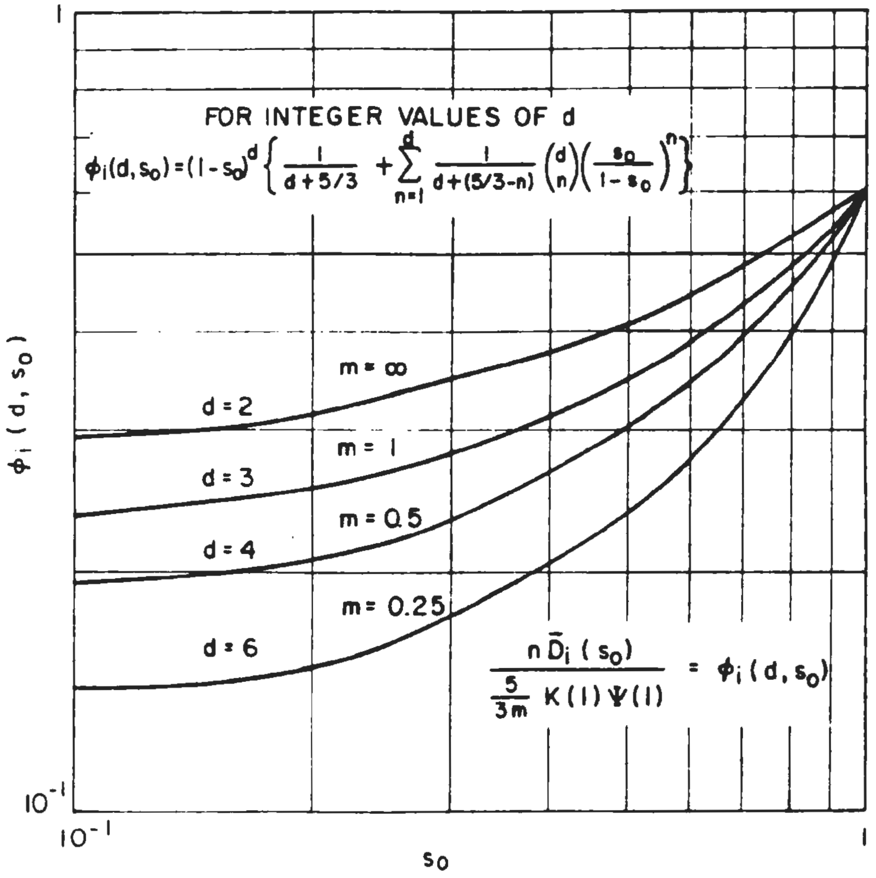


Figure HY-5

Dimensionless Infiltration Diffusivity

Source: [Eagleson, WRR, p.727, Figure 9]

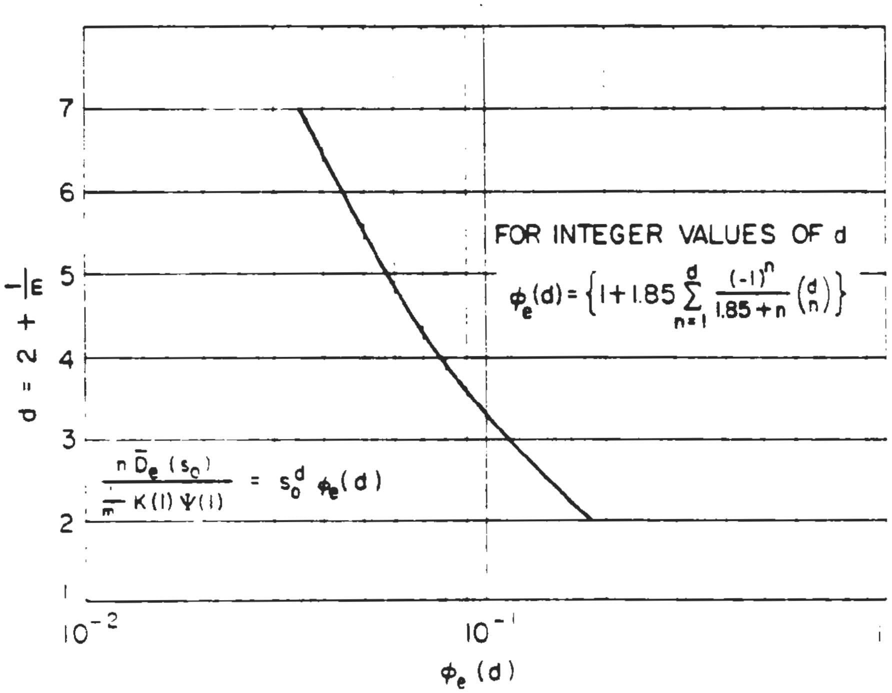


Figure HY-6

Dimensionless Exfiltration Diffusivity

Source: [Eagleson, WRR, p.727, Figure 10]

(2) OUTPUT parameters from the model are:

s_o, P_A, E_{TA}, S_A, R_{SA}, R_{gA},

An example of input and other climatic data for sub-humid (Clinton, Massachusetts) and an arid (Santa Paula, California) climate-soil system is shown in Table HY-2.

Representative independent soil properties nominal values covering a range of observations (Eagleson 1977) are given in Table HY-3. It is important to notice that there is no unique association of the particular c and n values with the tabulated value of k(1) for each soil. Derived (Eagleson 1979) climate-soil parameters for indicated climatic and soil input are given, as an example, in Table HY-4. The latter values are derived using Table HY-3 values.

Note: Model users should validate their model output based upon "water balance" data from a given site, and they should never rely upon the derived parameters of Tables HY-3 and HY-4. These tables should not give the impression, for example, that they contain all one needs to know about soil. That is, if the soil is clay it has the properties of the first column of Table HY-3. This is not the case of course, since soil stratification properties are of paramount importance and may drastically alter the k(1), n and c values of a site. The soil properties are critical to the moisture fluxes and are tremendously variable spatially. Use of point measured soil properties can yield results of only local (and hence not really averaged) character.

TABLE HY-2

Independent Soil and Climate Parameters for a Sub-Humid and an Arid Climate Soil System

		Location	
Parameter	Units	Clinton, Mass.	Santa Paula, Ca.
n	-	0.35	0.35
$k(1)$	cm^2	2.8×10^{-10}	1.2×10^{-9}
c	-	10	$5^{1)}$
m_{P_A}	cm	94.1	54.4
$\bar{e}_p$	cm/day	0.15	0.27
m_{t_r}	days	0.32	1.4
m_τ	days	365	212
m_ν	-	109	15.7
m_H	cm	1.0	3.0
Z	m	∞	∞
$\bar{T}_a$	^oC	8.4	13.8
m_{t_b}	days	3.0	10.4
κ	-	0.50	0.25
h_o	cm	0.1	0.1
k_v	-	1	1
ω	day^{-1}	0.30	0.084

Source: Eagleson [WRR,p.717, Table 1]

1)See comment on Table HY-3.

TABLE HY-3

INDEPENDENT SOIL PROPERTIES[1] FOR VARIOUS SOIL TYPES

Property (Variable)	Soil Type[2]			
	Clay	Clay-Loam	Silty-Loam	Sandy-Loam
k(1) [cm^2]	$1X10^{-10}$	$2.8X10^{-10}$	$1.2X10^{-9}$	$2.5X10^{-9}$
n	0.45	0.35	0.35	0.25
c	12	10	5[3]	4

Source: Eagleson 1977, p. 256.

[1] See limitation discussion in previous pages.

[2] Derived by using Table HY-4 values and the corresponding environments.

[3] Personal communication with Eagleson. In his publications c(silty-loam) = 6; however, later investigations indicated c = 4.5-5.5. An average value c = 5 is given here.

TABLE HY-4

DERIVED CLIMATE-SOIL PARAMETERS FOR A CLIMATE AND RELATED SOIL TYPES (OF TABLE HY-2)

Climate: $\alpha = 1.5 \times 10^{4}$ sec/m ; $\delta = 10^{-1}$ hr^{-1}

$\beta = 7 \times 10^{-3}$ hr^{-1} ; $m_H = 2.54$ cm

$m_\tau = 365$ days ; $m_\nu = 75$ events

$\overline{T}_a = 15$ °C

Derived Climate-Soil Parameters

Derived Parameter	Clay	Clay-Loam	Silty-Loam	Sandy-Loam
m	0.222	0.286	0.667	2
d	6.5	5.5	3.5	2.5
$\Psi(1)$, cm	25	19	166	200
$K(1)$, cm/sec	8.2×10^{-6}	2.32×10^{-5}	9.94×10^{-5}	2.08×10^{-4}
$\phi_e(d)$	0.0385	0.0494	0.0920	0.1430
$\phi_i(d,0)$	0.122	0.140	0.194	0.240
$\phi_i(d,1)$	0.6	0.6	0.6	0.6
$G(0)$	0.0621	0.174	0.746	1.560
$G(1)$	0.124	0.348	1.490	3.120
$\sigma(0)$	0.432	0.482	1.340	1.220
$\sigma(1)$	0	0	0	0
$\Gamma(\sigma(0)+1)$	0.886	0.886	1.200	1.110
$\Gamma(\sigma(1)+1)$	1	1	1	1
$\sigma(0)^{-\sigma(0)}$	1.44	1.42	0.68	0.79
$S_i(0)$, cm/sec$^{1/2}$	1.04×10^{-2}	1.27×10^{-2}	5.97×10^{-2}	5.15×10^{-2}
$S_i(1)$, cm/sec$^{1/2}$	0	0	0	0
$S_e(0)$, cm/sec$^{1/2}$	0	0	0	0
$S_e(1)$, cm/sec$^{1/2}$	4.54×10^{-3}	5.82×10^{-3}	3.19×10^{-2}	3.08×10^{-2}

Source: Eagleson [1978, 1979]

3.5 Water Balance Sensitivity

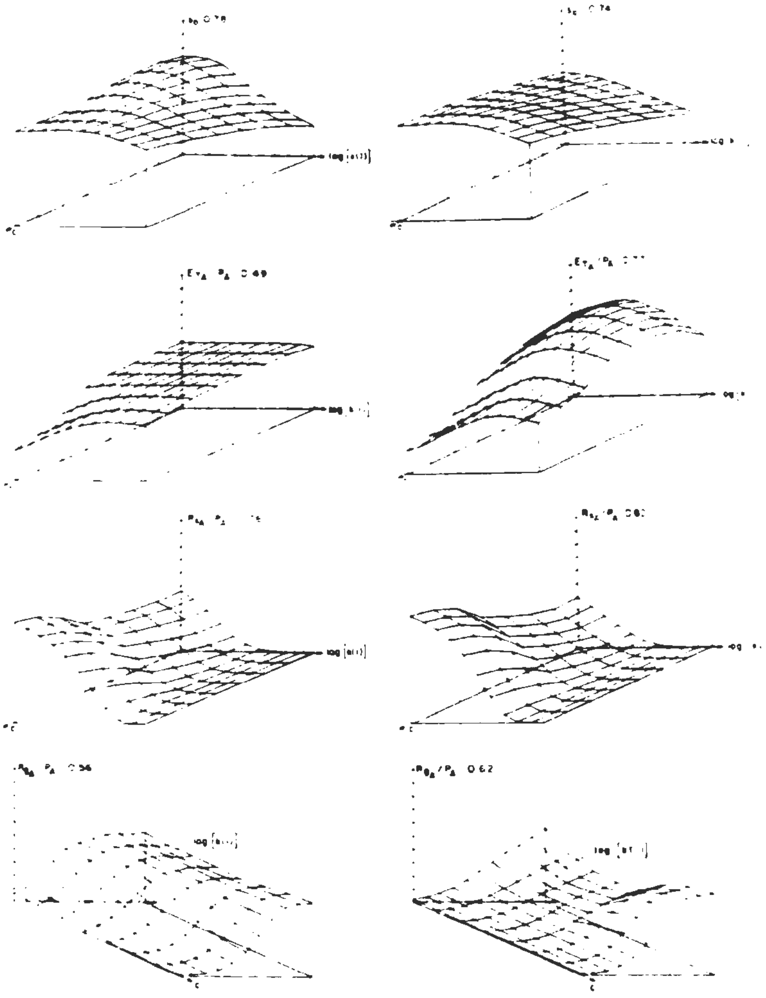
Equation HY-26 and its component equations were used by Eagleson (1979) in studying the sensitivity of the model to variation of the climatic or soil parameters. For the climatic parameters of Table HY-2 the sensitivity of the average annual water budget components is presented as a function of the soil permeability and soil porosity in Figures HY-7 and HY-8 for both locations, Clinton, Massachusetts and Santa Paula, California.

According to Eagleson, by comparing the two columns of Figure HY-7 we see contrasting behavior only in evapotranspiration and soil moisture. Beginning with the former, we see insensitivity of E_{TA} to soil properties in the sub-humid climate except when the soil gets very permeable. For the arid climate, however, E_{TA} is sensitive to the soil properties over their full range.

In the humid case, the supply of water is adequate and the soil moisture will be largest where the permeability readily admits water (and holds it against gravity). This requires a small σ which occurs for small k and large m (i.e., small c).

In the arid case where the evapotranspiration is controlled by the moisture supply to the surface, s_o will be largest where the moisture movement to the surface, as given by E, is smallest. This will occur for small k(1) and large d (i.e., large d).

The runoff behavior is qualitatively the same in both climates. For small k(1), the total yield is predominantly surface runoff because the water cannot enter the soil. This component increases with c due



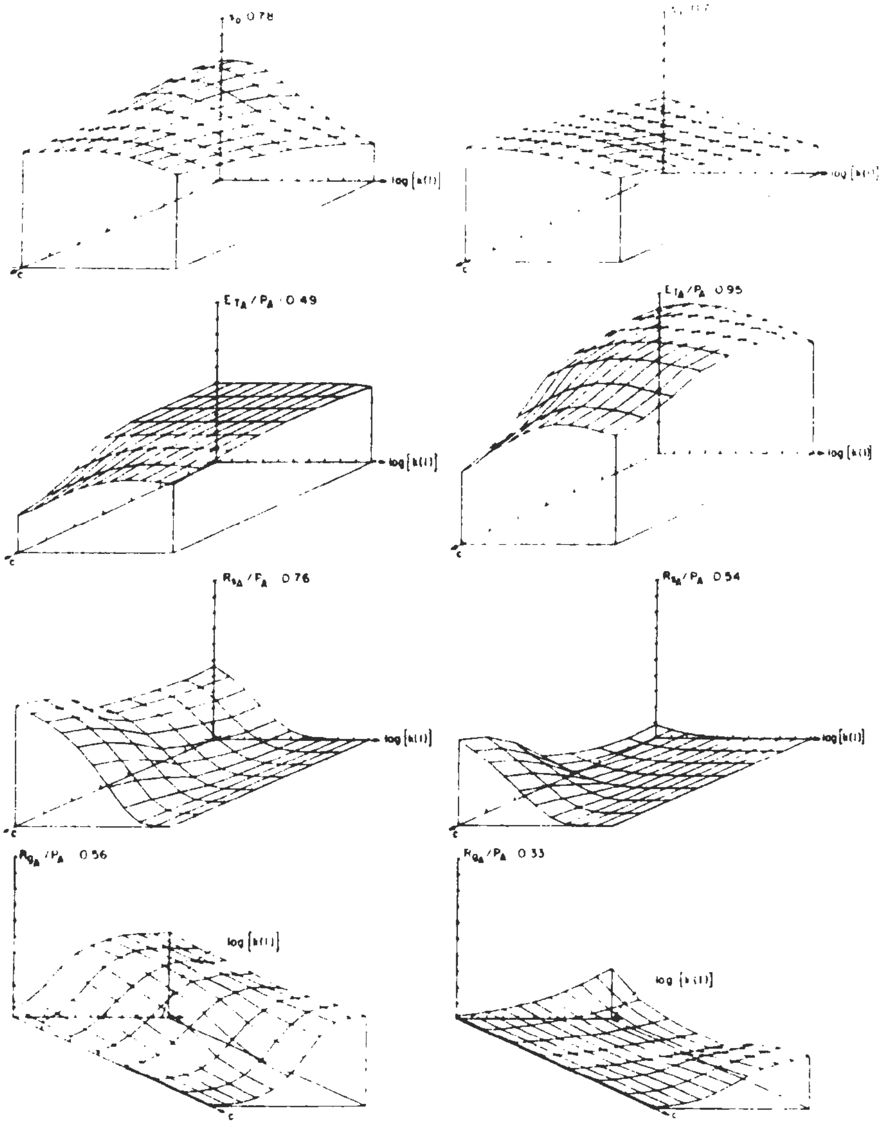
a. SUB-HUMID CLIMATE (CLINTON, MA)

b. ARID CLIMATE (SANTA PAULA, CA)

Figure HY-7

Sensitivity of Annual Water Budget to Changes in Soil Parameters ($M = 0, h_o = 0, w/\overline{e}_p << 1$)

Source: Eagleson (1979)



a CLINTON CLIMATE

b CLINTON CLIMATE WITH SANTA PAULA P_A

Figure HY-8

Effect on Annual Budget Due to
Decreasing Mean Annual Precipitation

Source: Eagleson (1979)

to decreasing permeability and it decreases with increasing k(1) due to increasing permeability. The groundwater component also increases with k(1). The "saddle" in the Santa Paula groundwater component with increasing c results from the behavior of the factor s_o^c where s_o is less than one and is increasing with c.

For additional information regarding the sensitivity analysis the reader is referred to the original publication of P. Eagleson [WRR, p.749].

3.6 Subroutine HYDROA

3.6.1 Equation Summary

The water balance model, as presented previously, has two distinctive working-steps:

(1) Based upon climatic data, the soil moisture, s_o, is determined;

(2) Based upon the soil moisture value, s_o, any desired seasonal water balance component is obtained.

Therefore:

(1) The soil moisture, s_o, is estimated by the first order conservation equation

$$\overbrace{\underbrace{[1}_{\text{Precip.}} - \underbrace{e^{-G-2\sigma}\,\Gamma(\sigma + 1)\sigma^{-\sigma}]}_{\text{Surface Runoff}}}^{\text{Infiltration}} = \underbrace{\frac{E[E_{PA}]}{m_{PA}}\; J(E)}_{\text{Evapotranspiration}} + \underbrace{\overset{\text{Groundwater:}}{\overbrace{\frac{m_\tau K(1)}{m_{PA}}\; s_o^{\,c}}^{\text{Recharge}} - \overbrace{\frac{Tw}{m_{PA}}}^{\text{Loss}}}}_{\text{Groundwater Runoff}} \qquad \text{(HY-32)}$$

in which:

$$G = \frac{\alpha}{2} K(1)[1 + s_o^{\,c}] - \alpha w \qquad \text{(HY-33)}$$

$$\sigma = \left[\frac{5n\eta^2 K(1)\Psi(1)(1 - s_o^{\,2})\phi_i(d, s_o)}{6\pi\delta m}\right]^{1/3} \qquad \text{(HY-34)}$$

$$J(E) \equiv 1-(+ \sqrt{2} \cdot E) \cdot e^{-E} + \sqrt{2E} \cdot \Gamma[3/2,E] \qquad \text{(HY-35)}$$

$$w = K(1) \; [1 + \frac{3}{2}(mc-1)] \; [\Psi(1)/Z]^{mc} \qquad \text{(HY-36)}$$

$$E = \frac{2\beta n K(1)\Psi(1)\phi_e(d)}{\pi m(\bar{e}_p-w)^2} \; s_o^{d+2} \qquad \text{(HY-37)}$$

The values of any desired seasonal water balance component are estimated by substituting a value for s_o in Equations H-32 through H-36, namely for:

Infiltration

$$I_A/P_A = 1 - e^{-G-2\sigma} \; \Gamma(\sigma + 1)\sigma^{-\sigma} \qquad \text{(HY-38)}$$

Surface Runoff

$$R_{sA}/P_A = e^{-G-2\sigma} \; \Gamma(\sigma + 1)\sigma^{-\sigma} \qquad \text{(HY-39)}$$

Evapotranspiration

$$E_{TA}/P_A = \frac{E_{PA}}{P_A} \; J(E) \qquad \text{(HY-40)}$$

Groundwater Runoff

$$R_{gA}/P_A = \frac{m_T K(1)}{P_A} \; s_o^c - \frac{Tw}{P_A} \qquad \text{(HY-41)}$$

Annual Yield

$$Y_A/P_A = \frac{R_{sA} + R_{gA}}{P_A} = 1-E_{PA}/P_A \qquad \text{(HY-42)}$$

Precipitation

$$P_A = \frac{E[E_{PA}]\ J(E) + m_\tau\ K(1)\ s_o^{\,c} - T \cdot w}{1 - e^{-G} \cdot \xi} \qquad \text{(HY-43)}$$

where: $\xi = e^{-2\sigma} . \frac{\Gamma(\sigma+1)}{\sigma}$

Equation HY-43 is another form of the water balance equation HY-32, that is employed in the step-by-step calculation procedure, section 3.6.3.

where:

$E[\ ]$ = expected value of [ ]

$\Gamma(\ )$ = Gamma function of ( ) (see Table HY-5)

$E[E_{PA}]$ = long-term expected (average) annual potential evapotranspiration (cm)

m_{PA} = average annual precipitation (cm)

G = gravitational infiltration parameter (Equation HY-33)

σ = capillary infiltration parameter (Equation HY-34)

$J(\ )$ = evaporation function (Equation HY-35)

E = evaporation parameter (Equation HY-37)

w = apparent velocity of capillary rise from water table (cm/sec)

c = pore disconnectedness index = $\ln[K(s_o)/K(1)]/\ln s_o$

T = time (year)

m_τ = long-term average length of annual rainy season (days)

$K(1)$ = saturated effective hydraulic conductivity (cm/sec)

s_o = long-term average effective soil moisture concentration in the unsaturated soil zone

α = reciprocal of mean storm intensity $\equiv m_i^{-1}$ (sec/cm)

Table HY-5

Values of the Gamma Function

x	$\Gamma(x)$	x	$\Gamma(x)$	x	$\Gamma(x)$
1.00	1.000	1.34	0.892	1.68	0.905
1.01	0.994	1.35	0.891	1.69	0.907
1.02	0.989	1.36	0.890	1.70	0.909
1.03	0.984	1.37	0.889	1.71	0.911
1.04	0.978	1.38	0.889	1.72	0.913
1.05	0.974	1.39	0.888	1.73	0.915
1.06	0.969	1.40	0.887	1.74	0.917
1.07	0.964	1.41	0.887	1.75	0.919
1.08	0.960	1.42	0.886	1.76	0.921
1.09	0.955	1.43	0.886	1.77	0.924
1.10	0.951	1.44	0.886	1.78	0.926
1.11	0.947	1.45	0.886	1.79	0.929
1.12	0.944	1.46	0.886	1.80	0.931
1.13	0.940	1.47	0.886	1.81	0.934
1.14	0.936	1.48	0.886	1.82	0.937
1.15	0.933	1.49	0.886	1.83	0.940
1.16	0.930	1.50	0.886	1.84	0.943
1.17	0.927	1.51	0.887	1.85	0.946
1.18	0.924	1.52	0.887	1.86	0.949
1.19	0.921	1.53	0.888	1.87	0.952
1.20	0.918	1.54	0.888	1.88	0.955
1.21	0.916	1.55	0.889	1.89	0.958
1.22	0.913	1.56	0.890	1.90	0.962
1.23	0.911	1.57	0.890	1.91	0.965
1.24	0.909	1.58	0.891	1.92	0.969
1.25	0.906	1.59	0.892	1.93	0.972
1.26	0.904	1.60	0.894	1.94	0.976
1.27	0.903	1.61	0.895	1.95	0.980
1.28	0.901	1.62	0.896	1.96	0.984
1.29	0.899	1.63	0.897	1.97	0.988
1.30	0.897	1.64	0.899	1.98	0.992
1.31	0.896	1.65	0.900	1.99	0.996
1.32	0.895	1.66	0.902	2.00	1.000
1.33	0.893	1.67	0.903		

Source: Eagleson, 1977

n = effective soil porosity = volume of active voids/total volume

η = reciprocal of mean storm depth $\equiv m_H^{-1}$ (cm^{-1})

$\Psi(1)$ = saturated soil moisture potential (cm) [equation HY-10]

$$= \frac{\sigma_w}{\gamma_w} \left[\frac{n}{k(1)}\right]^{1/2} \left(10^{-0.66-0.55/m-0.14/m^2}\right)^{1/2}$$

σ_w = surface tension of pore water (dynes/cm)

γ_w = specific weight of pore water ($dynes/cm^3$)

$k(1)$ = spatial average saturated effective intrinsic permeability of soil (cm) $\equiv K(1)\mu_w/\gamma_w$ (see Table HY-3)

μ_w = dynamic viscosity of pore fluid (poises)

$\phi_i(d,\tilde{s}_o)$ = dimensionless infiltration diffusivity (see Figure HY-5)

δ = reciprocal of mean storm duration ($days^{-1}$) $\equiv m_{tr}^{-1}$

m = $2/(c-3)$ pore size distribution index (Brook, R.H., et al; 1964)

β = reciprocal of mean interstorm period $\equiv m_{tr}^{-1}$

$\phi_e(d)$ = dimensionless exfiltration diffusivity (see Figure HY- 6)

$\overline{e}_p$ = potential rate of evaporation from a bare soil surface (cm/sec)

$d \quad = \quad (c + 1)/2$ = diffusivity index

$\xi(\sigma) \quad = \quad e^{-2\sigma} \cdot \Gamma(\sigma + 1)\sigma^{-\sigma}$; surface runoff function (see Figure HY-3)

With Equations HY-32 through HY-42 the average seasonal water balance can be displayed graphically in a variety of ways, one of which is illustrated in Figure HY-10 for an annual water cycle.

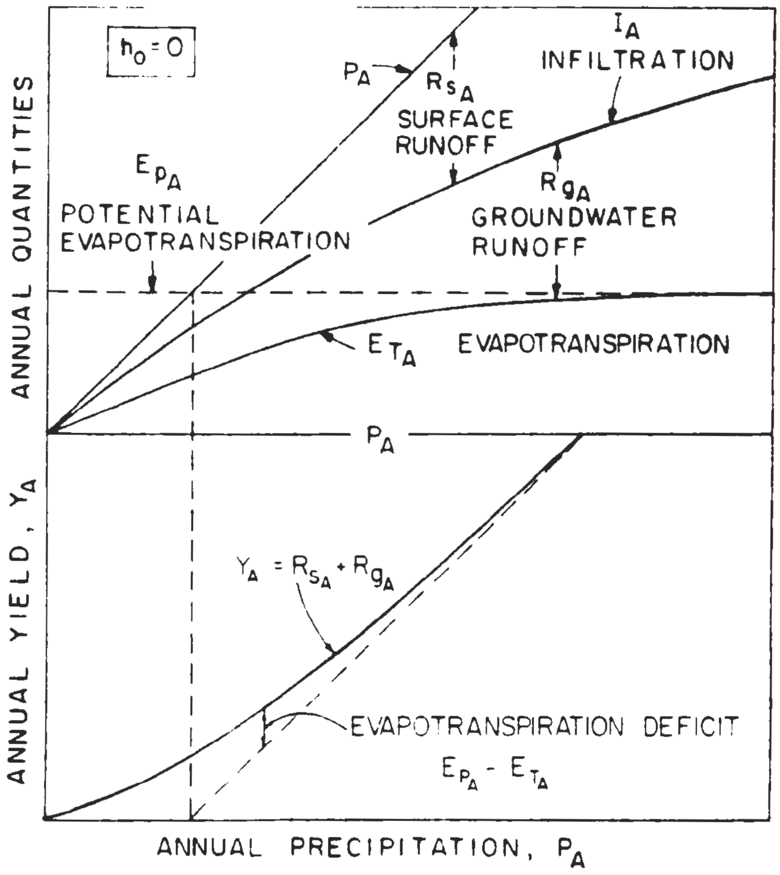


Figure HY-9

Climatic Influence of Annual Water Balance

Source: Eagleson (1979)

3.6.2 Input/Output Variables

INPUT data to HYDROA are categorized into the three groups of:

(1) Climatic data:

either: $\bar{e}_p$ (cm/day)

or: the data set

L	(°N)
$\bar{T}_a$	(°C)
$\bar{S}$	(fractional)
A	(-)
NN	(fractional)

(2) Storm data:

$T = 365$	(days)
m_{PA}	(cm)
m_{tr}	(day)
m_{ν}	(#)
m_{τ}	(days)

(3) Soil data:

$k(1)$	(cm^2)
c	(-)
n	(-)

Above variables are stored in arrays CLIMA1, CLIMA2 and SOIL1 of the SESOIL Data Base; see Appendix DF, Data Files.

OUTPUT data from HYDROA is the data set.

s_o	(-)
$P_A \equiv m_{PA}$	(cm)
I_A	(cm)
E_{TA}	(cm)
R_{sA}	(cm)
R_{gA}	(cm)
Y_A	(cm)

3.6.3 General Calculation Procedure.

The calculation of the annual water balance has the following major steps.

(1) Estimation of initial parameters

- 1.1 Estimation of climate parameters
- 1.2 Estimation of soil parameters
- 1.3 Estimation of potential evapotranspiration
- 1.4 Estimation (or input) of annual evapotranspiration

(2) Solution of the annual water balance equation HY-32

- 2.1 Solution of the water balance equation HY-32 (i.e. estimation of s_o) is best accomplished by employing an iterative procedure for s_o increments, that is by assuming an s_o and consequently estimating P_A via eq. HY-43.
- 2.2 Estimation of water balance components for the assumed s_o value.
- 2.3 Comparison of estimated P_A versus assumed m_{PA} to obtain the solution.

4.0 LEVEL2 - MONTHLY "ESTIMATED" HYDROLOGIC CYCLES

4.1 General

Subroutine HYDROM estimates the monthly (M) hydrologic cycle components of the soil compartment. HYDROM is based upon the theory of HYDROA discussed in the previous section.

4.2 Definitions

See Section 3.2.

4.3 Monthly Mathematical Analysis

4.3.1 Principal Assumptions

The principal assumptions made are:

(1) The assumptions made for the annual warer balance (see Section HY-3.3.1); and

(2) The response of the environment (eg. moisture content) at the end of a month with "constant" and "continuous" rain MPA is "similar" to the response of this environment at the end of a year with constant and continuous rain of the 12 (MPA). Mathematical Linearity of Processes (Dooge 1973) is assumed.

4.3.2 Theoretical Overall Approach

To reduce the averaging time of a simulation from a year to a month or shorter, traditionally modelers develop a numerical, finite-difference solution to the basic equations, thus "scaling down" the temporal resolution of equations.

To by-pass the numerical discretization difficulties of the literature, in SESOIL the temporal resolution of the equations is "scaled up." That is, the monthly subroutine HYDROM employs subroutine HYDROA which is now run 12 times in a year for 12 "typical" years. Each typical year has, for example, an annual precipitation that equals 12 times the precipitation of the month to be simulated. At the end of the "typical" year simulation, the annual output variables $P_{A,}$ I_A, E_{TA}, R_{SA}, R_{gA} are divided by 12 in order to estimate the monthly values of the month under consideration, while the annual output value s_o (moisture content) is kept at the typical annual year output value. However, because of the new time resolution issue, the change in soil moisture storage from month-to-month becomes important. To account for this moisture budget transfer (from time t-1 to time t) in the entire column, a moisture storage term $\Delta s_o = Z \cdot n(s_o(t)-s_o(t-1))$ has been added to the denominator of equation (HY-43) to balance (via precipitation) the deficit or surplus of moisture in the course of the months. The mathematical derivation of this logic can be traced from equation (HY-3) in conjunction with equation (HY-0) and will be documented in the future in this section.

In addition to the soil moisture storage issue, the authors had to retrieve solutions of equation HY-43 when $m_{PA}=0$ (no rain) because in the original Eagleson theory, when $m_{PA}=0$, $m_\gamma=0$ and in that case many parameters (eg. α, δ, σ, G) tend to ∞. The designed scheme will be presented in the revised documentation, but principally when $m_{pa}=o$, the $\sigma(t-1)$, $G(t-1)$ function of a previous time step (t-1) have been used for time step (t).

Finally the authors have accounted for a "smooth" soil anisotropy along the soil column by employing the theoretical background given in Freeze & Cherry (1979, p. 32). Documentation will also be presented in the near future.

Averaged annual estimates of the soil moisture content (s_o) calculated with both the subroutines HYDROA and HYDROM, gave an excellent correlation, thus leaving the authors to believe that the accuracy obtained from HYDROM is satisfactory.

Dec. 81

4.4 Input/Output Variables

INPUT data to HYDROM are the:

(1) Input data to HYDROA, and

(2) The 12 monthly storm depths $m_p(M)$; (cm)

Above variables are stored in arrays CLIMA1, CLIMA2 and SOILI of the SESOIL Data Base; see Appendix DF (Data Files).

OUTPUT data from HYDROM are 12 data sets (one for each month)

$s_o(M)$, $P(M)$, $I(M)$, $R_s(M)$, $R_g(M)$, $Y(M)$

$M = 1$ through 12; October through September

This data is stored in array HYDBAL.

5.0 MODEL EXTENSION

5.1 General

The hydrologic cycle routines (HYDROA, HYDROM) are based upon on analytic solution (versus numerical) approach and can be operated for monthly and annual simulations. The routines employ Eagleson's annual water balance model, the state of the art in analytic hydrologic research, which provides excellent theoretical insight to the coupling of the water balance components. This model is very easy to operate with a minimum of inputs. In addition the hydrologic cycle routines provide the feature of not requiring calibration procedure of non-physically based parameters (i.e. coefficients). Their hydrologic routines are suitable, for the time being, for:

- Seasonal (i.e. annual or monthly) simulations;
- Omission of snow or ice phenomena;
- Omission of energy and surface moisture storage in soil processes;
- Omission of vegetal influence on soil moisture movement;
- Linear superposition of moisture phenomena.

To remove the above constraints and reduce the seasonal period to less than a month (eg. storm-by-storm event), theoretically, it is necessary to formulate a finite difference solution to the basic equations. However, authors have a different approach to this issue, encompassing the use of the developed monthly routine (HYDROM) and the use of a finite difference moisture movement model. The latter will be "self-calibrational" based upon input information received from HYDROM.

For either vegetated or bare soils (but particularly the former), the effect of surface retained water and of moisture fluctuations to the fluctuations of the groundwater table is of importance and should be included in this model development. In certain climates, such as the

Pacific Northwest where the rain is intermittent drizzle with broken spells of sunshine, this fluctuation can be quite a significant item in the annual/monthly water balance estimates (Personal communication with Eagleson).

The phenomena of snow pack/melt and interception might be handled by assuming (in the future, however), in a semi-theoretical way, an increase (snow melt) or decrease (snow pack, interception) in precipitation. These water quantities can be separately estimated (see subsequent sections) and added or subtracted from the unit-term of equation HY-32. The snow pack/melt phenomenon might be also treated mathematically as increased "soil permeability," but additional thinking is required for this approach. A short discussion regarding above processes is given in the following sections.

5.2 Snow Pack/Melt

Two well known methods for modeling snow pack/melt phenomena are: (1) the Heat Balance Method; and (2) the Temperature Index, or Degree-Day Method. The first was developed by the U.S. Army Corps of Engineers and has been successfully applied in numerous cases. The Heat Balance Method requires extensive calculations, taking account of phenomena such as radiation, melt, condensation-convection melt, rain melt, snow density and compaction parameters, areal coverage, snow evaporation, snow pack heat and snow pack liquid water storage. The Temperature Index Method is extremely simple, but it has been reported to provide estimates which are of the same accuracy as those of the detailed Heat Balance Method (Novotny, 1976). SESOIL might employ, for example, the Temperature Index Method, adopted, however, to SESOIL'S theoretical needs:

$$S_m = \mathrm{abs}(k_s * \overline{T}_a) \qquad \text{(HY-44)}$$

in which:

S_m = snowmelt intensity(cm/day)

$\overline{T}_a$ = mean daily air temperature (°C); input variable
$T \leq 0°C$ (snow pack), $T > 0°C$ (snow melt)

k_s = snowmelt coefficient (cm/°C.day); input variable

abs = absolute value (i.e., $S_m \geq 0$)

When the average daily temperature is below freezing temperature (i.e., $T \leq 0°C$), precipitation becomes snowfall and accumulates as snow pack providing a minimum runoff. Conversely, when the average daily temperature is above freezing (i.e., $T > 0$), the snowmelt quantity is added to rainfall runoff (if any) for that period.

A simplified calculation procedure might be as follows:

Subtract (when $T \leq 0$) or add (when $T > 0$) the quantity $S^*_m = S_m \cdot P_A/\Delta t$

from the unit term on the left-hand side of Equation HY-32 (where Δt the simulation time step); and use the hydrologic cycle subroutines as previously described.

5.3 Interception

Interception is a function of the type and extent of vegetation, land use and meteorologic characteristics (wind, temperature, solar radiation, precipitation, etc.). In nature, all precipitation is assumed to enter interception storage until it is filled to capacity. Water is removed from the interception storage by transpiration, which may occur even during rain. For soil interception is modeled as a "one way" phenomenon, namely as a precipitation volume retained by vegetation, which for a particular season equals (Novotny et al, 1976);

$$I_r(A,M) = 2.54\ (a + b \cdot (P/2.54))^m \leq c \cdot P(A,M)/2.54 \qquad \text{(HY-45)}$$

where:

$I_r(A,M)$ = intercepted rainfall; annual, monthly (cm)
$P=P(A,M)$ = average seasonal precipitation (cm);
a,b,n = constants (Table HY-6)
c = % coefficient of average interception (Table HY-6)

A simplified calculation procedure might be as follows:

Subtract the quantity c of the above equation from the unit precipitation term on the left-hand side of Equation HY-32 and use the hydrologic routines (annual, monthly) as described in a previous section.

6.0 REFERENCES

References of this section only are given in appendix RE.

TABLE HY-6

Constants a, b, m of the Interception Equation (H-52)

Vegetal cover	a	$b \simeq c$	m
Orchards	0.04	0.18	1.00
Ash, in woods	0.02	0.18	1.00
Beech, in woods	0.04	0.18	1.00
Oak, in woods	0.05	0.18	1.00
Maple, in woods	0.04	0.18	1.00
Willow, shrubs	0.02	0.40	1.00
Hemlock and pine woods	0.05	0.20	0.50* $\simeq$ 1.00
Beans, potatoes, cabbage and other small hilled crops	0.02h**	0.15h	1.00
Clover and meadow grass	0.005h	0.08h	1.00
Forage, alfalfa, vetch, millet, etc.	0.01h	0.10h	1.00
Small grains, rye, wheat, barley	0.005h	0.05h	1.00
Corn	0.005h	0.005h	1.00

* This approximation is reasonable for the sole purpose of using the equation (HY-45); $I_r = c.P(A,M)/2.54$

** The symbol h refers to the height of the plant (h in m)

Source: Novotny, et al, 1978.

SW - soil washload

APPENDIX SW

TERRESTRIAL SOIL WASHLOAD SIMULATION[*]

Page

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[*] This subroutine is not operational in this version; therefore, little emphasis has been placed in its accurate documentation.

[**] Information abstracted from Foster et al (1980). The authors appreciate his contribution (see sections 1.4 Acknowledgements and SW-3.2 of this appendix).

LIST OF FIGURES

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1.0 INTRODUCTION

The SESOIL terrestrial washload simulation provides a quantitative seasonal prediction of soil sediment transport because of rainfall erosion.

Soil washload is the overland sediment transport of fine particles carried by surface runoff. Nutrients and pollutants can be adsorbed readily on fine soil particles and carried to receiving water bodies. In addition, sediment itself is a serious pollutant of surface water resources. The washload magnitude can be related to the available supply of solid particles in a watershed.

Washload is usually caused by land erosion and is defined by the American Geophysical Union (Konrad, et al, 1978) as the part of the sediment load composed of particles smaller than those found in appreciable quantities in the shifting portion of the streambed. The bedload portion is composed mostly of larger particles--sand and gravel--which originate from gulley and river bank erosion. It does not possess the high adsorptive capacity characteristic of clay and fine soil particles and may not be a significant nutrient or pollutant carrier.

Increased awareness of the ecological and financial consequences of severe erosion and resulting sedimentation on both urban and agricultural lands has increased the need for better methods of estimation deposition and sediment yield. Section 208 of Public Law 92-500 requires planning Agencies to develop plans for evaluating and controlling pollution, including sediment from nonpoint sources. Prediction equations for sediment yields are desirable in all these plans. [Neibling, W.H. and G.R. Foster, 1977.]

The mechanics of washload are very comples and it is impossible to formulate a realistic "all purpose" mathematical model at the micro-level, that will account for all variables describing the physics of transport. However, numerous mathematical algorithms for estimating sediment yield are available in the literature. The choice of an algorithm depends on the watershed characteristics, input data and objectives of the modeling effort, but in general, sediment washload can be estimated using: (1) empirical models; or (2) theoretically developed models.

Well known and widely used empirical models, formulated employing statistical techniques to measured sediment transport yields, are the Universal Soil Loss Equation (USLE) developed by the US Department of Agriculture [Wischmeier, W.H. and D.D. Smith, 1978], and the Raiting Curves Sediment Method (RCSM) [Novotny _et al_.]. Excellent discussions of such models have been presented in the literature by Novotny [Novotny, V., 1980] and Foster [Foster, G.R., 198].

Theoretically-developed sediment yield models can be categorized into stochastic yield models [Murota and Hashino, 1969; Woolhister and Todonivic, 1974], models using kinetic wave theory [Madsen and Grant, 1976] and models using the continuity mass transport equation [Foster and Meyer, 1972, and Adams, _et al_., 1976]. It is beyond the scope of this appendix to present a review of all models, rather an effort is made to shortly document employed models to performing "annual" and "monthly" sediment simulation. SESOIL employs: (1) USLE for annual simulations; and (2) two theoretically developed sediment yield models for monthly simulations.

2.0 "ANNUAL" SEDIMENT YIELD SIMULATIONS

2.1 General

Subroutine SEDIMA (Sediment Annual) of the model simulates annual sediment (soil) losses for a particular area. SEDIMA is employed by both LEVEL0 and LEVEL1 SESOIL simulations. Simulations are performed via the Universal Soil Loss Equation (USLE) as developed and documented by the US Department of Agriculture. [Wischmeier and Smith, 1978.]

The USLE initially developed for areas (regions) east of the Rocky Mountains has been applied to the entire United States for both urban and agricultural areas. The USLE enables planners to predict the average rate of soil erosion for each feasible alternative combination of crop systems and management practices in association with a specified soil type, rainfall pattern, and topography. The equation has been also applied to construction sites and other non-agricultural uses.

The USLE does not predict deposition, does not estimate sediment yields from gully, streambank and streambed erosion; it is applicable only for annual sediment transport predictions mainly originating from small watersheds subject to sheet and rill erosion. In case the USLE has to be applied to specific storm events or time periods, less than a year, two recent reports [Foster, G.R. et al., 1977; Oustand, C.A. et al., 1975] are recommended by the equation developers [Wischmeier and Smith, 1978]. SESOIL, however, does not employ for monthly or after-each-rainfall-event sediment simulations the USLE; therefore, above issue is not of concern.

In the following sections a summary of the USLE theory is presented in order to make this appendix a self-contained document for SESOIL users. Additional details regarding the USLE are to be found in the original publication.

2.2 Universal Soil Loss Equation (USLE)

2.2.1 General

The USLE is

$$A = R\ K\ L\ S\ C\ P \qquad \text{(SW-1)}$$

Several studies [Roehl, 1962; Denfro, 1975; Novotny, 1980] have shown that the upland erosion estimated either by an erosion model or extrapolated from measurements on small plots, does not equal the sediment nor pollutant yield measured at the watershed outlet. This fact is applicable to the USLE theory as well. To overpass these differences, a sediment delivery ratio factor D, was introduced by Novotny [Novotny, *et al.*, 1978] to account for resettling of particulate matter after or during the overland flow. Thus, the USLE equations is formulated as:

$$SYA = R\ K\ L\ S\ C\ P\ D \qquad \text{(SW-2)}$$

where

SYA = annual sediment yield of basin

A = estimated soil loss by the USLE

R = rainfall and runoff factor

K = soil erodibility factor

L = slope-length factor

S = slope-steepness factor

C = cover and management factor

P = support practice factor

D = sediment delivery factor

Above factors, their units, and their numerical values for practical application (related to LEVEL0 and LEVEL1 simulations) are discussed in the following sections. A numerical example for sediment yield delivered by an agricultural small watershed in Clinton, Massachusetts is presented in section 2.4.

2.2.2 Rainfall and Runoff Factor (R)

The factor R encompasses a rainfall erosion index unit factor and a factor for runoff from snowmelt or applied water where such runoff is significant.

Data have shown that the rainfall factor used to estimate the average annual soil loss must include the cumulative effects of many moderate-sized storms as well as the effects of the occasional severe ones. The latter ones are represented by a rainfall erosion index (EI) theoretically presented for "single rainfall events" by the equation:

$$R_r = EI/100 \qquad \text{(SW-3)}$$

with

$$EI = 210 + 89 \log_{10} I_{30} \qquad \text{(SW-4)}$$

where

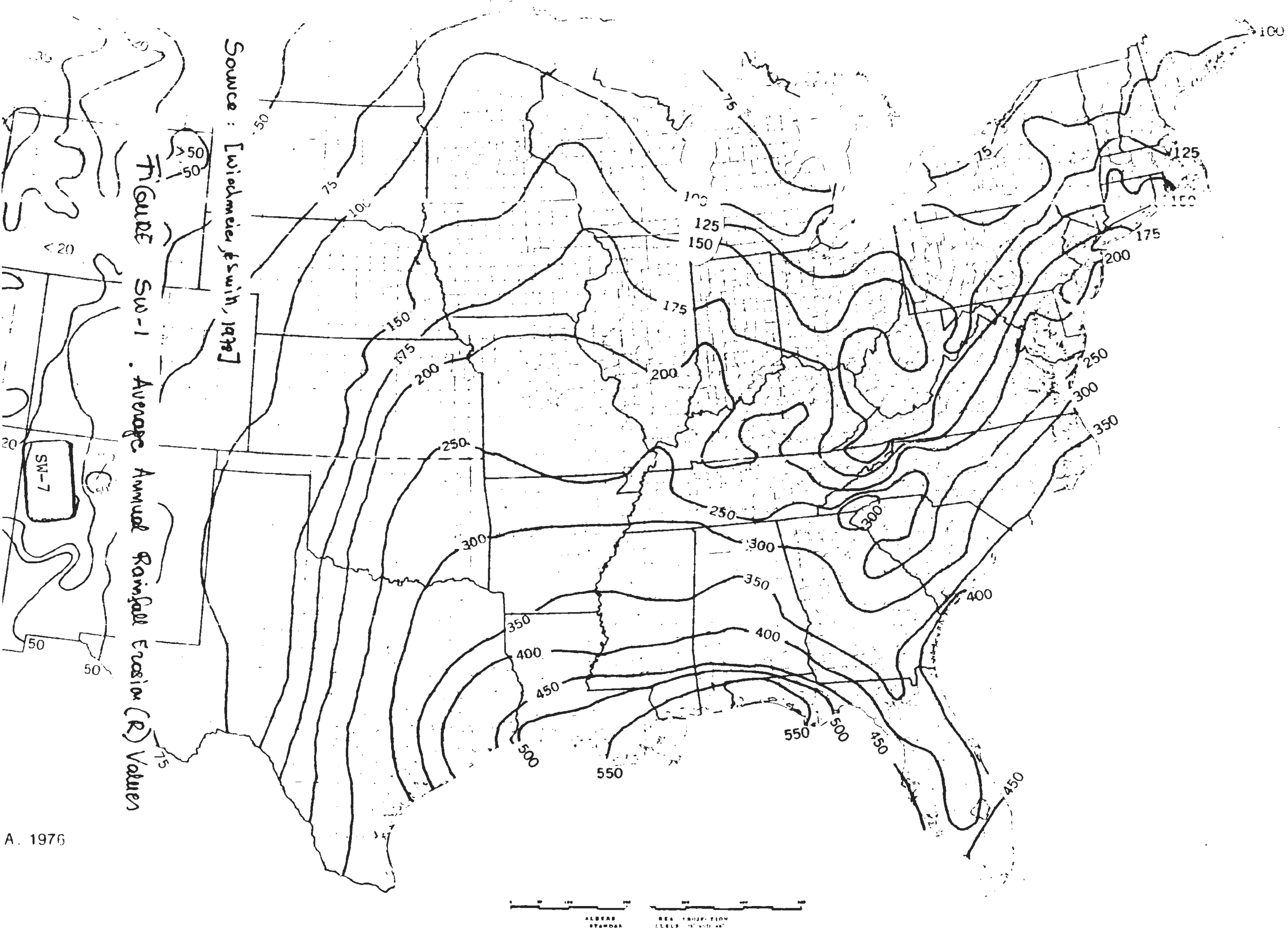
R_r = R factor for single storm events [cm/hr]

E = total energy of rain [metric-ton meters/ha/cm of rain]

I_3 = maximum 30-minutes rainfall intensity [cm/hr]

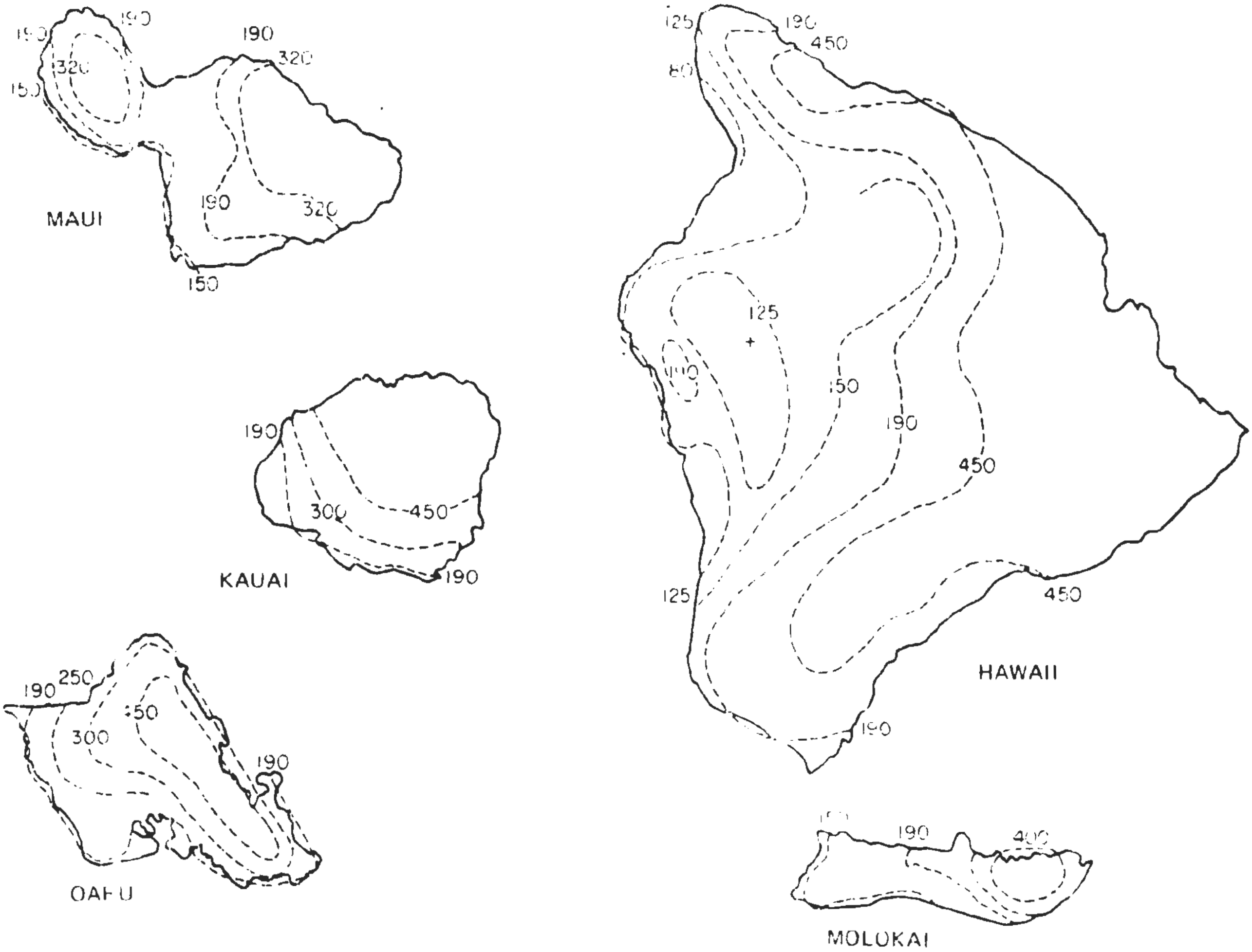
100 = units conversion factor (from english to metric)

However, for long-term and annual simulations the local value of the above index generally equals R for the USLE. R-values have been compiled by the equation developers, and can be obtained for use for both LEVEL0 and LEVEL1 simulations from the isoerodent map [Wischmeier and Smith, 1978, p. 7] presented in figures SW-1 and SW-2.



Source: [Wischmeier & Smith, 1978]

Figure SW-1. Average Annual Rainfall Erosion (R) Values



Source: [Wischmeier & Smith, 1978]

<u>FIGURE SW-2</u> Annual Rainfall Erosion (R) values, Hawai

2.2.3 Soil Erodibility Factor (K)

The K factor in the USLE represents the soil loss rate per erosion index unit for a specified soil as measured on a unit plot, which is defined as a 21.8 m (72.6 ft) length of uniform 9% slope continuously in clean-tilled fallow.

The K factor in the USLE is a quantitative value experimentally determined on a "unit" plot arbitrarily defined. Representative values of K for various soil types and texture classes can be obtained from tables prepared by soil scientists using the latest available research information and data. Table SW-1 and SW-2 are two examples.

For soils containing less than 70% silt and very fine sand, the following regression relationship has been derived by the USLE developer:

$$K = 2.1 \times 10^{-2} M^{1.14} (10^{-4}) (12-a) + 3.25 (b-2) + 2.5 (c-3) \qquad \text{(SW-5)}$$

where:

M = particle size parameter [mm]

a = % of soil organic matter [-]

b = soil structure code used in soil classification

c = profile permeability class

Above equation is presented for practical application and is in figure SW-3. In tests against measured K values ranging from 0.03 to 0.69, 65% of the nomograph solutions differed from the measured K values by less than 0.02 and 95% of them by less than 0.04.

TABLE SW-1

Computed K Values for Soils on Erosion Research Stations

TABLE 1 —Computed K values for soils on erosion research stations

Soil	Source of data	Computed K
Dunkirk silt loam	Geneva, N Y	[1]0.69
Keene silt loam	Zanesville, Ohio	48
Shelby loam	Bethany, Mo	41
Lodi loam	Blacksburg, Va	39
Fayette silt loam	LaCrosse, Wis	[1]38
Cecil sandy clay loam	Watkinsville, Ga	36
Marshall silt loam	Clarinda, Iowa	33
Ida silt loam	Castana, Iowa	33
Mansic clay loam	Hays, Kans	32
Hagerstown silty clay loam	State College, Pa	31
Austin clay	Temple, Tex	29
Mexico silt loam	McCredie, Mo	28
Honeoye silt loam	Marcellus, N Y	28
Cecil sandy loam	Clemson, S C.	28
Ontario loam	Geneva, N Y	27
Cecil clay loam	Watkinsville, Ga	26
Boswell fine sandy loam	Tyler, Tex	25
Cecil sandy loam	Watkinsville, Ga	23
Zaneis fine sandy loam	Guthrie, Okla	22
Tifton loamy sand	Tifton, Ga	10
Freehold loamy sand	Marlboro, N J	08
Bath flaggy silt loam with surface stones > 2 inches removed	Arnot, N Y	[1]05
Albia gravelly loam	Beemerville, N J	03

[1] Evaluated from continuous fallow All others were computed from rowcrop data

Source: [Wischmeier & Smith, 1978]

TABLE SW-2

Table SW-2

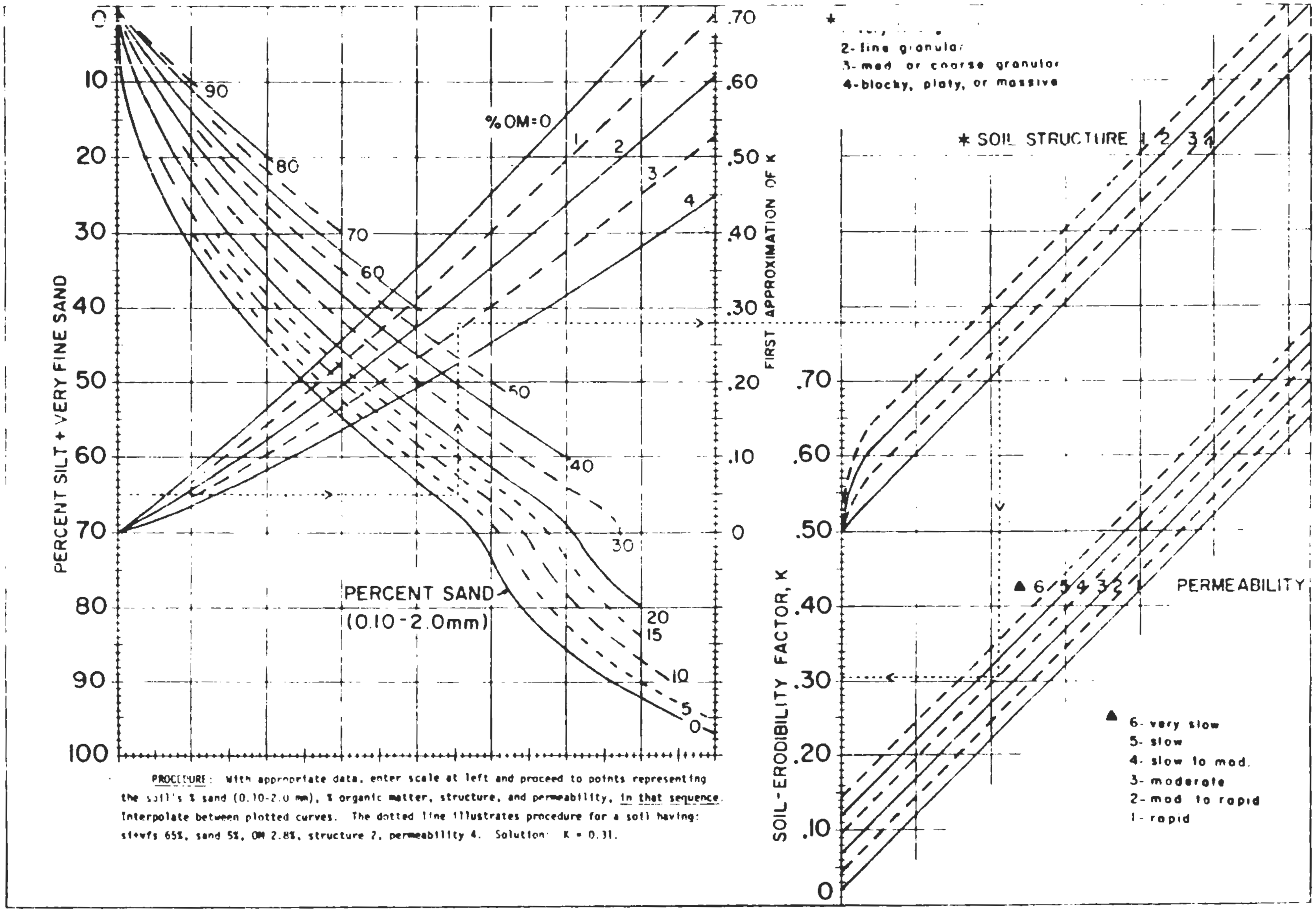
T~~ABLE 7~~—*Approximate values of the soil erodibility factor, K, for 10 benchmark soils in Hawaii*

Order	Suborder	Great group	Subgroup	Family	Series	K
Ultisols	Humults	Tropohumults	Humoxic Tropohumult ,	Clayey, kaolinitic, isohyperthermic	Waikane	0.10
Oxisols	Torrox	Torrox	Typic Torrox	Clayey, kaolinitic, isohyperthermic	Molokai	.24
Oxisols	Ustox	Eutrustox	Tropeptic Eutrustox	Clayey, kaolinitic, isohyperthermic	Wahiawa	.17
Vertisols	Usterts	Chromusterts	Typic Chromusterts	Ver, fine, montmorillonitic, isohyperthermic	Lualualei	28
Aridisols	Orthids	Camborthids	Ustollic Camborthids	Medial, isohyperthermic	Kawaihae (Extremely stony phase)	32
Inceptisols	Andepts	Dystrandepts	Hydric Dystrandepts	Thixotropic, isothermic	Kukaiau	.17
Inceptisols	Andepts	Eutrandepts	Typic Eutrandepts	Medial isohyperthermic	Naalehu (Variant)	.20
Inceptisols	Andepts	Eutrandepts	Entic Eutrandepts	Medial, isohyperthermic	Pakini	.49
Inceptisols	Andepts	Hydrandepts	Typic Hydrandepts	Thixotropic, isohyperthermic	Hilo	10
Inceptisols	Tropepts	Ustropepts	Vertic Ustropepts	Very fine kaolinitic, isohyperthermic	Waipahu	20

SOURCE, El Swaify and Dangler (9)

Figure SW-3

K-Values [Wischmeier & Smith, 1978]



PROCEDURE: With appropriate data, enter scale at left and proceed to points representing the soil's % sand (0.10-2.0 mm), % organic matter, structure, and permeability, in that sequence. Interpolate between plotted curves. The dotted line illustrates procedure for a soil having: si+vfs 65%, sand 5%, OM 2.8%, structure 2, permeability 4. Solution: K = 0.31.

~~FIGURE 3~~ 7.--The soil-erodibility nomograph. Where the silt fraction does not exceed 70 percent, the equation is $100 K = 2.1 M^{1.14} (10^{-4}) (12 - a) + 3.25 (b - 2) + 2.5 (c - 3)$ where $M = $ (percent si + vfs) (100 — percent c), a = percent organic matter, b = structure code, and c = profile permeability class.

2.2.4 Topographic Factor (LS)

Both the length and the steepness of the land slope affect the rate of soil erosion by rain. The two effects have been evaluated separately in research and are presented in the USLE by:

> L, the slope length factor, which is the ratio of soil loss from the field slope length to that from a 21.8 m (72.6 ft) length under identical conditions; and
>
> S, the slope-steepness factor, which is the ratio of soil loss from the field slope gradient to that from a 9% slope under otherwise identical conditions.

LS, therefore, is the expected ratio of soil loss per unti area from a field slope that from a 21.8 m (72.6 ft) length of uniform (9% slope under otherwise identical conditions. The following equation was derived [Wischmeier and Smith; 1978].

$$LS = (0.045_{\lambda})^{m} (65.41 \sin^{2}\Theta + 4.56 \sin\Theta + 0.065) \qquad \text{(SW-6)}$$

where

λ = slope length [m]
Θ = angle of slope
$m = 0.5$ for $4.5\% < \Theta < 4.5\%$
0.4 for $3.5\% < \Theta$
0.3 for $\% < \Theta < 3.5\%$
0.2 for $\Theta < 1\%$

A graphical presentation of equation (SW-6) is presented in figure SW-4. Those who prefer a table may use table SW-3. For irregular slopes, the LS values (figure SW-4, table SW-3) have to be adjusted [Wischmeier and Smith, 1978, p. 16]:

(1) by using table SW-4, and
(2) as shown in table SW-5

Figure SW-4, LS - Values

Source: [Wischmeier & Smith, 1978]

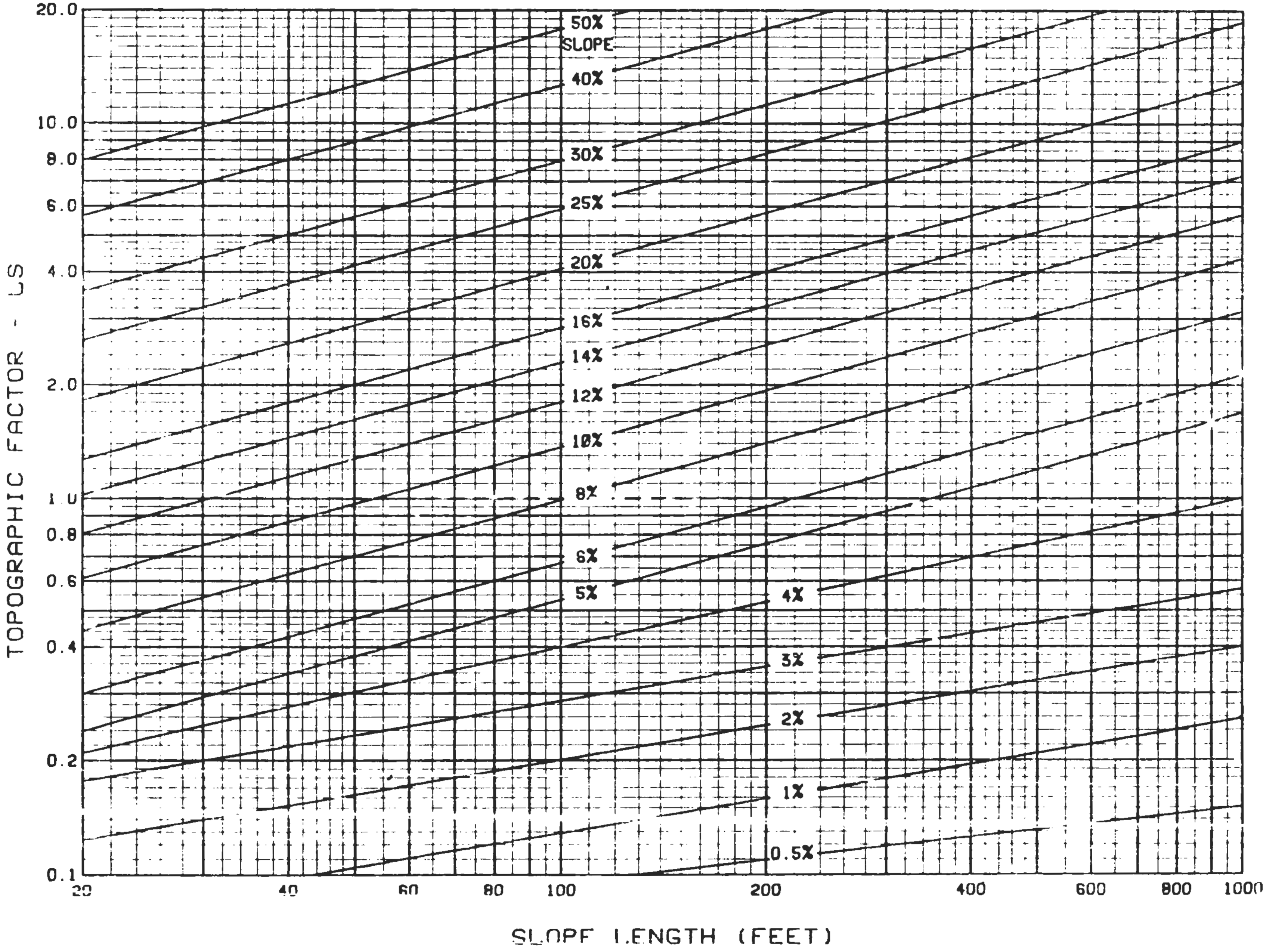


FIGURE 4.—Slope-effect chart (topographic factor, LS). LS = $(\lambda/72.6)^m (65.41 \sin^2\theta + 4.56 \sin\theta + 0.065)$ where λ = slope length in feet; θ = angle of slope; and m = 0.2 for gradients < 1 percent, 0.3 for 1 to 3 percent slopes, 0.4 for 3.5 to 4.5 percent slopes, and 0.5 for slopes of 5 percent or steeper.

TABLE SW-3

LS values

TABLE SW3—*Values of the topographic factor,* **LS**, *for specific combinations of slope length and steepness*[1]

Percent slope	Slope length (feet)											
	25	50	75	100	150	200	300	400	500	600	800	1,000
0.2	0.060	0.069	0.075	0.080	0.086	0.092	0.099	0.105	0.110	0.114	0.121	0.126
0.5	073	.083	090	096	104	110	119	126	132	137	145	152
0.8	086	098	107	113	123	130	141	149	156	162	171	179
2	133	163	185	201	227	248	280	305	326	344	376	402
3	.190	.233	264	287	325	354	400	437	466	492	536	573
4	.230	303	357	400	471	528	621	697	762	820	920	1.03
5	268	379	464	536	656	758	928	1.07	1.20	1.31	1.52	1.69
6	336	476	583	.673	824	952	1.17	1.35	1.50	1.65	1.90	2.13
8	496	701	859	992	1.21	1.41	1.72	1.98	2.22	2.43	2.81	3.14
10	.685	968	1.19	1.37	1.68	1.94	2.37	2.74	3.06	3.36	3.87	4.33
12	903	1.28	1.56	1.80	2.21	2.55	3.13	3.61	4.04	4.42	5.11	5.71
14	1.15	1.62	1.99	2.30	2.81	3.25	3.98	4.59	5.13	5.62	6.49	7.26
16	1.42	2.01	2.46	2.84	3.48	4.01	4.92	5.68	6.35	6.95	8.03	8.98
18	1.72	2.43	2.97	3.43	4.21	3.86	5.95	6.87	7.68	8.41	9.71	10.9
20	2.04	2.88	3.53	4.08	5.00	5.77	7.07	8.16	9.12	10.0	11.5	12.9

[1] $LS = (\lambda/72.6)^m (65.41 \sin \theta + 4.56 \sin \theta + 0.065)$ where λ slope length in feet, m 0.2 for gradients < 1 percent, 0.3 for 1 to 3 percent slopes, 0.4 for 3.5 to 4.5 percent slopes, 0.5 for 5 percent slopes and steeper, and θ - angle of slope (For other combinations of length and gradient, interpolate between adjacent values or see fig SW-4).

TABLE SW-4

TABLE -- *Estimated relative soil losses from successive equal-length segments of a uniform slope*[1]

Number of segments	Sequence number of segment	Fraction of soil loss		
		m = 0.5	m = 0.4	m = 0.3
2	1	0.35	0.38	0.41
	2	65	.62	.59
3	1	19	22	24
	2	35	35	.35
	3	46	43	.41
4	1	12	14	17
	2	23	24	.24
	3	30	29	.28
	4	.35	.33	.31
5	1	09	.11	12
	2	.16	.17	18
	3	21	21	21
	4	25	24	23
	5	28	27	.25

[1] Derived by the formula

$$\text{Soil loss fraction} = \frac{j^{m+1} - (j-1)^{m+1}}{N^{m+1}}$$

where j = segment sequence number, m = slope length exponent (0.5 for slopes ≥ 5 percent, 0.4 for 4 percent slopes, and 0.3 for 3 percent or less), and N = number of equal-length segments into which the slope was divided

Source: [Wischmeier & Smith, 1978]

TABLE SW-5

Adjustment of LS-factor, irregular slopes

Segment I c	*Table 3*	*Table 4*	**K**	*Product*
1	1 07	0 19	0 27	0 055
2	2 74	35	32	307
3	5 12	46	37	871
			KLS -	1 233

Segment	*Percent slope*	*Table 3*	*Table 4*	*Product*
1	5	1 07	0 19	0 203
2	10	2 74	35	959
3	15	5 12	46	2 355
			LS =	3 517

2.2.5 Cover and Management Factor (C)

The factor C represents the ratio of soil loss from an area with specified cover and management to that from an identical area in tilled continuous fallow.

This factor represents the combined effect of all the interrelated cover and management variables. Deriving the appropriate C values for a given locality requires knowledge of how the erosive rainfall in that locality is likely to be distributed through the 12 months of the year and how mud erosion protects the growing plants, crop residues and selected management practices will provide at the time when erosive rains are most likely to occur.

For an optimal derivation of C values, the reader is referred to the corresponding chapter of the original research. [Wischmeier and Smith, 1978, p. 17.] The estimation of the C-factor is the most time consuming effort when employing the USLE. C-values can be estimated for: (1) Agricultural areas, (2) Construction areas, (3) Pasture, Range and Idle Land, and (4) Woodland. Some information is presented below.

Agricultural Areas

Tables SW-6 through SW-11 provide details needed by a trained agronomist to develop simple handbook tables of C values for conditions in specific climatic areas. The tables are self-explanatory and within their broad limits of accuracy these tables can supply the research data needed to complete the estimation of C. The procedure is not that straightforward for site specific applications; however, it is well explained in a "problem-procedure" on page 29 of the original work.

Construction Areas

Applied mulches immediately restore protective cover on denuded areas and drastically reduce C that has a maximum value C=1. Soil loss ratios for various percentages of cover are presented in table SW-12.

Pasture, Range, and Idle Land

Factor C values for a specific combination of cover conditions on these types of land may be obtained from table SW-13.

Source: [Wischmeier & Smith, 1978]

TABLE SW-6

~~TABLE 5.~~—Ratio of soil loss from cropland to corresponding loss from continuous fallow

Line No.	Cover, crop sequence, and management[1]	Spring residue[2]	Cover after plant[3]	Soil loss ratio[4] for cropstage period and canopy cover[5]: F	SB	1	2	3:80	90	96	4L
		Lb	Pct	Pct	Pct	Pct	Pct	Pct	Pct	Pct	Pct
	CORN AFTER C, GS, G OR COT IN MEADOWLESS SYSTEMS										
	Moldboard plow, conv till										
1	RdL, sprg TP	4,500		31	55	48	38			20	23
2		3,400		36	69	52	41		24	20	30
3		2,600		43	64	56	43	32	25	21	37
4		2,000		51	68	60	45	33	25	22	47
5	RdL, fall TP	HP'		44	65	53	38			20	
6		GP		49	70	57	41		24	20	
7		FP		57	74	61	43	32	25	21	
8		LP		65	78	65	45	32	26	22	
9	RdR, sprg TP	HP		66	74	65	47			22	56
10		GP		67	75	65	47		27	23	62
11		FP		68	76	67	48	35	27		69
12		LP		69	77	68	49	35			74
13	RdR, fall TP	HP		76	82	70	49			22	
14		GP		77	83	71	50		27	23	
15		FP		78	85	72	51	35	27		
16		LP		79	85	73	52	35			
17	*Wheeltrack pl, RdL, TP'*	4,500			31	27	25			18	23
18		3,400			36	32	30		22	18	30
19		2,600			43	36	32	29	23	19	37
20		2,000			51	43	36	31	24	20	47
21	*Deep off set disk or disk plow*	4,500	10		45	38	34			20	23
22		3,400	10		52	43	37		24	20	30
23		2,600	5		57	48	40	32	25	21	37
24		2,000			61	51	42	33	26	22	47
25	*No-till plant in crop residue'*	6,000	95		2	2	2			2	14
26		6,000	90		3	3	3			3	14
27		4,500	80		5	5	5			5	15
28		3,400	70		8	8	8		8	6	19
29		3,400	60		12	12	12	12	9	8	23
30		3,400	50		15	15	14	14	11	9	27
31		2,600	40		21	20	18	17	13	11	30
32		2,600	30		26	24	22	21	17	14	36
	Chisel, shallow disk, or fld cult as only tillage										
33	On moderate slopes	6,000	70		8	8	7			7	17
34			60		10	9	8			8	17
35			50		13	11	10			9	18
36			40		15	13	11			10	19
37			30		18	15	13			12	20
38			20		23	20	18			16	21
39	Do	4,500	70		9	8	7			7	18
40			60		12	10	9			8	18
41			50		14	13	11			9	19
42			40		17	15	13			10	20
43			30		21	18	15			13	21
44			20		25	22	19			16	22
	CORN AFTER WC OF RYEGRASS OR WHEAT SEEDED IN C STUBBLE										
	WC reaches stemming stage										
79	No till pl in killed WC	4,000			7	7	7		7	6	(')
80		3,000			11	11	11	11	9	7	
81		2,000			15	15	14	14	11	9	
82		1,500			20	19	18	18	14	11	
	Strip till one-fourth row space										
83	Rows U/D slope	4,000			13	12	11		11	9	('')
84		3,000			16	17	16	16	13	10	
85		2,000			23	22	20	19	15	12	
86		1,500			28	26	24	22	17	14	
87	Rows on contour''	4,000			10	10	10		10	8	('')
88		3,000			15	15	15	15	12	9	
89		2,000			20	20	19	19	15	12	
90		1,500			25	24	23	22	17	14	
91	TP, conv seedbed	4,000		36	60	52	41		24	20	(')
92		3,000		43	64	56	43	31	25	21	
93		2,000		51	68	60	45	33	26	22	
94		1,500		61	73	64	47	35	27	23	
	WC succulent blades only										
95	No-till pl in killed WC	3,000			11	11	17	23	18	16	('')
96		2,000			15	15	20	25	20	17	
97		1,500			20	20	23	26	21	18	
98		1,000			26	25	27	27	22	19	
99	Strip till one-fourth row space	3,000			18	18	21	25	20	17	( )
100		2,000			23	23	25	27	21	18	
101		1,500			28	28	28	28	22	19	
102		1,000			33	33	31	29	23	20	
	CORN IN SOD-BASED SYSTEMS										
	No till pl in killed sod										
103	3 to 5 tons hay yld				1	1	1		1	1	1
104	1 to 2 tons hay yld				2	2	2	2	2	2	2
	Strip till, 3-5 ton M										
105	50 percent cover, tilled strips				2	2	2		2	2	4
106	20 percent cover, tilled strips				3	3	3		3	3	5
	Strip till, 1-2 ton M										
107	40 percent cover, tilled strips				4	4	4	4	4	4	6
108	20 percent cover, tilled strips				5	5	5	5	5	5	7
	Other tillage after sod			('')	('')	('')	('')	('')	('')	('')	('')
	CORN AFTER SOYBEANS										
109	*Sprg TP, conv till*	HP		40	72	60	48			25	29
110		GP		47	78	65	51		30	25	37
111		FP		56	83	70	54	40	31	26	44
112	*Fall TP, conv till*	HP		47	75	60	48			25	
113		GP		53	81	65	51		30	25	
114		FP	--	62	86	70	54	40	31	26	

TABLE SW-6 (Continued)

45	Do	3,400	60		13	11	10		10	8	20
46			50		16	13	12		12	9	24
47			40		19	17	16		14	11	25
48			30		23	21	19		17	14	26
49			20		29	25	23		21	16	27
50			10		36	32	29		24	20	30
51	Do	2,600	50		17	16	15	15	13	10	29
52			40		21	20	19	19	15	12	30
53			30		25	23	22	22	18	14	32
54			20		32	29	28	27	22	17	34
55			10		41	36	34	32	25	21	37
56	Do	2,000	40		23	21	20	20	15	12	37
57			30		27	25	24	23	19	15	39
58			20		35	32	30	28	22	18	42
59			10		46	42	38	33	26	22	47
	On slopes > 12 percent										
60	Lines 33-59 times factor of				1 [illegible]	1 3	1 1	1 0	1 0	1 0	1 0
	Disk or harrow after spring chisel or fld cult										
	Lines 33-59 times factor of										
61	On moderate slopes				1 1	1 1	1 1	1 0	1 0	1 0	1 0
62	On slopes > 12 percent				1 4	1 4	1 2	1 0	1 0	1 0	1 0
	Ridge plant										
	Lines 33-59 times factor of										
63	Rows on contour				7	7	7	7	7	7	7
64	Rows U/D slope < 12 percent				7	7	1 0	1 0	1 0	1 0	1 0
65	Rows U/D slope > 12 percent				9	9	1 0	1 0	1 0	1 0	1 0
	Till plant										
	Lines 33-59 times factor of										
66	Rows on contour[11]				7	85	1 0	1 0	1 0	1 0	1 0
67	Rows U/D slope < 7 percent				1 0	1 0	1 0	1 0	1 0	1 0	1 0
	Strip till one fourth of row spacing										
68	Rows on contour[11]	4,500	60		12	10	9			8	23
69		3,400	50		16	14	12		11	10	27
70		2,600	40		22	19	17	17	14	12	30
71		2,000	30		27	23	21	20	16	13	36
72	Rows U/D slope	4,500	60		16	13	11			9	23
73		3,400	50		20	17	14		12	11	27
74		2,600	40		26	22	19	17	14	12	30
75		2,000	30		31	26	23	20	16	13	36
	Vari-till										
76	Rows on contour[11]	3,400	40		13	12	11			11	22
77		3,400	30		16	15	14	14	13	12	26
78		2,600	20	-	21	19	19	19	16	14	34
115	Fall & sprg chisel or cult	HP	30		40	35	27			23	29
116		GP	25		[illegible]	39	33		27	23	37
117		GP	20		51	44	39	34	27	23	37
118		FP	15		58	51	44	36	28	23	44
119		LP	10		67	59	48	36	28	23	54
120	*No till pl in crop resd*	HP	40		25	20	19		14	11	26
121		GP	30		[illegible]	27	[illegible]	[illegible]	[illegible]	14	[illegible]
122		FP	20		44	38	32	27	23	18	40
	BEANS AFTER CORN										
123	*Sprg TP, RdL, conv till*	HP		33	60	52	38		20	17	('')
124		GP		39	64	56	41		21	18	
125		FP		45	68	60	43	29	22		
126	*Fall TP, RdL, conv till*	HP		45	69	57	39		20	17	('')
127		GP		52	73	61	41		21	18	
128		FP		59	77	65	43	29	22		
	Chisel or fld cult			('')	('')	('')	('')	('')	('')	('')	('')
	BEANS AFTER BEANS			('')	('')	('')	('')	('')	('')	('')	('')
	GRAIN AFTER C, G, GS, COT[13]										
129	*In disked residues*	4,500	70		12	12	11	7	4	2	('')
130		3,400	60		16	14	12	7	4	2	
131			50		22	18	14	8	5	3	
132			40		27	21	16	9	5	3	
133			30		32	25	18	9	6	3	
134			20		38	30	21	10	6	3	
135	Do	2,600	40		29	24	19	9	6	3	('')
136			20		43	34	24	11	7	4	
137			10		52	39	27	12	7	4	
138	Do	2,000	30		38	30	23	11	7	4	('')
139			20		46	34	26	12	7	4	
140			10		56	43	30	13	8	5	
141	*In disked stubble, RdR*				79	62	42	17	11	6	('')
142	*Winter G after fall TP, RdL*	HP		31	55	48	31	12	7	5	('')
143		GP		36	60	52	33	13	8	5	
144		FP		43	64	56	34	14	9	5	
145		LP	-	53	68	60	38	15	10	6	
	GRAIN AFTER SUMMER FALLOW										
146	*With grain residues*	200	10		70	55	43	18	13	11	('')
147		500	30		43	34	23	13	10	8	
148		750	40		34	27	18	10	7	7	
149		1,000	50		26	21	15	8	7	6	
150		1,500	60		20	16	12	7	5	5	
151		2,000	70	-	14	11	9	7	5	5	
152	*With row crop residues*	300	5		82	65	44	19	14	12	('')
153		500	15	-	62	49	35	17	13	11	
154		750	23	-	50	40	29	14	11	9	
155		1,000	30	-	40	31	24	13	10	8	
156		1,500	45		31	24	18	10	8	7	
157		2,000	55		23	19	14	8	7	5	
158		2,500	65		17	14	12	7	5	4	
	POTATOES										
159	*Rows with slope*			43	64	56	36	26	19	16	
160	*Contoured rows, ridged when canopy cover is about 50 percent*[11]			43	64	56	18	13	10	8	

See footnotes, ~~p 24~~ next page

Footnotes for table ~~5~~ Sw-6

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[1] Symbols B, soybeans, C, corn, conv till plow, disk and harrow for seedbed, cot, cotton, F rough fallow fld cult, field cultivator, G small grain, GS grain sorghum, M, grass and legume meadow, at least 1 full year, pl, plant, RdL, crop residues left on field, RdR crop residues removed, SB seedbed period, sprg spring, TP plowed with moldboard, WC, winter cover crop, — insignificant or an unlikely combination of variables

[2] Dry weight per acre after winter loss and reductions by grazing or partial removal 4,500 lbs represents 100 to 125 bu corn, 3,400 lbs, 75 to 99 bu, 2,600 lbs, 60 to 74 bu, and 2 000 lbs, 40 to 59 bu, with normal 30 percent winter loss For RdR or fall-plow practices, these four productivity levels are indicated by HP, GP, FP and LP, respectively (high good fair and low productivity) In lines 79 to 102, this column indicates dry weight of the winter-cover crop

Percentage of soil surface covered by plant residue mulch after crop seeding The difference between spring residue and that on the surface after crop seeding is reflected in the soil loss ratios as residues mixed with the topsoil

The soil loss ratios given as percentages, assume that the indicated crop sequence and practices are followed consistently One year deviations from normal practices do not have the effect of a permanent change Linear interpolation between lines is recommended when justified by field conditions

Cropstage periods are as defined on p 18 The three columns for cropstage 3 are for 80 90, and 96 to 100 percent canopy cover at maturity

Column 4L is for all residues left on field Corn stalks partially standing as left by some mechanical pickers If stalks are shredded and spread by picker, select ratio from table 5 C When residues are reduced by grazing, take ratio from lower spring-residue line

Period 4 values in lines 9 to 12 are for corn stubble (stover removed)

[8] Inversion plowed, no secondary tillage. For this practice, residues must be left and incorporated

[9] Soil surface and chopped residues of *matured* preceding crop undisturbed except in narrow slots in which seeds are planted

[10] Top of old row ridge sliced off, throwing residues and some soil into furrow areas Reridging assumed to occur near end of cropstage 1

[11] Where lower soil loss ratios are listed for rows on the contour, this reduction is in addition to the standard field contouring credit The *P* value for contouring is used with these reduced loss ratios

[12] Field-average percent cover, probably about three-fourths of percent cover on undisturbed strips

[13] If again seeded to WC crop in corn stubble, evaluate winter period as a winter grain seeding (lines 132 to 148) Otherwise, see table 5 C

[14] Select the appropriate line for the crop, tillage, and productivity level and multiply the listed soil loss ratios by sod residual factors from table 5 D

[15] Spring residue may include carryover from prior corn crop

[16] See table 5 C

[17] Use values from lines 33 to 62 with appropriate dates and lengths of cropstage periods for beans in the locality

[18] Values in lines 109 to 122 are best available estimates, but planting dates and lengths of cropstages may differ

[19] When meadow is seeded with the grain, its effect will be reflected through higher percentages of cover in cropstages 3 and 4

[20] Ratio depends on percent cover. See table 5-C

[21] See item 12, table 5 B.

TABLE SW-6 (Continued)

TABLE SW-7

TABLE ~~5-A~~ --Approximate soil loss ratios for cotton

Practice Number	Tillage operations			
	Expected final canopy percent cover	65	80	95
	Estimated initial percent cover from defoliation – stalks down	30	45	60
		Soil loss ratio[1]		
COTTON ANNUALLY		Percent		
1	*None*			
	Defoliation to Dec 31	36	24	15
	Jan 1 to Feb or Mar tillage			
	Cot Rd only	52	41	32
	Rd & 20 percent cover vol veg	32	26	20
	Rd & 30 percent cover vol veg	26	20	14
2	*Chisel plow soon after cot harvest*			
	Chiseling to Dec 31	40	31	24
	Jan 1 to sprg tillage	56	47	40
3	*Fall disk after chisel*			
	Disking to Dec 31	53	45	37
	Jan 1 to sprg tillage	62	54	47
4	*Chisel plow Feb Mar, no prior tillage*			
	Cot Rd only	50	42	35
	Rd & 20 percent vol veg	39	33	28
	Rd & 30 percent vol veg	34	29	25
5	*Bed (hip) Feb Mar no prior tillage*			
	Cot Rd only	100	84	70
	Rd & 20 percent vol veg	78	66	56
	Rd & 30 percent vol veg	68	58	50
	Split ridges & plant after hip, or Disk & plow after chisel (SB)			
	Cot Rd only	61	54	47
	Rd & 20 percent vol veg	53	47	41
	Rd & 30 percent vol veg	50	44	38
	Crop stage 1			
	Cot Rd only	57	50	43
	Rd & 20 percent vol veg	49	43	38
	Rd & 30 percent vol veg	46	41	36
	Crop stage 2	45	39	34
	Crop stage 3	40	27	17
6	*Bed (hip) after 1 prior tillage*			
	Cot Rd only	110	96	84
	Rd & 20 percent veg	94	82	72
	Rd & 30 percent veg	90	78	68
	Split ridges after hip (SB)			
	Cot Rd only	66	61	52
	Rd & 20 to 30 percent veg	61	55	49
	Crop stage 1			
	Cot Rd only	60	[illegible]	49
	Rd & 20 to 30 percent veg	56	51	46
	Crop stage 2	47	44	38
	Crop stage 3	42	30	19
7	*Hip after 2 prior tillages*			
	Cot Rd only	116	106	98
	Rd & 20 30 percent veg	108	[illegible]	88
	Split ridges after hip (SB)	67	62	57
8	*Hip after 3 or more tillages*	120	110	102
	Split ridges after hip (SB)	68	[illegible]	59
9	*Conventional moldboard plow and disk*			
	Fallow period	42	39	36
	Seedbed period	68	[illegible]	59
	Crop stage 1	63	59	55
	Crop stage 2	49	46	43
	Crop stage 3	44	[illegible]	[illegible]
	Crop stage 4 (See practices 1 2 and 3			

COTTON AFTER SOD CROP

For the first or second crop after a grass or grass and legume meadow has been turnplowed multiply values given in the last five lines above by sod residual factors from table 5 D

COTTON AFTER SOYBEANS

Select values from above and multiply by 1 25

Source : [ ]

Footnotes

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[1] *Alternate procedure for estimating the soil loss ratios*

The ratios given above for cotton are based on estimates for reductions in percent cover through normal winter loss and by the successive tillage operations Research is underway in Mississippi to obtain more accurate residue data in relation to tillage practices This research should provide more accurate soil loss ratios for cotton within a few years

Where the reductions in percent cover by winter loss and tillage operations are small, the following procedure may be used to compute soil loss ratios for the preplant and seedbed periods Enter figure 6 with the percentage of the field surface covered by residue mulch, move vertically to the upper curve and read the mulch factor on the scale at the left Multiply this factor by a factor selected from the following tabulation to account for effects of land use residual, surface roughness and porosity

Productivity level	No tillage	Rough surface	Smoothed surface
High	0.66	0.50	0.56
Medium	71	54	61
Low	75	58	65

[2] Values for the seedbed period on slopes of less than 3 percent should be [illegible] the value computed above for rough surface

[3] Rd crop residue [illegible] volunteer vegetation

TABLE SW-8

TABLE ~~5-~~B.—*Soil loss ratios for conditions not evaluated in table 5*

COTTON

See table 5-A

CROPSTAGE 4 FOR ROWCROPS

Stalks broken and partially standing: Use col 4L

Stalks standing after hand picking Col 4L times 1.15

Stalks shredded without soil tillage See table 5-C

Fall chisel Select values from lines 33-62, seedbed column

CROPSTAGE 4 FOR SMALL GRAIN:

See table 5-C

DOUBLE CROPPING

Derive annual C value by selecting from table 5 the soil loss percentages for the successive cropstage periods of each crop

ESTABLISHED MEADOW, FULL-YEAR PERCENTAGES:

Grass and legume mix,	3 to 5 t hay	0.4
Do.	2 to 3 t hay	.6
Do.	1 t hay	1.0
Sericea, after second year		1.0
Red clover		1.5
Alfalfa, lespedeza, and second-year sericea		2.0
Sweetclover		2.5

MEADOW SEEDING WITHOUT NURSE CROP:

Determine appropriate lengths of cropstage periods SB, 1, and 2 and apply values given for small grain seeding

PEANUTS

Comparison with soybeans is suggested

PINEAPPLES.

Direct data not available Tentative values derived analytically are available from the SCS in Hawaii or the Western Technical Service Center at Portland, Oreg (Reference 5)

SORGHUM

Select values given for corn, on the basis of expected crop residues and canopy cover

SUGARBEETS:

Direct data not available Probably most nearly comparable to potatoes, without the ridging credit.

SUGARCANE.

Tentative values available from sources given for pineapples

SUMMER FALLOW IN LOW-RAINFALL AREAS, USE GRAIN OR ROW CROP RESIDUES

The approximate soil loss percentage after each successive tillage operation may be obtained from the following tabulation by estimating the percent surface cover after that tillage and selecting the column for the appropriate amount of initial residue The given values credit benefits of the residue mulch, residues mixed with soil by tillage, and the crop system residual

Percent cover by mulch	Initial residue (lbs/A)			
	>4,000	3,000	2,000	1,500
90	4	—	—	—
80	8	[1]8		
70	12	13	[1]14	
60	16	17	[1]18	[1]19
50	20	22	24	[1]25
40	25	27	30	32
30	29	33	37	39
20	35	39	44	46
10	47	55	63	58

[1] For grain residue only

WINTER COVER SEEDING IN ROW CROP STUBBLE OR RESIDUES

Define cropstage periods based on the cover seeding date and apply values from lines 120 to 145

Source : [ ]

TABLE SW-9

TABLE ~~5-C~~ —*Soil loss ratios (percent) for cropstage 4 when stalks are chopped and distributed without soil tillage*

	Corn or Sorghum		Soybeans		
Mulch cover[1]	**Tilled seedbed**	**No till**	**Tilled seedbed[2]**	**No till in corn rd[3]**	**Grain Stubble[4]**
20	48	34	60	42	48
30	37	26	46	32	37
40	30	21	38	26	30
50	22	15	28	19	22
60	17	12	21	16	17
70	12	8	15	10	12
80	7	5	9	6	7
90	4	3		-	4
95	3	2	—	- -	3

[1] Part of a field surface directly covered by pieces of residue mulch

This column applies for all systems other than no till

Cover after bean harvest may include an appreciable number of stalks carried over from the prior corn crop

[4] For grain with meadow seeding, include meadow growth in percent cover and limit grain period 4 to 2 mo. Thereafter, classify as established meadow

Source : [ ]

Table SW-10

TABLE 5 D - *Factors to credit residual effects of turned sod*[1]

Crop	Hay yield	Factor for cropstage period				
		F	SB and 1	2	3	4
	Tons					
First year after mead						
Row crop or grain	3 5	0 25	0 40	0 45	0 50	0 60
	2-3	30	45	.50	55	65
	1-2	35	50	55	60	70
Second year after mead						
Row crop	3 5	70	80	.85	90	.95
	2 3	75	.85	90	95	1 0
	1-2	80	.90	95	1.0	1 0
Spring grain	3 5		75	80	.85	.95
	2 3		80	85	90	1 0
	1-2		.85	90	95	1 0
Winter grain	3 5		60	70	85	95
	2-3		65	75	90	1 0
	1-2	-	70	85	95	1.0

[1] These factors are to be multiplied by the appropriate soil loss percentages selected from table 5 They are directly applicable for sod forming meadows of at least 1 full year duration, plowed not more than 1 month before final seedbed preparation

When sod is fall plowed for spring planting the listed values for all cropstage periods are increased by adding 0 02 for each additional month by which the plowing precedes spring seedbed preparation For example, September plowing would precede May disking by 8 months and 0 02(8 1), or 0 14, would be added to each value in the table For nonsod forming meadows, like sweetclover or lespedeza, multiply the factors by 1 2 When the computed value is greater than 1 0, use as 1 0

TABLE SW-11

TABLE 6.—Percentage of the average annual **EI** which normally occurs between January 1 and the indicated dates.[1] Computed for the geographic areas shown in figure ~~7~~ below

Area No	Jan		Feb.		Mar		Apr		May		June		July		Aug		Sept		Oct		Nov		Dec.	
	1	15	1	15	1	15	1	15	1	15	1	15	1	15	1	15	1	15	1	15	1	15	1	15
1	0	0	0	0	0	0	1	2	3	6	11	23	36	49	63	77	90	95	98	99	100	100	100	100
2	0	0	0	0	1	1	2	3	6	10	17	29	43	55	67	77	85	91	96	98	99	100	100	100
3	0	0	0	0	1	1	2	3	6	13	23	37	51	61	69	78	85	91	94	96	98	99	99	100
4	0	[illegible]	1	[illegible]	2	3	4	7	12	18	27	38	48	54	62	69	76	83	90	94	97	98	99	100
5	0	[illegible]	2	3	4	6	8	13	21	29	37	46	54	63	65	69	74	81	87	92	95	97	96	99
6	0	0	0	0	1	1	1	2	6	16	29	39	46	53	60	67	74	81	88	95	99	99	100	100
7	0		1	2	3	4	6	8	13	25	40	45	56	62	67	72	76	80	85	91	97	98	99	99
8	0		3	5	7	10	14	20	28	37	48	56	61	64	68	72	77	81	86	89	92	95	98	99
9	0	[illegible]	4	6	9	12	17	23	30	37	43	49	54	58	62	66	70	74	78	82	86	90	94	97
10	0		2	4	6	8	10	15	21	29	38	47	53	57	61	65	70	76	83	88	91	94	96	98
11	0		3	5	7	9	11	14	18	27	35	41	46	51	57	62	68	73	79	84	89	93	96	98
12	0	[illegible]	0	0	1	1	2	3	5	9	15	27	38	50	62	74	84	91	95	97	96	99	99	100
13	0	0	0	1	1	2	3	5	7	12	19	33	48	57	65	74	82	88	93	96	98	99	100	100
14	0	0	0	1	2	3	4	6	9	14	20	28	39	52	63	72	80	87	91	94	97	98	99	100
15	0	0	1	2	3	4	6	8	11	15	22	31	40	49	59	69	78	85	91	94	96	98	99	100
16	0	[illegible]	2	3	4	6	8	10	14	18	25	34	45	56	64	72	79	84	89	92	95	97	98	99
17	0	[illegible]	2	3	4	5	6	8	11	15	20	28	41	54	65	74	82	87	92	94	96	97	98	99
18	0		2	4	6	8	10	13	19	26	34	42	50	58	63	68	74	79	84	89	93	95	97	99
19	0		3	6	9	12	16	21	26	31	37	43	50	57	64	71	77	81	85	88	91	93	95	97
20	0	[illegible]	3	5	7	10	13	16	19	23	27	34	44	54	63	72	80	85	89	91	93	95	96	98
21	0	[illegible]	6	10	13	16	19	23	26	29	33	39	47	58	68	75	80	63	86	88	90	92	95	97
22	0	[illegible]	6	9	13	17	21	27	33	38	44	49	55	61	67	71	75	78	81	84	86	90	94	97
23	0	1	5	7	10	14	18	23	27	31	35	39	45	53	60	67	74	80	84	86	88	90	93	95
24	0	1	6	9	12	16	20	24	28	33	38	43	50	59	69	75	80	84	87	90	92	94	96	97
25	0		3	5	7	10	13	17	21	24	27	33	40	46	53	61	69	78	89	92	94	95	97	98
26	0	[illegible]	4	6	8	12	16	20	25	30	35	41	47	56	67	75	81	85	87	89	91	93	95	97
27	0		2	3	5	7	10	14	18	22	27	32	37	46	58	69	80	89	93	94	95	96	97	99
28	0		3	5	7	9	12	15	18	21	25	29	36	45	56	68	77	83	88	91	93	95	97	99
29	0		2	3	4	5	7	9	11	14	17	22	31	42	54	65	74	83	89	92	95	97	98	99
30	0	[illegible]	2	3	4	5	6	8	10	14	19	26	34	45	56	66	76	82	86	90	93	95	97	99
31	0	0	0	1	2	3	4	5	7	12	17	24	33	42	55	67	76	83	89	92	94	96	98	99
32	0	1	2	3	4	5	6	8	10	13	17	22	31	42	52	60	68	75	80	85	89	92	96	98
33	0	1	2	4	6	8	11	13	15	18	21	26	32	38	46	55	64	71	77	81	85	89	93	97

[1] For dates not listed in the table, interpolate between adjacent values.

Source: [ ]

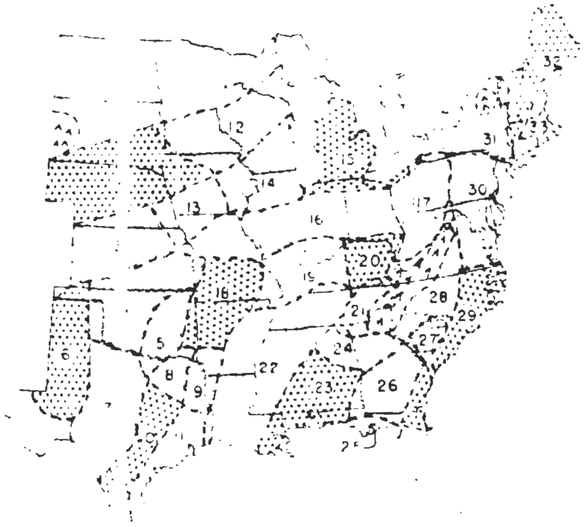


FIGURE ~~7~~.—Key map for selection of applicable EI distribution data from table SW-11

TABLE SW-12

TABLE 9.—*Mulch factors and length limits for construction slopes*[1]

Type of mulch	Mulch Rate	Land Slope	Factor C	Length limit[2]
	Tons per acre	*Percent*		*Feet*
None	0	all	1.0	—
Straw or hay	1 0	1 5	0 20	200
tied down by	1 0	6-10	20	100
anchoring and				
tacking	1.5	1-5	12	300
equipment	1 5	6-10	12	150
Do	2 0	1 5	06	400
	2 0	6 10	06	200
	2 0	11 15	07	150
	2 0	16 20	11	100
	2 0	21 25	14	75
	2 0	26 33	17	50
	2 0	34 50	20	35
Crushed stone	135	<16	05	200
¼ to 1½ in	135	16 20	05	150
	135	21 33	05	100
	135	34 50	05	75
Do	240	<21	02	300
	240	21 33	02	200
	240	34 50	02	150
Wood chips	7	<16	08	75
	7	16 20	08	50
Do	12	<16	05	150
	12	16 20	05	100
	12	21 33	05	75
Do	25	<16	02	200
	25	16 20	02	150
	25	21 33	02	100
	25	34 50	02	75

[1] From Meyer and Ports (24). Developed by an interagency workshop group on the basis of field experience and limited research data.

[2] Maximum slope length for which the specified mulch rate is considered effective. When this limit is exceeded, either a higher application rate or mechanical shortening of the effective slope length is required.

[3] When the straw or hay mulch is not anchored to the soil, C values on moderate or steep slopes of soils having K values greater than 0 30 should be taken at double the values given in this table.

Source [ ]

Table SW-13

TABLE 10.—*Factor C for permanent pasture, range, and idle land*[1]

Vegetative canopy		Cover that contacts the soil surface						
Type and height[2]	Percent cover		Percent ground cover					
		Type[4]	0	20	40	60	80	95+
No appreciable canopy		G	0 45	0 20	0.10	0 042	0 013	0 003
		W	45	24	15	.091	.043	011
Tall weeds or short brush with average drop fall height of 20 in	25	G	36	17	09	038	.013	003
		W	36	20	13	083	041	011
	50	G	26	13	07	035	012	.003
		W	26	16	11	076	039	011
	75	G	17	10	06	032	011	003
		W	17	12	09	.068	038	011
Appreciable brush or bushes with average drop fall height of 6½ ft	25	G	40	18	09	040	013	003
		W	40	22	14	087	042	011
	50	G	34	.16	08	.038	.012	003
		W	34	19	13	082	.041	011
	75	G	28	14	08	036	012	003
		W	28	17	12	078	040	011
Trees, but no appreciable low brush Average drop fall height of 13 ft	25	G	42	19	10	041	013	003
		W	42	23	14	089	042	011
	50	G	39	18	09	040	013	003
		W	39	21	14	087	042	011
	75	G	36	17	09	039	012	003
		W	36	20	13	084	041	011

---

[1] The listed C values assume that the vegetation and mulch are randomly distributed over the entire area

Canopy height is measured as the average fall height of water drops falling from the canopy to the ground Canopy effect is inversely proportional to drop fall height and is negligible if fall height exceeds 33 ft

Portion of total area surface that would be hidden from view by canopy in a vertical projection (a bird's eye view)

G cover at surface is grass grasslike plants decaying compacted duff or litter at least 2 in deep

W cover at surface is mostly broadleaf herbaceous plants (as weeds with little lateral root network near the surface) or undecayed residues or both

Source : []

Woodland Areas

Three categories of woodland can be can be considered separately: (1) undisturbed forest land; (2) woodland that is grazed, burned, or selectively harvested; and (3) forest lands that have site specific preparation treatments for re-establishment after harvest.

Factor C values for undisturbed forest land may be obtained from table SW-14. Factor C-values for mechanically prepared woodland sites can be obtained from table SW-15.

Table SW-14

TABLE ~~11~~ — *Factor C for undisturbed forest land*[1]

Percent of area covered by canopy of trees and undergrowth	Percent of area covered by duff at least 2 in deep	Factor C
100-75	100-90	0001 001
70-45	85-75	002 004
40-20	70-40	003 009

[1] Where effective litter cover is less than 40 percent or canopy cover is less than 20 percent, use table 6 Also use table 6 where woodlands are being grazed, harvested, or burned

The ranges in listed C values are caused by the ranges in the specified forest litter and canopy covers and by variations in effective canopy heights.

Table SW-15

TABLE ~~12~~.—Factor C for mechanically prepared woodland sites

Site preparation	Mulch cover[1]	Soil condition and weed cover[2]							
		Excellent		Good		Fair		Poor	
		NC	WC	NC	WC	NC	WC	NC	WC
	Percent								
Disked, raked, or bedded[4]	None	0.52	0.20	0.72	0.27	0.85	0.32	0.94	0.36
	10	33	15	46	20	54	24	60	26
	20	24	12	34	17	40	20	44	22
	40	17	11	23	14	27	17	30	19
	60	11	08	15	11	18	14	20	15
	80	05	04	07	.06	.09	08	10	09
Burned	None	.25	10	26	10	31	12	45	17
	10	23	10	24	10	26	11	36	16
	20	19	10	19	10	21	11	27	14
	40	14	09	14	09	15	09	17	11
	60	08	06	09	07	10	08	11	08
	80	04	04	05	04	05	04	06	05
Drum chopped	None	16	07	17	07	20	.08	29	11
	10	15	07	16	07	17	08	23	13
	20	12	06	12	06	14	07	18	09
	40	09	06	.09	06	10	06	11	07
	60	06	05	06	05	07	05	07	05
	80	03	03	03	03	03	03	04	04

---

[1] Percentage of surface covered by residue in contact with the soil

[2] *Excellent* soil condition—Highly stable soil aggregates in topsoil with fine tree roots and litter mixed in

Good—Moderately stable soil aggregates in topsoil or highly stable aggregates in subsoil (topsoil removed during raking), only traces of litter mixed in

Fair—Highly unstable soil aggregates in topsoil or moderately stable aggregates in subsoil, no litter mixed in

Poor—No topsoil, highly erodible soil aggregates in subsoil, no litter mixed in

[3] NC—No live vegetation

WC—75 percent cover of grass and weeds having an average drop fall height of 20 in For intermediate percentages of cover, interpolate between columns

[4] Modify the listed C values as follows to account for effects of surface roughness and aging

First year after treatment multiply listed C values by 0.40 for rough surface (depressions >6 in), by 0.65 for moderately rough and by 0.90 for smooth (depressions <2 in)

For 1 to 4 years after treatment multiply listed factors by 0.7

For 4+ to 8 years use table 6

More than 8 years use table 7

For first 3 years use C values as listed

For 3+ to 8 years after treatment use table 6

More than 8 years after treatment use table 7

2.2.6 Support Practice Factor (P)

The P factor is the ratio of soil loss within a support practice like contouring, stripcropping, or terracing to that with straight-row farming up and down the slope.

The P factor is related to the C factor and to practices that can slow the runoff water. The most important of these supporting cropland practices are contour tillage, stripcropping on the contour and terrace systems.

Current recommendation for contouring are presented in table SW-16. Effects of contour stripcropping are shown in table SW-17. Terracing effects are presented in table SW-18.

Table SW-16

TABLE ~~11~~—P values and slope-length limits for contouring

Land slope percent	P value	Maximum length
		Feet
1 to 2	0 60	400
3 to 5	50	300
6 to 8	50	200
9 to 12	60	120
13 to 16	70	80
17 to 20	80	60
21 to 25	90	50

Limit may be increased by 25 percent if residue cover after crop seedlings will regularly exceed 50 percent

table SW-17

TABLE ~~14~~ P values maximum strip widths, and slope-length limits for contour stripcropping

Land slope percent	P values			Strip width	Maximum length
	A	B	C		
				Feet	Feet
1 to 2	0 30	0 45	0 60	130	800
3 to 5	25	38	50	100	600
6 to 8	25	38	50	100	400
9 to 12	30	45	60	80	240
13 to 16	35	52	70	80	160
17 to 20	40	60	80	60	120
21 to 25	45	68	90	50	100

P values

A For 4-year rotation of row crop small grain with meadow seeding and 2 years of meadow A second row crop can replace the small grain if meadow is established in it

B For 4-year rotation of 2 years row crop winter grain with meadow seeding and 1 year meadow

C For alternate strips of row crop and small grain

Adjust strip-width limit generally downward to accommodate widths of farm equipment

Table SW-18

TABLE ~~15~~—P values for contour-farmed terraced fields[1]

Land slope (percent)	Farm planning		Computing sediment yield[3]	
	Contour factor	Stripcrop factor	Graded channels sod outlets	Steep backslope underground outlets
1 to 2	0 60	0 30	0 12	0 05
3 to 8	50	25	10	05
9 to 12	60	30	12	05
13 to 16	70	35	14	05
17 to 20	80	40	16	06
21 to 25	90	45	18	06

Slope length is the horizontal terrace interval The listed values are for contour farming No additional contouring factor is used in the computation

Use these values for control of interterrace erosion within specified soil loss tolerances

These values include entrapment efficiency and are used for control of offsite sediment within limits and for estimating the field's contribution to watershed sediment yield

2.2.7 Sediment Delivery Factor (D)

The D factor is the ratio of the watershed sediment yield (SY) versus the upland erosion potential (A); D - SY/A.

Many factors and processes contribute to its estimation, such as redeposition of the particulates in the surface water runoff, storage, trapping of the sediment by vegetation and its residues, local scouring and redeposition in rills and channels, and possibly other yet unidentified. [Novotny, V., 1980.]

For D, the following formula has been proposed in the literature [Williams, 1975]:

$$D = e^{-bt(d_{50})^{1/2}} \qquad \text{(SW-7)}$$

where:

D = sediment delivery factor

b = decay constant (or routine coefficient)

t = travel time between two sections of a channel

d_{50} = mean particle diameter of sediment.

A graphical presentation of sediment delivery ratio as a function of the watershed size is shown in figure SW-5 [Roehl, 1972]. The statistical relationships relying on the morphological characteristics of the watershed have limited applicability for estimating long term (annual or more) deliveries. Furthermore, their reliability for "event" deliveries is almost nil as demonstrated by Berkowitz. [Berkowitz, 1979.] Another relation of D to the storm characteristics (EI) and the runoff volume (V) is shown in figure SW-6 [Berkowitz, 1979]. An interesting discussion regarding D is presented by Novotny. [Novotny, 1980.]

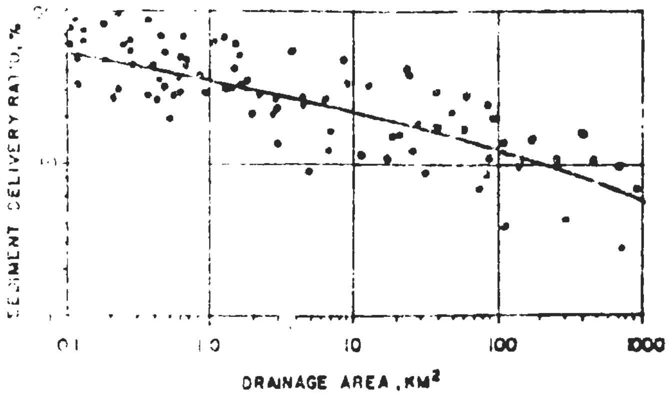


Figure Sw-5

~~Figure 1.~~ Delivery Ratio Relationship to the Watershed Size (from Roehl, 1962).

Figure sw-5 :

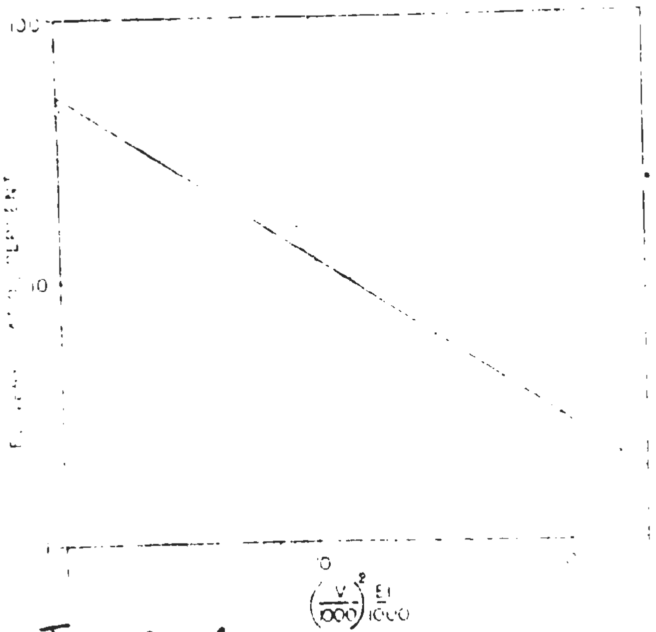


Figure Sw-6:

7. Relation of Sediment Delivery Ratio to Storm Characteristics. Data from [illegible], 1979

2.3 Subroutine SEDIMA

2.3.1 General

Subroutine SEDIMA (Sediment Annual) estimates the annual sediment washload of the soil compartment due to rain, based upon the USLE-theory previously outlined. It is "important" to keep in mind that all the sediment of the compartment will reach an adjacent receiver that has to be at a distance not exceeding 330 meters (1000 ft), as mandate by the assumption of the USLE. If the receiver happens to be at a greater distance, then it might be assumed that only the 330 m area will contribute sediment.

2.3.2 Input/Output Parameters

Input parameters and their associated units (metric system) for subroutine SEDIMA are:

R_m [cm/hr] = R x 10^{-2}; figure SW-1 for R index

K_m [t/ha/EI unit] = 1.292 K; figure SW-3 for K

$(LS)_m$ = LS ; figure SW-4 for LS

C_m = C ; see section 2.2.5 for C

P_m = P ; see section 2.2.6 for P

D_m = D ; see section 2.2.7 for D.

Output from SEDIMA is:

SYA [tons/ha]

2.3.3 Parameter Units

Metric equivalents were not included in the general procedures and tables presented in the original USLE documentation [Wischmeier and Smith, 1978]. Metric untis can then be selected so that each factor will have a counterpart whose values will be expressed in numbers that are easy to handle and to combine in computations.

It is recommended, however, by the USLE designers rather to converting into metric individual empirically derived parameters (especially R), to converting into metric the USLE as a whole. The overall converting formula (1 t/ha = 2.242 tons per acre) for the metric (m) system is:

$$SYA_m = 0.446\ SYA \qquad \text{(SW-8)}$$

A_m = t/ha/yr = 0.1 kg/m^2/yr

A = tons/acre as estimated by the USLE.

2.4 Numerical Example

Annual soil loss from a particular field area is estimated by LEVEL0 and LEVEL1 SESOIL operations by inputing the values of R, K, LS, C, P and D. These variables describe both the average climate of the area and the agricultural or field conditions, and can be obtained from the tables of the previous sections, as demonstrated by the following numerical example [see also Wischmeier and Smith, p.40].

Assume, for example, a field on Russell silt loam soil in the Topeka area, Kansas. The dominant slope is assumed 8% with a length of 200 ft. Fertility and crop management on this field are such that crop yields are rarely less than 85 bu corn, 40 bu wheat, or 4 t alfalfa-brome hay. The probability of meadow failure is slight.

The USLE equation factors are obtained as follows:

(1) Factor R is taken from the isoerodent map of figure SW-1. Topeka, Kansas, in north-east Kansas, lies between isoerodents 200 and 250. By linear (graphical) interpolation R = 205.

(2) Factor K can be obtained: (a) from a table (SW-1, SW-2) of K values derived either by direct research measurements, or (b) by use of the soil erodibility nomograph (figure SW-3). For the Russell silt loom soil, K=0.37 (figure SW-3).

(3) Factor LS is obtained from figure SW-4, the slope-effect chart, where an 8% slope along a 200 ft distance gives LS = 1.41.

If the field was continuously in clean tilled fallow and the delivery factor was assumed D = 1, the average annual soil loss from the dominant slope would equal (equation SW-8):

$$SYA = 0.446\ (205)(0.37)(1.41) = 47.69\ \text{t/ha/yr}$$

However, for the present agricultural area we need to account for the effects of the cropping and management system and support practices existing in the field, this effect being represented by factors C, P and D as follows:

(4) Factor C for the field may be: (a) either derived by the procedures described in the original USLE theory [Wischmeier and Smith, p. 28] using data of tables 5 and 6; or (b) obtained from centrally prepared C value tables available from the SCS (Soil Classification System). Let us assume for the present example that $C = 0.085$ [Wischmeier and Smith, p. 40].

(5) Factor $P = 1.0$, because rows and tillage are in the direction of the land slope. However, if farming were on the contour, the average P value would have been $P = 0.5$ (see section 2.2.6).

(6) Finally the sediment delivery factor can be assumed $D = 80\%$ (see section 2.2.7) without having any particular justification for its value in this illustrative example.

Thus, total annual sediment yield of the field is estimated to (equation SW-8)*

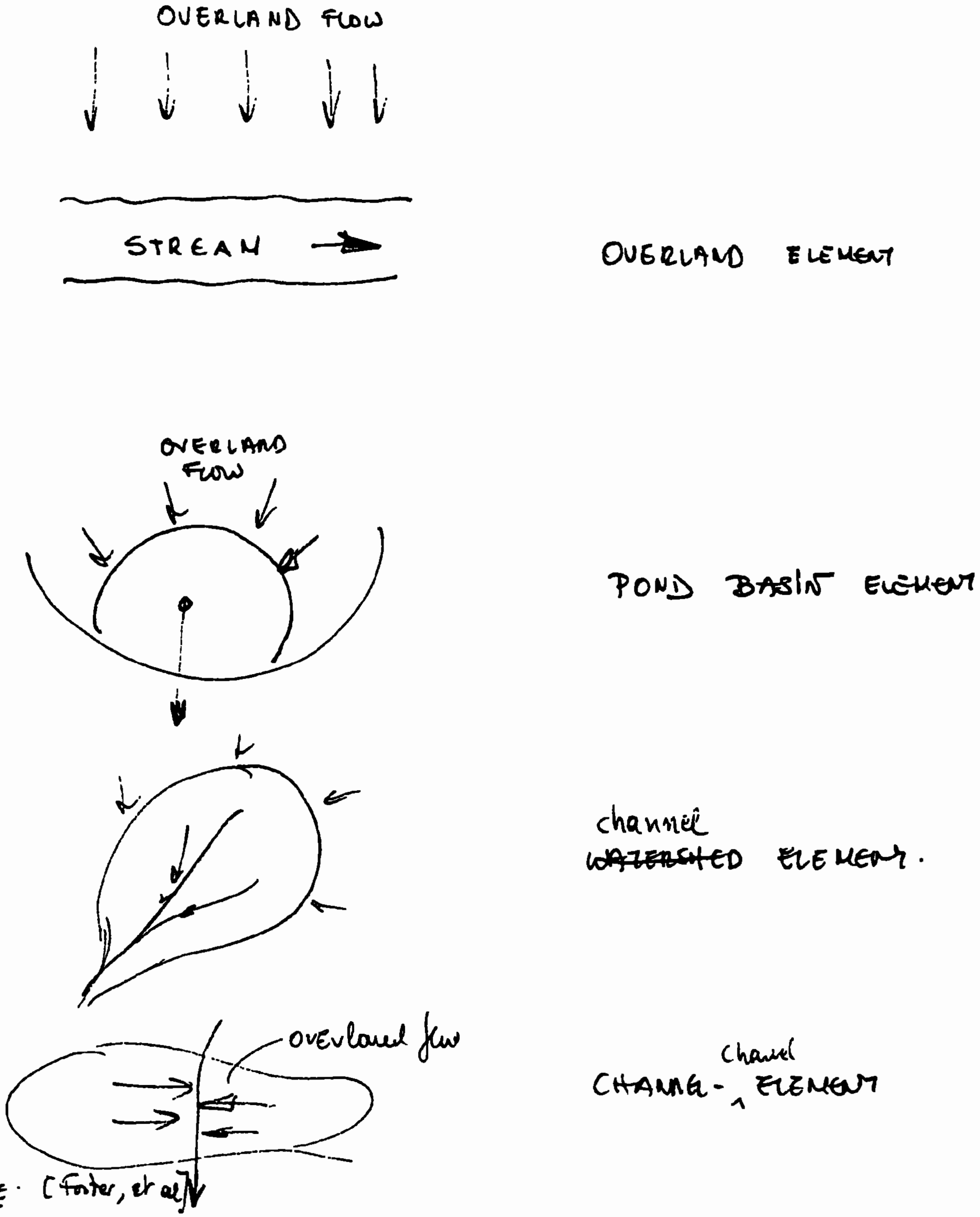
$$SYA = 0.446\ (205)(0.37)(1.41)(0.085)(1.0)(0.80) = 3.24\ \mathrm{t/ha/yr}$$

The USLE may also be used to compute the average soil loss for each crop in the rotation or for a particular cropstage period, during annual simulations. For such additional information regarding C, and P values, the reader is referred to the original work. [Wischmeier and Smith, p. 41.]

2.5 Discussion

The USLE is designed to predict longtime-average soil losses for specified conditions. Best predictions are "averaged-annual" losses from small watersheds, because the USLE factors are more difficult to evaluate for large mixed watersheds. Under "small" watersheds it is meant watersheds with adjacent receivers at a distance not exceeding 330 m (1000 ft), as shown in figure SW-7. For larger watershed simulations it can be assumed that only one portion of the watershed delivers sediment to the receiver, because upland erosion will be deposited within the watershed, thus, not contributing to the sediment yield of the basin. For large watersheds, factor D (delivery factor) becomes of paramount importance, and USLE predictions should be calibrated or validated with field data.

The USLE does not consider the basic processes of soil detachment, transport and deposition separately and does not account for various basin forms as schematically shown in figure SW-7. Therefore, above equation is employed only for LEVEL0 and LEVEL1 (annual simulation) of SESOIL. For more site specific, accurate and monthly sediment simulations, the user has to employ LEVEL2 of SESOIL, whose sediment routine is described in the following section.



Source · [Foster, et al]

Figure SW-7 . Typical field elements

3.0 "MONTHLY" WASHLOAD SIMULATIONS

3.1 OBJECTIVE

The objective of this section is to select and document the most appropriate sediment transport routine to meet the following criteria; the routine should: (1) represent the state-of-the-art, (2) be physically based and not require calibration, (3) be driven by a limited number of input parameters, (4) simulate sediment detachment, transport and deposition, (5) account for various basin shapes, (6) be applicable to an entire watershed and to discrete portions of the watershed as well, and (7) account for both long-term (monthly) and short-term (peaks within a month) simulations.

3.2 BACKGROUND/ACKNOWLEDGMENTS

Numerous factors and processes have been reported in the literature as providing statistically significant correlations to the attenuation of sediment and particulate pollutants from nonpoint sources. These factors include: (1) the effect of rainfall energy, that detaches the soil particles from small rills and keeps them in movement as long as the overland flow persists, (3) the effect of vegetation, that slows down the flow and filters out the particles during shallow flow conditions, (4) infiltration, which filters out the particles from the overland flow, (5) small depressions and surface roughnesses in which particles can settle due to reduction of velocity, and (6) change of slope of the overland flow. [Novotny, V.; 1980.]

The number of available sediment transport formulas in the literature is extremely large. Some of these formulas have not received extensive application, others are too complicated or require knowledge of the concentration of the suspended load and, therefore, have not been suitable for hydrologic simulations. A comprehensive analysis and evaluation of sediment transport theories have been conducted by Alonso [Alonso, C.V.; 1980] with reference to flume and silt data (Table SW-19).

Theories examined range from simplified formulas to sophisticated modeling packages accounting for the micromechanics of sediment movement. Following the testing of the formulas presented in Table SW-19, Foster, G.R. et al [1980] developed a model to estimate sediment yield from field-size areas. The model summarizes the state-of-the-art in erosion and sediment yield modeling with appropriate simplifications required to couple the governing equations.

SESOIL employs the sediment yield model as developed by Foster et al, however, adapted to the statistical needs of SESOIL for monthly yield and maximum yield of individual rainstorms within a month. Interested readers are advised to the original work of Foster. [Foster, G.R. et al; 1980, Knisel, W.G.; 1980], since the following sections have been mainly

TABLE SW-19. SUMMARY OF AVAILABLE SEDIMENT TRANSPORT FORMULAS

Type	Predicted load	Author(s) and reference	Date
Deterministic	Bed	DuBoys, (11)	1879
Deterministic	Bed	Schoklitsh, (26)	1934
Deterministic	Bed	Meyer-Peter, (22)	1934
Deterministic	Bed	Straub, (29)	1935
Deterministic	Bed	Waterways Experiment Station, (31)	1935
Deterministic	Bed	Shields, (28)	1936
Deterministic	Bed	Schoklitsh, (27)	1943
Deterministic	Bed	Kalinske, (19)	1947
Empirical	Total	Inglis, (18)	1947
Deterministic	Bed	Meyer-Peter and Muller, (23)	1948
Stochastic	Bed	Einstein, (13)	1950
Stochastic	Total	Einstein, (13)	1950
Stochastic	Bed	Einstein and Brown, (7)	1950
Stochastic	Total	Colby and Hembree, (10)	1955
Deterministic	Bed	Bagnold, (2)	1956
Deterministic	Total	Egiazaroff, (12)	1957
Deterministic	Total	Bogardi, (6)	1958
Deterministic	Total	Laursen, (21)	1958
Deterministic	Bed	Rottner, (25)	1959
Deterministic	Bed	Yalin, (37)	1963
Empirical	Total	Blench, (5)	1964
Stochastic	Total	Colby, (9)	1964
Stochastic	Total	Bishop, Simons and Richardson, (4)	1965
Deterministic	Total	Bagnold, (3)	1966
Stochastic	Total	Wilson, (36)	1966
Deterministic	Total	Chang, Simons and Richardson, (8)	1967
Deterministic	Total	Engelund and Hansen, (14)	1967
Deterministic	Total	Graf, (15)	1968
Deterministic	Total	Toffaleti, (30)	1968
Deterministic	Total	Ackers and White, (1)	1973
Deterministic	Total	Yang, (39)	1973

Source: [Alonso, C.V.; 1980]

"abstracted" from his work. The author of this section gratefully acknowledges the assistance received by Professor Foster (Agricultural Engineering Department, Purdue University, West Lafayette, Indiana 47907) while working out the adaptation for SESOIL of his sediment yield theory.

3.3 OVERVIEW OF THE MONTHLY WASHLOAD MODEL

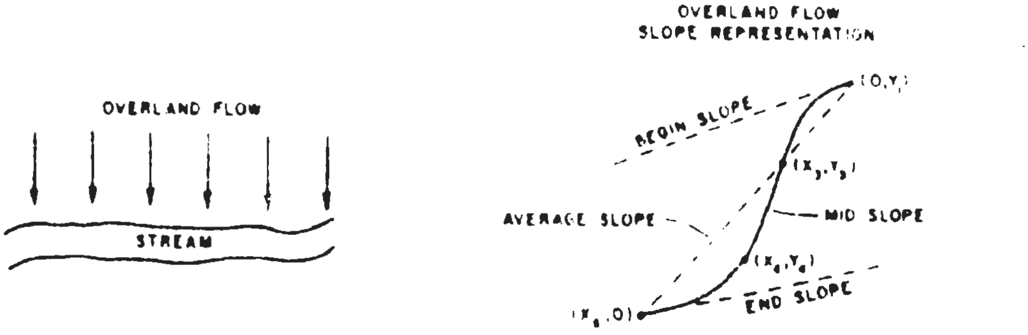
Erosion of soil particulates and their transport can be broken down into four processes [Foster and Meyer; 1972]: (1) detachment by rainfall, (2) detachment by overland flow, (3) transport by rainfall, and (4) transport by overland flow. On a given field, either detachment or sediment transport capacity may limit sediment yield depending on topography, soil characteristics, cover, and rainfall/runoff rate and amounts.

Control of sediment yield by detachment or transport can change from season to season, from storm to storm, and even within a storm. The relationship for detachment is different from the one for transport so that they cannot be lumped together into a single equation. Furthermore, the interrelation between detachment and transport is nonlinear and interactive for each storm, or each storm category, which prevents using separate equations to linearly accumulate the amount of detached sediment transport capacity over several storms. Therefore, to simulate erosion and sediment yield and to satisfy the need for a continuous simulation model, a rather fundamental approach was selected by Foster et al [1980] where separate equations are used for soil detachment and sediment transport.

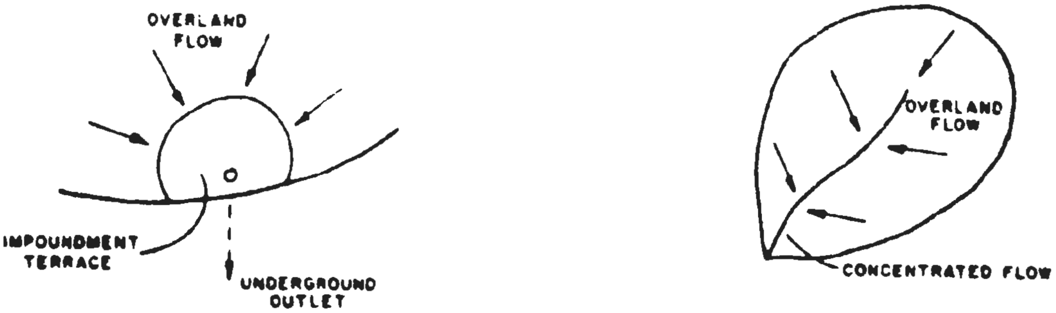
Every model is a representation and a simplification of a real environmental situation. Various techniques, including plains and channels, square grids, converging sections, and stream cubes have been used to represent subsections of an area. [Foster et al; 1980.] Most erosion/sediment yield models have adequate degrees of freedom to fit observed data. Some models, depending on their representation scheme, distort parameter values more than others do. Distortion of parameter values greatly reduces the transfer ability of parameter values from one area to another. An objective, therefore, in Foster's model, was the development of a theory representing the field in a way minimizing parameter distortion. In addition, a minimum number of input parameters have to be compiled by the user, the simulation being performed with the aid of theoretically derived equations rather than the employment of massive input data sets and calibration coefficients to account for the processes previously described.

Regarding the possible shape of elements and the calling sequence used to represent field-size areas, Foster et al distinguish between overland flow, channel flow, and impoundment (pond) elements as shown in Figure SW-8.

The model user selects the best combination of elements and enters the appropriate sequence number according to Table SW-20. Computation starts in the uppermost element, which is always an overland flow element and proceeds downslope. Sediment concentration (for each particle type) is the output from each element which becomes the input to the next element in the sequence.

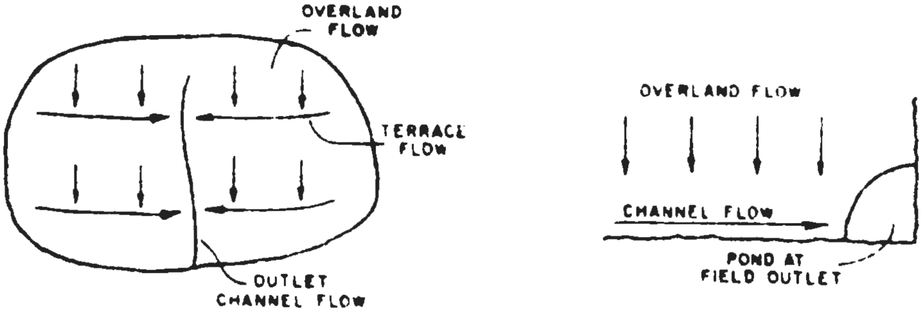


(1) OVERLAND FLOW
SEQUENCE AND SLOPE REPRESENTATION



(2) OVERLAND FLOW
POND SEQUENCE

(3) OVERLAND FLOW
CHANNEL SEQUENCE



(4) OVERLAND FLOW
CHANNEL-CHANNEL SEQUENCE

(5) OVERLAND FLOW
CHANNEL-POND SEQUENCE

Source: [Foster, G.R. et al; 1980]

FIGURE SW-8. SCHEMATIC REPRESENTATION OF TYPICAL FIELD SYSTEMS IN THE FIELD-SCALE EROSION/SEDIMENT YIELD MODEL

TABLE SW-20. POSSIBLE ELEMENTS AND THEIR CALLING SEQUENCE USED TO REPRESENT FIELD-SIZED AREA

Sequence number	Elements and their sequence
1	Overland
2	Overland-Pond
3	Overland-Channel
4	Overland-Channel-Channel
5	Overland-Channel-Pond
6	Overland-Channel-Channel-Pond

Source: [Foster, G.R. _et al_; 1980]

3.4 MODEL MATHEMATICS

3.4.1 Basic Concepts and Equations

Sediment load is a function of the sediment quantity available: (1) after detachment by precipitation energy, and (2) by the transport capacity of overland flow. Quasi-steady state conditions can be assumed, so that a single rainfall and runoff rate characteristics of each storm (or storm series) can be used in computational procedures. [Foster and Meier; 1975.] The major sequence of computation is shown in Figure SW-9.

Sediment transport downslope of an area can be described with the steady state equation of sediment mass continuity [Foster, G.R. et al; 1980]:

$$dq_s/dx = D_L + D_F \qquad \text{(SW-10)}$$

where:

q_s = sediment load per unit width per unit time

x = distance (location)

D_L = lateral sediment inflow (mass/unit area/unit time)

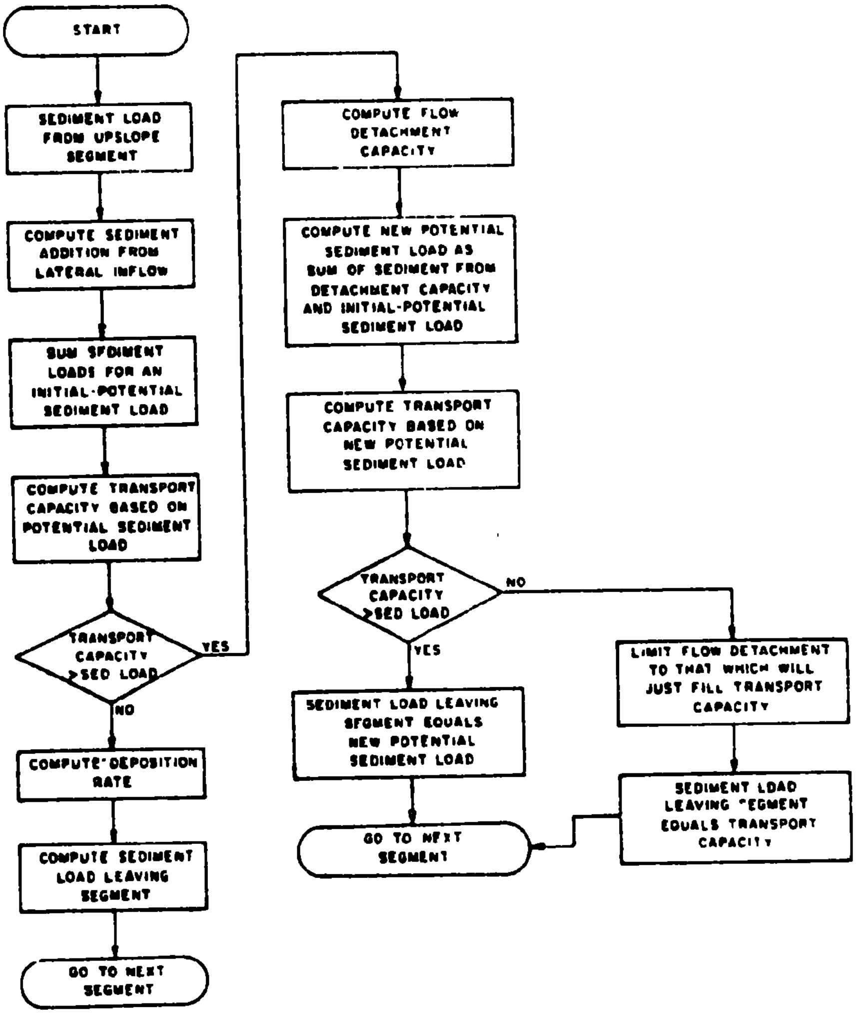
D_F = sediment detachment or deposition by overland flow (mass/unit area/unit time)

Lateral sediment inflow to a watershed segment may originate from interill erosion on overland flow elements, or from overland flow (or a channel, if two channel segments are in a sequence) for the channel elements. Flow in rills on overland flow areas or in channels, transports the sediment load downslope. Lateral sediment inflow can be independently assumed of whether the flow is detaching or depositing.

During simulations of a watershed segment (overland flow element or in a channel), the initial "potential sediment load" is estimated. This load equals the sum of the sediment load from the: (1) immediate upslope segment and (2) the lateral inflow. If:

(1) the initial potential sediment load is less than the "transport capacity" of the overland flow, detachment takes place at a rate: "equal or less" the detachment capacity of the flow. When this detachment takes place, it adds particles having the particle size distribution for detached sediments. No sorting is assumed to take place during detachment;

(2) the initial potential sediment load is greater than the transport capacity of the overland flow, deposition is assumed to take place.



Source: Foster, G.R. et al; 1980]

FIGURE SW-9. FLOW CHART FOR DETACHMENT-TRANSPORT-DEPOSITION COMPUTATIONS WITHIN A SEGMENT OF OVERLAND FLOW OR CONCENTRATED FLOW ELEMENTS

Sediment deposition within a segment is described in the simulation by:

$$D = \alpha(T_c - q_s) \quad , \text{ and} \qquad \text{(SW-11)}$$

$$\alpha = \varepsilon V_s / q_w$$

where:

D = sediment deposition rate (mass/unit area/unit time)

α = first order reaction coefficient (length^{-1})

T_c = transport capacity (mass/unit width/unit time)

ε = 0.5 for overland flow, and
1.0 for channel flow

V_s = soil particle fall velocity

$q_w = q_L \cdot x$; discharge rate of runoff per unit width (volume/width/time).

Sediment detachment and deposition by flow is simulated in a segment in four independent cases (processes):

(1) deposition over the entire segment

(2) detachment in the upper boundary and deposition in the lower boundary of the segment

(3) deposition on the upper end and detachment in the lower end of the segment

(4) detachment all along the segment.

Above cases are described mathematically [Foster, G.R. *et al*; 1981] as follows:

Case (1): takes place when:

$$T_c < q_s \quad \text{all along the segment} \qquad \text{(SW-12)}$$

where:

$$D = [\phi/(1+\phi)]\ (dT_c/dx - D_L)[1-(x_u/x)^{1+\phi}] + D_u(x_u/x)^{1+\phi}$$

$$\phi = \varepsilon V_s / q_L$$

$$dT_c/dx = \text{constant over segment} \qquad \text{(SW-13)}$$

$$D_u = \alpha(T_{cu} - q_{su})$$

$$q_s = T_c - (D/\alpha)$$

in which:

T_c = transport capacity

q_s = sediment load at distance x

D = deposition rate

ϕ = depositing coefficient

V_s = soil particle fall velocity

q_L = discharge rate

D_L = lateral sediment inflow

x_u = distance (location)

D_u = deposition rate at x_u

T_{cu} = transport capacity at x_u

q_{su} = sediment load at x_u

α = first order reaction coefficient

Case (2) takes place when:

$T_c < q_s$ within the segment

$T_{cu} > q_{su}$ and (SW-14)

$dT_c/dx < 0$

If $dT_c/dx < 0$ for a segment where $T_{cu} > q_{su}$, T_c may decrease below q_s within the segment. The point location where $q_s = T_c$ is determined (defined) as x_{db} (x_u in equation SW-13), with $D_u = 0$. Deposition and sediment load are estimated from equations SW-13.1, SW-13.2 and SW-13.5 (equations group SW-13).

Case (3) takes place when:

$T_c > q_s$ within the segment

$T_{cu} < q_{su}$ and (SW-14)

$dT_c/dx > 0$

At a point (location) x_{de} "deposition" may end. In this case $D_u = 0$, $T_c = q_s$. Downslope, detachment and "sediment load" take place.

Deposition ends at:

$$x_{de} = x_u \left\{ 1 - [(1+\phi)/\phi][D_u/(dT_c/\partial x - D_L)] \right\}^{1/(1+\phi)} \quad \text{(SW-15)}$$

Sediment load is given by:

$$q_s = (D_{Fu} + D_{Lu} + D_{FL} + D_{LL})\ \Delta x/2 + q_{su} \quad \text{(SW-16)}$$

where:

x_{de} = location where deposition ends

x_u = distance

ϕ = deposition coefficient

D_u = deposition rate at x_u ; see equation (SW-13.4)

T_c = transport capacity

D_L = lateral sediment inflow

q_s = sediment load

u,L = segment subscripts; u = upper, L = lower

D_F = D_{Fu}, D_{FL} ; sediment detachment or deposition

D_L = D_{Lu}, D_{LL} ; lateral sediment inflow

Δx = length of segment where detachment occurs

q_{su} = sediment load from upper segment

in which:

Δx is from x_{de} to the lower end of segment

q_{su} is at x_{de}, which is T_c at x_{de} ; ie $q_{su}(x_{de}) = T_c$

<u>Case (4)</u> takes place when:

$T_c > q_s$ over the entire segment.

Sediment load is estimated with equation SW-16.

3.4.2 Modeling Issues

Eroded sediment is a mixture of particles having various sizes and densities. Simulations are performed for each particle type.

Equations describing: (a) sediment characteristics, (b) flow detachment capacity, (c) rainfall erosivity, (d) effects of overland slope, (e) sediment transport capacity, and (f) other parameters are presented [Foster, G.R.; 1980] in the following sections for the:

(1) overland flow element
(2) channel element
(3) impoundment element

The following four sections describe sedimentation characteristic issues, and issues relating to the modeling of the three elements; overland, channel and impoundment.

3.4.3 Sediment Characteristics

Eroded sediment is a mixture of primary particles and aggregates of various sizes. Size distribution is either an input to the model, or can be estimated by the model analytically if distribution is not given. In the latter case the model assumes 5 particle size distributors derived from surveys of existing data as described in the following paragraph.

Typical sediment characteristics assumed for detached sediment before disposition, typical for midwestern silt loam soil are presented in Table SW-21. Equations employed to estimate particle size distributions are presented in Table SW-22. Particle sizes assumed to derive the equations for the particle size distributions are presented in Table SW-23. Primary particle composition of the sediment load is estimated for small and large aggregates with the equations presented in Table SW-24.

TABLE SW-21. SEDIMENT CHARACTERISTICS ASSUMED FOR DETACHED SEDIMENT BEFORE DEPOSITION; ASSUMED TYPICAL OF MANY MIDWESTERN SILT LOAM SOILS

Particle Type	Diameter (mm)	Specific Gravity (g/cm^3)	Fraction of Total Amount (mass basis)
Primary clay	0.[illegible]2	2.60	0.05
Primary silt	.010	2.65	.08
Small aggregate	.030	1.80	.50
Large aggregate	.500	1.60	.31
Primary sand	.200	2.65	.06

Source: [Foster, *et al.*; 1980]

TABLE SW-22. EQUATIONS EMPLOYED TO DESCRIBE PARTICLE SIZE DISTRIBUTION

$$PSA = (1.0 - ORCL)^{2.49}\ ORSA$$

$$PSI = 0.13\ ORSI$$

$$PCL = 0.2\ ORCL \qquad \text{(SW-14)}$$

$$SAG = \begin{cases} 2\ ORCL & ORCL < 0.25 \\ 0.28(ORCL - 0.25) + 0.5 & 0.25 \leq ORCL \leq 0.50 \\ 0.57 & 0.5 < ORCL \end{cases}$$

$$LAG = 1.0 - PSA - PSI - PCL - SAG$$

where:

ORCL, ORSI, ORSA: Fractions for primary clay, silt, sand in the original soil mass

PCL, PSI, PSA, SAG, LAG: Fractions for primary clay, silt, sand, small and large aggregates in the detached sediment

$LAG \geq 0.0$: In case $LAG < 0.0$ multiply all other parameters with a coefficient to make $LAG = 0.0$

Source: [Foster, et al.; 1980]

TABLE SW-23. ASSUMED TYPICAL DIAMETERS OF PARTICLE SIZES

$$
\begin{aligned}
\mathrm{DPCL} &= 0.002 \text{ mm} \\
\mathrm{DPSI} &= 0.010 \text{ mm} \\
\mathrm{DPSA} &= 0.20 \text{ mm} \\
\mathrm{DSAG} &= \begin{cases} 0.03 \text{ mm} & \mathrm{ORCL} < 0.25 \\ 0.20(\mathrm{ORCL} - 0.25) + 0.03 \text{ mm} & 0.25 \leq \mathrm{ORCL} \leq 0.60 \\ 0.1 \text{ mm} & 0.60 < \mathrm{ORCL} \end{cases} \\
\mathrm{DLAG} &= 2(\mathrm{ORCL}) \text{ mm}
\end{aligned}
\tag{SW-15}
$$

where DPCL, DPSI, DPSA, DSAG, and DLAG are, respectively, the diameters of the primary clay, silt, and sand, and the small and large aggregates in sediment. The assumed specific gravities are shown in Table SW-21.

Source: [Foster, G.R. et al; 1980]

TABLE SW-24. EQUATIONS EMPLOYED FOR PARTICLE COMPOSITION OF SEDIMENT LOAD*

Small aggregates:

$$CLSAG = SAG \cdot ORCL/(ORCL + ORSI)$$

$$SISAG = SAG \cdot ORSI/(ORCL + ORSI) \qquad (SW\text{-}16)$$

$$SASAG = 0.0$$

Large aggregates:**

$$CLLAG = ORCL - PCL - CLSAG$$

$$SILAG = ORSI - PSI - SIAG \qquad (SW\text{-}17)$$

$$SALAG = ORSA - PSA$$

where CLSAG, SISAG, and SASAG = gractions of the total for the sediment of, respectively, primary clay, silt, and sand in the small aggregates in the sediment load, and CLLAG, SILAG, and SALAG are corresponding fractions for the large aggregates.

---

*The text of this table was "quoted" from Foster, G.R, *et al*. [1980].

**If the clay in the large aggregate expressed as a fraction for that particle alone is less than 0.5 times ORCL, the distribution of the particle types is recomputed so that this constraint can be met. A sum, SUMPRI, is computed whereby:

$$SUMPRI = PCL + PSI + PSA.$$

The fractions PSA, PSI, and PCL are not changed. The new SAG is:

$$SAG = (0.3 + 0.5\ SUMPRI)(ORCL + ORSI)/[1 - 0.5\ (ORCL + ORSI)].$$

Above equation is derived given previously determined values for PCL, PSI, and PSA; the sum of primary clay fractions for the total sediment equals the clay fraction in the original soil, and the assumption that the fraction of primary clay in LAG equals half of the primary clay in the original soil.

The model also computes an enrichment ratio using specific surface areas for organic matter, clay, silt, and sand. Organic matter is distributed among the particle types based on the proportion of primary clay in each type. Enrichment ratio is the ratio of the total specific surface area for the sediment to that for the original soil.

Although these relationships are approximations to the data found in the literature (Young, R.A.; 1978), they represent the general trends.

3.4.4 Overland Flow Element

Detachment on interrill and rill areas and transport and deposition by rill flow are the erosion-transport processes on the overland flow element. Detachment equations are presented in Table SW-25 (Equation 18.1 and 18.2). Mathematical expressions for the storm erosivity (EI) and slope length exponent (m) of above equations are also presented in Table SW-25 (Equation 18.3 through 18.4).

Sediment transport capacity is described by the Yalin equation [Yalin, S.; 1963]; however, it has been modified by Foster and Meyer [1972] to account for various particle sizes and types. All equations employed are presented in Table SW-26. Foster, G.R., et al. [1980], presented six computational steps to redistribute the transport capacity when excess and deficits of sediment occur.

Regarding the computational procedure the authors [Foster, et al.; 1980] established a sequential simulation starting with the upper end of a slope and routing sediment downslope, as in most discretized sediment models. Computations take place for each particle size type. Concentration multiplied by the runoff volume and overland flow area represented by the overland flow profile gives the sediment yield for the stone on the overland area of the field.

The overland flow is represented by a typical land profile selected from possible overland flow paths. Its shape may be uniform, convex, concave, or a combination of these shapes. Inputs are total slope length, average steepness, the slope at the upper end of the profile, the slope at the lower end of the profile and location of end points of a miduniform section.

Given the above information, the model establishes segments along the profile. The procedure is illustrated by the convex shape shown in Figure SW-10. Coordinates of points A, C, and D are given, as are slopes S_b and S_m. A quadratic curve will pass through point C tangent to the line CD and through point E tangent to line AB. The location of point E is the intersection of a line having a slope equal to the average of S_b and S_m with line AB. If x_2 is less than x_1, x_3 is shifted downslope so that $x_1 = x_2$. [Foster, et al.; 1980].

TABLE SW-25. OVERLAND FLOW ELEMENT EQUATIONS (Equation category SW-18; for notation see next page)

$$D_{Li} = 4.57\,(EI)(s + 0.014)\,KCP\;\sigma_p/V_u \qquad \text{(SW-18.1)}$$

$$D_{Fr} = (6.86 \times 10^6)\,m\;V_u\sigma_p^{1/3}\left(x/22.1\right)^{m-1}s^2KCP\left(\sigma_p/V_u\right) \qquad \text{(SW-18.2)}$$

where:

$$EI \begin{cases} = 0.103\;V_R^{1.51} & \text{or} \\ = 0.0276\;V_R I & \text{or} \\ = e = 11.9 + 8.73\left(\log_{10} i\right) & \text{(if hyetograph is available)} \end{cases} \qquad \text{(SW-18.3)}$$

$$m \begin{cases} = 1.0 + 3.912/\ln(x); & x > 50\text{m} \\ = 2 & ;\; x \leq 50\text{m} \end{cases} \qquad \text{(SW-18.4)}$$

where:

D_{Li} = interrill detachment rate ($g/m^2/s$)

D_{Fr} = rill detachment capacity rate ($g/m^2/s$)

EI = EI_{30} = Wischmeier's rainfall erosivity (N/h) expressed as total rainstorm energy (E) times 30-minute (I_{30}) intensity[1/]

m = slope length exponent (-)

s = sine of slope angle

K = USLE soil erodibility factor (gh/Nm^2)[2/]

TABLE SW-25. OVERLAND FLOW ELEMENT EQUATIONS (Continued)

C = soil loss ratio of the USLE cover-management factor

P = USLE contouring factor[3]

σ_p = peak runoff rate expressed as volume/area/time (m/s)

V_u = runoff volume/area (m)

x = distance downslope (m)

V_R = volume of rainfall (mm)[4]

I = maximum 30-minute intensity (mm/h)

e = rainfall energy per unit of rainfall (J/m^2/mm of rain)[5]

i = rainfall intensity (mm/h)

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[1] EI[English]*1.702 = EI[metric; N/h]

[2] Units of K must be carefully noted. K[English]*131.7 = K[metric; gh/Nm^2]

[3] Only the contouring part of P is used.

[4] Equation SW-18.3a was derived from 2700 data points (r^2=0.56)

[5] EI≃e [Foster, *et al*.; 1980]

Source: [Foster, G.R. et al; 1980]

TABLE SW-26. DIMENSIONLESS SEDIMENT TRANSPORT CAPACITY EQUATION OF S. YALIN [1963] (SESOIL Equation Category SW-19; For notations, see next page)

Single Particle Equation:

$$P_s = \frac{W_s}{(S_g)g\rho_w dV_*} = 0.635\ \delta[1 - \frac{1}{\sigma}\ln(1 + \sigma)] = P_s$$

where:

$$\sigma = \delta A$$

$$\delta = \frac{Y}{Y_{cr}} - 1 \text{ (when } Y < Y_{cr},\ \delta = 0)$$

(SW-19)

$$A = 2.45(S_g)^{-0.4}(Y_{cr})^{1/2}$$

$$Y = \frac{V^2_*}{(S_g - 1.0)\ gd}$$

$$V_* = (gRS_f)^{1/2}$$

Modified Multiparticle Supporting Equations:

- $T = \sum_{i=1}^{n_s} \delta_i$

(SW-20)

- $(N_e)_i = N_i\ (\delta_i/T)$
- $(P_e)_i = P_i\delta_i/T$
- $(W_{si}) = (P_e)_i\ (S_g)_i\rho_w g d_i V_*$

where:

$$\tau_{soil} = \gamma y s(n_{bov}/n_{cov})^{0.9}$$

$$y = \left[q_w n_{bov}/s^{0.5}\right]^{0.6}$$

TABLE SW-26. DIMENSIONLESS SEDIMENT TRANSPORT CAPACITY EQUATION OF S. YALIN [1963] (Continued)

where:

P_s = nondimensional transport

W_s = transport capacity (mass/unit time/unit flow width)

S_g = particle specific gravity

g = acceleration due to gravity ($g=9.81$ m/sec^2)

ρ_w = mass density of fluid (water)

V_* = sheer velocity = $(\tau/\rho_w)^{1/2}$

τ = sheer stress

0.635 = constant from Shield's diagram

σ, A, δ = defined dimensionless expressions

Y = actual lift force given by Yalin

Y_{cr} = critical lift force given by Shield's diagram as a function of the particle Reynolds number

d = particle diameter

R = hydraulic radius

S_f = slope of energy gradeline

i = sediment particle type

T = total value of δ's in the mixture

n_s = number of particle types in the mixture

$(Ne)_i$ = number of transported particles of type i in a mixture

N_i = number of particles transported in sediment of uniform type i for a δ_i.

$(Pe)_i$ = effective P for particle type i in a mixture

$(Ps)_i$ = the P_s calculated for uniform material i

$(W_s)_i$ = transport capacity of each particle type in a mixture

τ_{soil} = sheer stress acting on soil

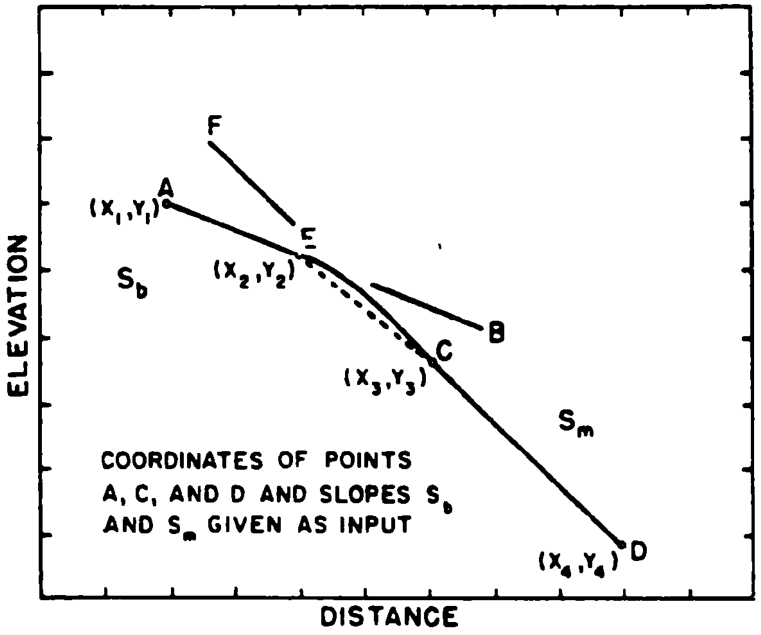
γ = weight density of water

y = flow depth for bare smooth soil

n_{bov} = Manning's coefficient (n) for bare soil; =0.01 for overland flow; =0.03 for channel flow

n_{cor} = total Manning's (n) for rough surfaces or soil covered by mulch or vegetation

q_w = discharge rate per unit width



Source: [Foster, et al.; 1980]

FIGURE SW-10. SCHEMATIC REPRESENTATION OF CONVEX SLOPE PROFILE FOR OVERLAND FLOW

3.4.5 Channel Element

The channel element (Figure SW-8) is used to represent flow in terrace channels, diversions, major flow concentrations whose topography has caused overland flow to converge, grass waterways, row middles or graded rows, etc. This element does not describe gully or large channel erosion [Foster, G.R.; et al; 1980].

The spatially varied flow equation of the channel element is given in Table SW-27. Equation system (SW-21) is solved for a range of typical values C_1, C_2, C_3 for subcritical flow, and regression curves are derived for the components of the normalized friction slope of the channels (SSF). Curves are fitted to the solutions in order to reduce computation time.

The equation for: (1) the detachment capacity (D_{Fc}) by flow over a loosely tilled seedbed; (2) the erosion rate in the channel (E_{ch}); (3) the width of the channel (W) at any time after the channel has eroded to the nonerodible layer; (4) the final width of the channel (W_f); (5) the hydraulic radius due to soil (R_{soil}); (6) the shear stress acting in the soil (τ_{soil}); and (7) the shear stress acting on the soil cover (τ_{cov}) are given in Table SW-28 (equations SW-22 to SW-28).

TABLE SW-27

SPATIALLY VARIED FLOW EQUATION; CHANNEL ELEMENT

$$dy_*/dx_* = [S_* - C_2\ x_*^{2}/y_*^{16/3} - C_3\ x_*/y_*^{4}]/[1 - C_3\ x_*^{2}/y_*^{5}]$$

$$C_1 = [Z^{5/2}/2(Z^2+1)^{1/2}]^{2/3}$$

$$C_2 = [Q_e\ n\ L_{eff}/C_1 y_e^{19/6}]^2 \tag{SW-21}$$

$$C_3 = 2\ \beta\ Q_e^{2}/g\ z^2\ y_e^{5}$$

where:

$y = y/y_e$

y = flow depth

y_e = flow depth at the end of the channel

$S_* = sL_{eff}/y_e$

s = channel slope

x = distance along channel

$x_* = x/L_{eff}$

L_{eff} = effective channel length (i.e., the length of the channel if it is extended upslope to where discharge would be zero with the given lateral inflow rate

C_1, C_2, C_3 = constants

m = Manning coefficient

z = side slope of channel

Q_c = discharge at end of channel

β = energy coefficient (app. 1.56)

g = 9.81 m/sec^2; acceleration of gravity

TABLE SW-28

OTHER EQUATIONS DESCRIBING SEDIMENT TRANSPORT

$$D_{Fc} = K_{ch} (1.35 \bar{\tau} - \tau_{cr})^{1.05} \qquad \text{(SW-22)}$$

$$E_{ch} = W_{ac} K_{ch} (1.35 \bar{\tau} - \tau_{cr})^{1.05} \qquad \text{(SW-23)}$$

$$(dW/dt)_i = 2 k_{ch} (\tau_b - \tau_{cr})^{1.05}/\rho_{soil} \qquad \text{(SW-24)}$$

$$W_f = [Qn/S_f^{1/2}]^{3/8} [(1 - 2 x_{cf})/ x_{cf}^{5/3}] \qquad \text{(SW-25)}$$

$$R_{soil} = (Vn_{bch}/S_f^{1/2})^{3/2} \qquad \text{(SW-26)}$$

$$\tau_{soil} = \gamma R_{soil} S_f \qquad \text{(SW-27)}$$

$$\tau_{cov} = \gamma [V(n_t - n_{bch}) S_f^{1/2}]^{3/2} \qquad \text{(SW-28)}$$

where:

D_{Fc} = rate of sediment detachment by flow in channel (mass/area/time; i.e., $kg/m^2/s$)

K_{ch} = soil erodibility factor of the USLE $(m^2/N)^{1.05}(kg/m^2/s)]$

$\bar{\tau}$ = average shear stress (N/m^2) of the flow in the channel.

τ_{cr} = critical shear stress (N/m^2) below which erosion is negligible.

E_{ch} = rate of soil loss per unit channel length (mass/unit/channel length/unit time)

W_{ac} = width of an eroding channel at equilibrium

W_i = width at time $t=t_i$

W = width at time t

$(dW/dt)_i$ = rate that channel widens at $t=t_i$

TABLE SW-28 (Continued)

τ_b = shear stress in a channel at a nonerodible boundary

ρ_{soil} = man density of soil

W_f = final channel width

Q = discharge rate (m^3/s)

n = Manning friction coefficient

S_f = Friction slope for flow hydraulics in a channel

x_{cf} = Normalized distance around wetted perimeter where $\tau=\tau_{cr}$ at nonerodible boundary

R_{soil} = hydraulic radius due to soil

τ_{cov} = shear stress at which the cover starts to move

n_t = total Manning coefficient

n_{bch} = Manning coefficient for a base channel.

3.4.6 Impoundment (Pond) Element

The impoundment or pond element (Figure SW-8) describes deposition behind impoundments (including parallel tile outlet terraces) that drain after each storm. The pond element (receiver) is the last element of an element series.

The equations for: (1) the sediment fraction (F_{pi}) deposed in an impoundment and (2) the runoff volume (V_{out}) out of an impoundment are presented in Table SW-29.

3.4.7 Discussion

Discussion regarding use of the model will be presented later.

TABLE SW-29

SUPPORTING EQUATIONS; IMPOUNDMENT ELEMENT

$$F_{pi} = A_1[\exp(B_1 d_u) - \exp(B_1 d_1)]/(B\,\Delta d) \qquad \text{(SW-29)}$$

$$V_{out} = 0.95\ V_{in} \exp\ (Z_r) \qquad \text{(SW-39)}$$

where:

$A_1 = 1.136 \exp\ (Z_s)$

$B_1 = -0.152 \exp\ (Y_s)$

$Z_s = Z_s\ (f_a, C_{or}, V_{ro}, I_p)$

$Y_s = Y_s\ (f_a, C_{or}, V_{ro}, I_p)$

$C_{or} = 0.15\ d_{or}^2 \cong (7.02 \times 10^4)\ Q_p/y_d^{1/2}$

$Z_r = Z_r\ (f_a, C_{or}, V_{ro}, I_p)$

in which:

F_{pi} = fraction passed for particle i

A_1, B_1 = coefficients

d_u = equivalent sand diameter of upper end of a sediment particle class; (mm)

d_1 = equivalent sand diameter of lower end of a sediment particle class: (mm)

Δd = width of a particle class; (mm)

V_{out} = volume of runoff discharged (out of impoundment); (m^3/storm)

V_{in} = runoff volume into impoundment; (m^3/storm)

Z_r = exponent in equation for runoff reduction by an impoundment; (-)

Z_s = exponent in equation for deposition in an impoundment; (-)

Y_s = exponent in deposition equation of an impoundment; (-)

f_a = coefficient in surface area-depth relationship for impoundment

V_{ro} = runoff/volume (m^3/storms)

3.5 Subroutine SEDIMM

- 3.5.1 General
- 3.5.2 Input/Output Parameters
- 3.5.3 Data Files
- 3.5.4 Discussion

3.6 Sensitivity Analysis of SEDIMM

- 3.6.1 General
- 3.6.2 Hydrologic Parameters
- 3.6.3 Sediment Yield Parameters
- 3.6.4 Discussion

3.7 Conclusions

Sections 3.5 and 3.6 will be presented in the draft report of this contract. Section 3.7 will be presented at a later time.

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SR - soil resuspension

APPENDIX SR

SOIL RESUSPENSION*

TABLE

FIGURES

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*Contribution from Diane Gilbert.

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1.0 INTRODUCTION

The transport by wind of ground surface particles is called soil resuspension or wind erosion. In many geographical areas the amount of material (fugitive dust) involved is significant; therefore, sediment associated pollutant load entrained by the air can also be significant. "Fugitive dust processes" involve mechanical disturbances on the ground surface causing atmospheric pollution dishcarges. The physics of soil resuspension are complex, with several dependent variables.

This appendix is not intended to thoroughly describe the fugitive dust (soil resuspension) mechanics; rather it provides generalized background information on the nature of the process, the assumptions made for the mathematical modeling developed, and examples of the soil-resuspension routine of SESOIL. Alternative modeling approaches are possible. This routine is not operational in the 1981 version of SESOIL; therefore no special attention is given to the drafting of this appendix. However, in case of interest, a potential model user should contact the SESOIL model developer (Dr. M. Bonazountas, (617) 864-5770 x5871), since coding of this routine is a minor task.

2.0 MATHEMATICAL MODELING

2.1 General

The Soil Resuspension model (SR) estimates the amount of soil lost from the surface layer due to wind erosion. The amount of pollutant carried with the resuspended particles is proportional to the soil loss and the concentration of adsorbed pollutant on soil particles. Depending upon data availability, or the desired degree of accuracy, the model output provides estimates of: (1) the monthly soil loss, (2) the average annual loss, or (3) the annual loss as the sum of monthly losses.

Figure SR-1 shows the overall module structure of SESOIL. The module accounts internally for a check for average wind speeds below a "critical velocity" and passes on to the next time step if the critical condition is not met. A similar check is carried out for frozen or snow-covered ground conditions; this check is carried out differently for the annual as opposed to monthly time step analysis.

2.2 Mathematical Approach

Soil resuspension has been described and analyzed by Chepil and Woodruff (1963), Woodruff and Siddoway (1965) and Evans and Cooper (1980) among others. This subroutine is based primarily on the work of Chepil, Woodruff, and Siddoway in the development of an erosion equation and upon the work of Evans and Cooper in application of the equation to estimate particulate emissions from various open sources.

The amount of soil eroded by wind, E, as estimated by Chepil and Woodruff (1963) is:

$$E = f(I, K, C, L, V) \qquad \text{(SR-1)}$$

The variables are:

- I: soil erodibility index (tons/acre/season)
  This parameter is based upon the percentage of soil fractions larger than 0.84 mm (A) as determined by dry sieving.

  The value for I, as used in equation SR-1, however, is given in tons/acre/month (or year). For flat sites, values of I are provided in Table SR-1 for various soil types covering the range of particle sizes.

- K: soil ridge roughness factor
  K is approximated from the soil ridge height (in inches) using Figure SR-2 or Equation SR-2.

$$K = ah^2 + bh + 1 \qquad \text{(SR-2)}$$

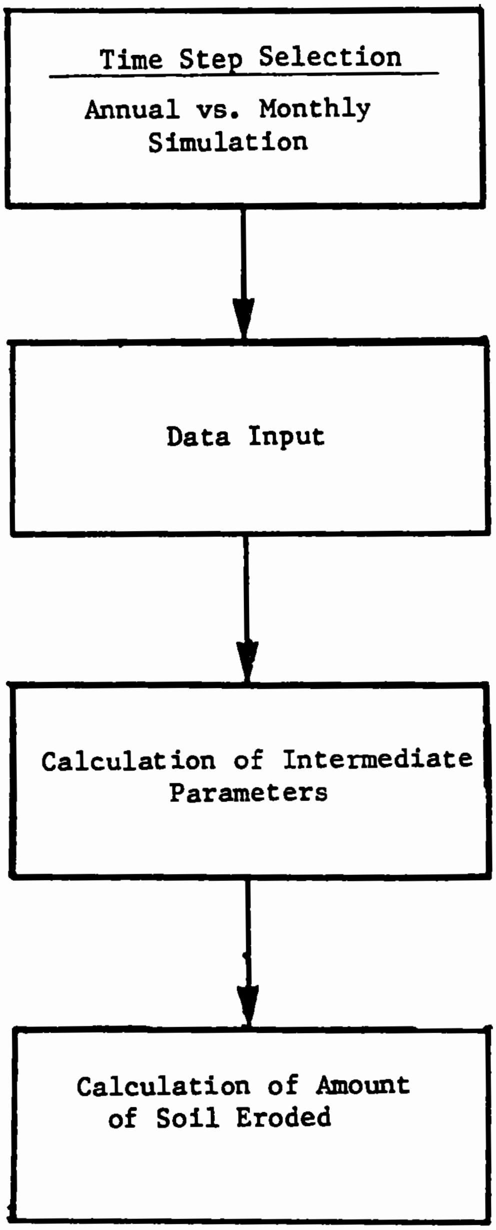

FIGURE SR-1: THE SOIL RESUSPENSION MODULE STRUCTURE

TABLE SR-1

SOIL ERODIBILITY INDEX (I)

	I	
Soil Types	(Tons/Acre/Year)	t/A/mo
Sand	436	36
Loam	207	17
Loamy Sand	180	15
Sandy Loam	156	13
Sandy-clay-loam	129	11
Silt Loam	91	7.6
Clay, Silty-clay	60	5
Sitly-clay-loam	59	4.9
Clay Loam	44	3.7
Sandy-clay	31	2.6
Silt	11	0.92

Source: Evans and Cooper 1980.

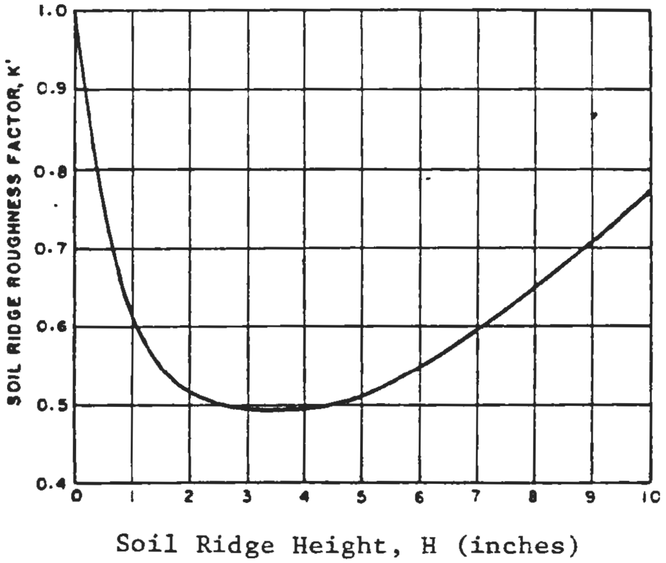

FIGURE SR-2: RELATIONSHIP OF SOIL RIDGE ROUGHNESS FACTOR K, FROM HEIGHT OF SOIL RIDGES where h is the height (in inches of the soil ridges and must be less than 10. Parameters "a" and "b" will be determined for the operational version of SESOIL, which will not require any user interaction.

- C: climatic factor
  The relationship defining C is based upon work by Thornthwaite (1931) in establishing a P-E (precipitation-evaporation) index. The general equation for C is:

$$C = \frac{0.0026 \left(\frac{30}{z}\right)^{3/2} \cdot v_z^3}{((P/T)-10)^{2.222}} \qquad \text{(SR-3)}$$

where

z = height of mean wind velocity measurement (ft)

v_z = mean wind speed at elevation z (ft/sec)

P = mean precipitation (inches)

T = mean temperature (°F)

This relationship was derived from the equation correcting for wind speeds not measured at 30 ft elevation (e.g. SR-4), the equation for determining P-E (e.g. SR-5), and the original relationship for C (e.g. SR-6).

$$\bar{V}_{30} = \left(\frac{30}{z}\right)^{1/2} \cdot \bar{v}_z \qquad \text{(SR-4)}$$

$$P\text{-}E = 11((P/T)-10)^{1.111} \qquad \text{(SR-5)}$$

$$C = 34.483 \frac{(V_{30})^3}{(P\text{-}E)^2} \qquad \text{(SR-6)}$$

- L: field length factor
  This parameter is dependent upon the values of I, K, and C already determined and upon dimensions of the site. These latter are used to find the equivalent (or unsheltered) field length, L. Graphs provided by Woodruff and Siddoway (1965) (Figure SR-3) are

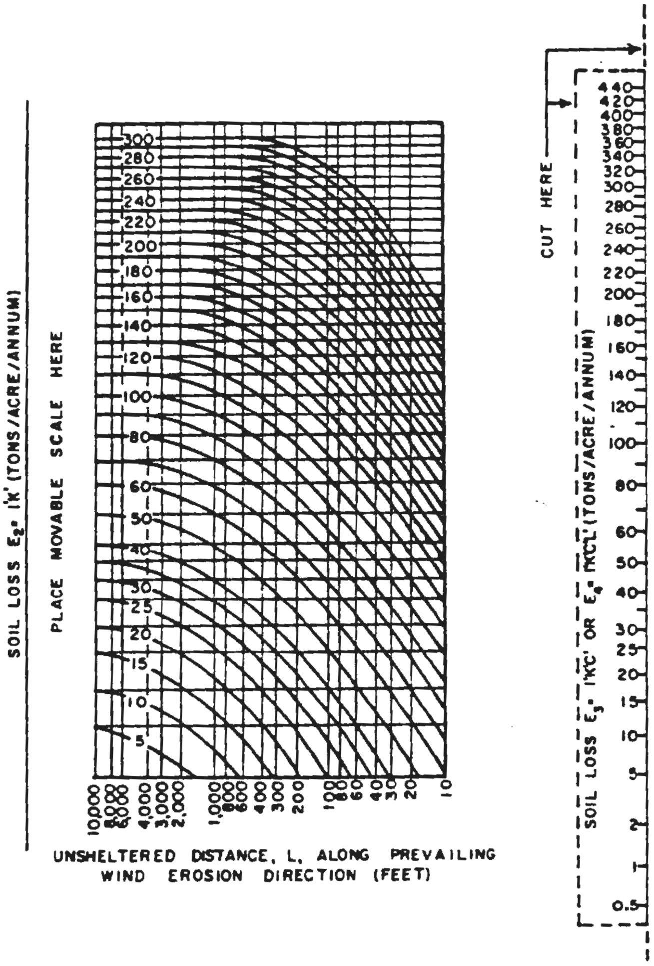

FIGURE SR-3: RELATIONSHIP BETWEEN L, 1, K, C AND E used to determine an intermediate value for E as f(I, K, C, L).[1]

The field length factor is used to account for the shielding effect of barriers around the site. A boundary barrier, such as wind break or building can reduce wind speed in the upwind direction and may even cause an adjacent dead spot, i.e. $\bar{v}_o = 0$. Within the site itself, due to the presence of barriers, effective length of field exposed to the wind may, therefore, be decreased.

- V: vegetative cover factor
  The presence of vegetation reduces erosion through the combined action of three mechanisms: increased soil moisture held in root zone, physical presence of the roots, and raising of the mean aerodynamic surface above the ground surface. The latter phenomenon reduces the movement of air (i.e. wind velocity) at the ground surface.

  This parameter is a function of I, K, C, and L, found graphically from a family of curves representing different values of V (Figure SR-4).[1]

2.3 The SESOIL Subroutine

A simplified flowchart for the SR simulation subroutine is shown on the next page (Figure SR-5). In order to keep this figure simple, the details of time step decisions and summation of monthly erosion are omitted.

The SR subroutine requires input data for parameters which are not used by other subroutines. These parameters are:

- SOI = the soil erodability index, I; (tons/acre/month)
- WVZ = mean wind velocity at elevation z; (ft/sec)
- WEZ - elevation, z, of wind velocity (WVZ) measurement; (ft)
- SRH - soil ridge height; (inches)
- DFG = days the ground is frozen per month; (days)
- APW = angle of prevailing wind

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[1] In the final, fully automated version of SR, this graph will not be necessary. It is shown here to demonstrate the relationships between the variables.

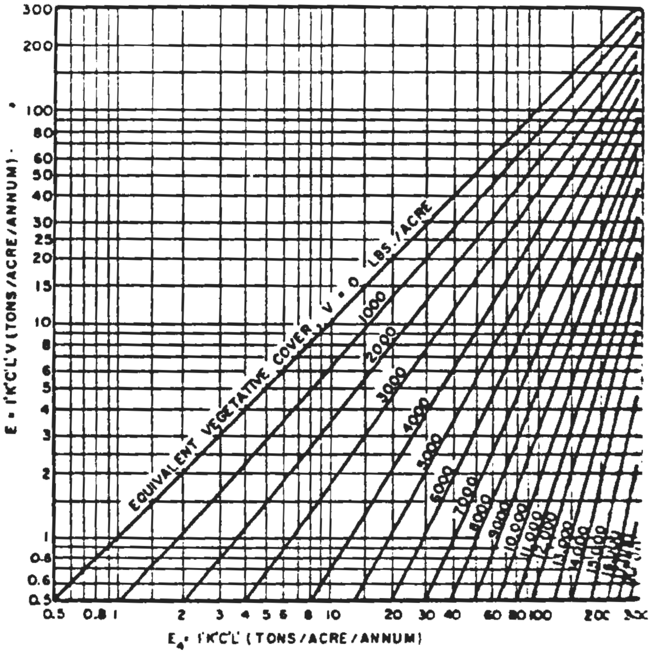

FIGURE SR-4: RELATIONSHIP BETWEEN I, K, C, L, U AND E

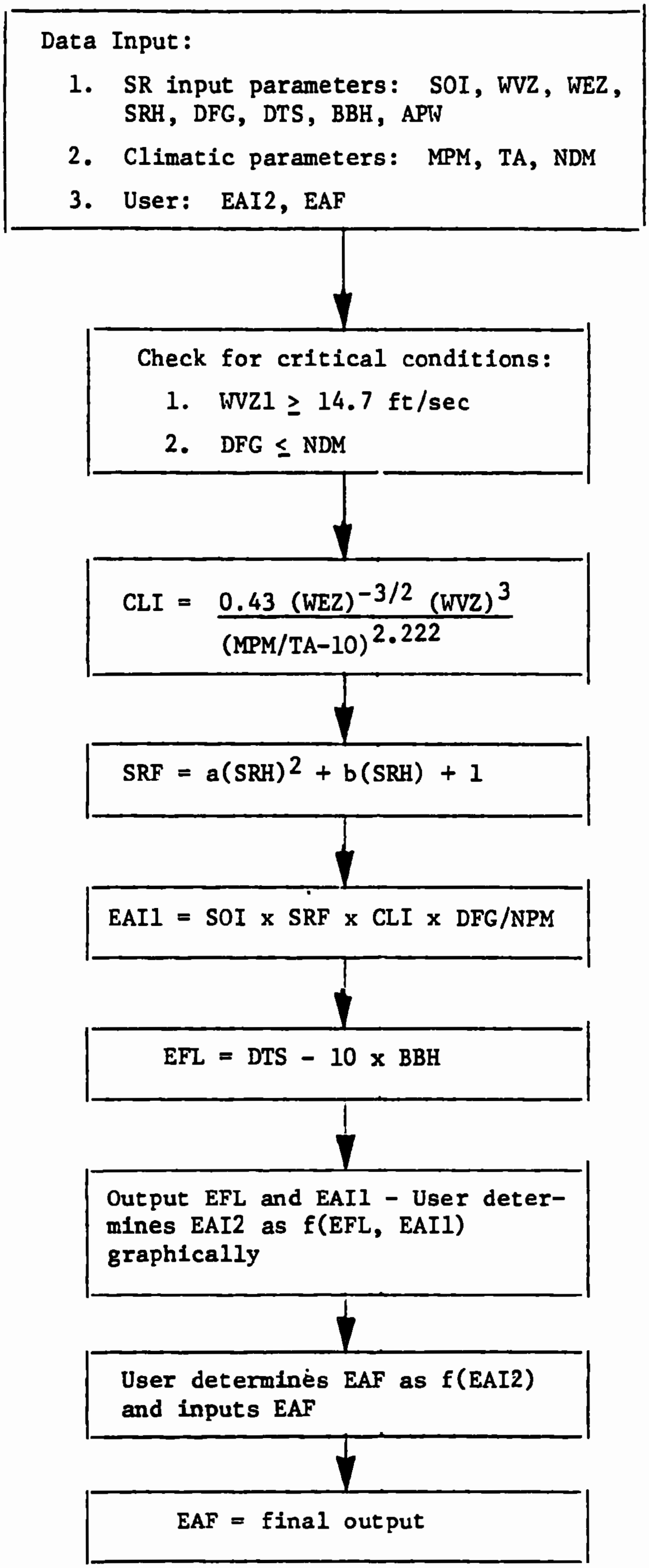

FIGURE SR-5: SIMPLIFIED FLOWCHART FOR SR SUBROUTINES

- DTS = distance across field to site under analysis (ft)
- BBF = boundary barrier height (ft)

The subroutine requires data for two parameters already incorporated into SESOIL: MPM, the mean monthly precipitation (MPM) and the mean monthly temperature (TA). The subroutines which use MPM and TA as inputs require them in units of cm and °C, respectively, Therefore, the SR subroutine will read the appropriate values from the data files and automatically convert MPM from cm to inches and TA from °C to °F as part of calculating the climatic index C.

The subroutine, as currently assembled, requires user inputs to find the final eroded amount: EAF. Those inputs are necessary because a single equation expressing the eroded amount, as a function of <u>all</u> the variables, has not yet been derived. The relationship between E and V is of the form $E = f(e)^V$, while that between E and L is of the form $E = f(1 - b)$. The vegetative cover factor (V) is called VCF and the field length factor (L) is named FLF in the SR subroutine.

The FLF is a function of I, K, and C as well as the physical dimensions of the site/field relative to the prevailing wind direction. Therefore, the model outputs an intermediate value for E, defined as EAI1, and a value for the unsheltered wind distance or equivalent field length (EFL). These two are applied to Figure SR-3 to determine a second intermediate value for E, called EAI2.

The final value for E, defined as EAF, is also user determined as the relation for the VCF is handled graphically based upon EAI2. The user must then input EAF so it can be integrated into the pollutant cycle subroutine. Figure SR-4 is used for this purpose.

The time steps used in the SR subroutine correspond to the four levels of simulation used by SESOIL: monthly - time-specific, monthly - general, annual - time-specific, and annual - general.

Note: The final version of the SR subroutine will not require user input as we will determine the mathematical relationships involved to allow SR to run unaided.

2.4 Subroutine Parameters

Input Parameters

- Climatic Parameters

  MPM = mean precipitation (inches)
  TA = mean temperature (°F)

- Soil Erosion Parameters

SOI = soil erodability (I) (tons/acre/month)

WVZ = mean wind velocity at elevation z (ft/sec)

WEZ = elevation z at which WVZ was measured (ft)

SRH = soil ridge height (inches)

DFG = days of frozen or snow-covered ground per month

DTS = perpendicular distance across field to site of analysis (ft)

BBH = boundary barrier height (ft)

APW = angle of prevailing wind (°)

NDM = number of days in the current month

- User Specified Parameters

EAI2 = second intermediate value for eroded amount

EAF = eroded amount -- final value

- Program Parameters (not user inputs)

CLI = climatic index, C

SRF = soil ridge height factor

EFL = equivalent field length

EAI1 = first intermediate value for eroded amount

3.0 EXAMPLES OF APPLICATIONS

3.1 Waste Disposal

For the simple and probably commonly-encountered situation of a waste disposal site, the following assumptions may be made:

1. Soil types will vary greatly, thus relying upon the specification of a value for 1 for each site.
2. The site will be flat and have no ridges, thus SRH = 1.
3. C will be determined by the data input for the site.
4. The site will be of sufficient size to eliminate any reductions in the equivalent field length. Thus F(L) = 100% or a factor of one.
5. No vegetation will be present at the site of recent pollutant (waste) application. Thus f(V) = 100% or a factor of one.

Thus equation SR-1 reduces in this case to

$$E = \frac{0.43\ (z)^{-3/2}\ (\bar{v}_z)^3}{((P/T)-10)^{2.222}}$$

Assumption 4 is based upon the fact that EFL = DTS if not the analytical location is at least 6000 feet from the site's boundary along the direction of the wind <u>and</u> if $I > 30$; if $I > 130$, and the location of analysis is 2000 feet from the edge, then boundary barrier effects do not reduce EFL.

3.2 Agricultural Application of Wastes

Whether liquid or sludge wastes have been applied to agricultural lands, there will likely be a residual pollutant load in the surface soil layer. While some amount of the residues may be taken up by the crop, the possibility of erosion exists. In this case, a value for SRH and determination of the VCF is necessary. The user must specify from Figure SR-2 (or equation SR-2) a value for SRH during data initialization and use Figure SR-3 during the program. Similarly, if the site does not meet the size limitations described in application 3.1 above, the procedure for EAI2 is necessary -- also to be input by the user during the program. Because this function is particularly difficult to utilize with any degree of accuracy from Figure SR-4, it is recommended that assumption 4 always be made.

4.0 REFERENCES

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VO - volatilization

APPENDIX VO

DIFFUSION AND VOLATILIZATION

1.0 INTRODUCTION

Diffusion and dispersion (terminology is given in Section 2.0) are two processes by which molecules of a compound in a region of high concentration move into a region of lower concentration. Diffusion occurs most readily in gases, less so in liquids, and least in solids. Volatilization is a form of diffusion that occurs when a compound moves from the soil environment into the atmosphere. For many pollutants, volatilization is an important mechanism for their loss from the soil.

The rate at which a chemical volatilizes from the soil is affected by many factors, such as soil properties, chemical properties, and environmental conditions. The magnitude of these factors and the complexity of their interactions are such that assumptions must be made in order to develop volatilization mathematical models. Many models are available in the literature, and some of these models can be applied only to specific environmental situations and only for the chemicals for which they were developed. Obviously, all models do not provide the same numerical results when employed to provide answers to a particular problem.

This appendix is not intended to thoroughly describe the dispersion, diffusion and volatilization processes of chemical species in soils; rather, it provides: background information on the nature of these processes, a short discussion on the physicochemical parameters affecting volatilization, a short discussion of available volatilization models and a presentation of the volatilization models employed in SESOIL. Additional information regarding diffusion and volatilization is given by Freeze and Cherry (1979) and Thomas (1981).

2.0 BACKGROUND

2.1 General

In order to select a volatilization model, it is important to understand the mechanism of movement of chemicals in the soil matrix and from the soil to the atmosphere. An elucidation of this mechanism will also aid in enumerating the factors affecting volatilization and the complexity of their interaction.

It is known that flow regimes of soils have the ability to transport dissolved substances known as solutes. Solutes are transported by advection, at an average rate equal to the average linear velocity of the flow regime. In addition, there is a tendency for the solute to spread out from its path both longitudinally and transversally. This phenomenum is called mechanical dispersion, or dispersion. Diffusion is a dispersion process of importance only at low flow regime velocities. Throughout this appendix only the terminology of diffusion will be used.

2.2 Diffusion/Volatilization

Substantial information in this section has been obtained from Freeze and Cherry (1979).

Diffusion in solution is the process whereby ionic or molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradient. Diffusion occurs in the absence of any bulk hydraulic movement of the solution. If the solution is flowing, diffusion is a mechanism, along with mechanical dispersion, that causes mixing of ionic or molecular constituents. Diffusion ceases only when concentration gradients become nonexistent. The process of diffusion is often referred to self-diffusion, molecular diffusion, or ionic diffusion.

The mass of diffusing substance passing through a given cross section per unit time is proportional to the concentration gradient (Fick's first law), or

$$F = -D(dc/dx) \qquad \text{(VO-1)}$$

where

F = solute mass flux along x; ($ug/cm^2 \cdot s$)

D = diffusion coefficient of pollutant in aqueous solution; (cm^2/s)

c = solute concentration of pollutant; (ug/mL)

dc/dx = concentration gradient; (-)

x = direction

The diffusion coefficients for electrolytes, for example, in aqueous solutions are well known. The major ions in saturated soil layer (groundwater) of NA^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, HCO_3^- have diffusion coefficients in the range of $1x10^{-9}$ to $2x10^{-9}$ m^2/s at 25°C. The coefficients are temperature-dependent and at 5°C, for example, they are about 50% smaller. In unsaturated soil zones, estimation of the overall diffusion coefficient (aqueous, vapor phase) is more complicated as will be discussed in a later section.

In summary, it is important to realize that both diffusion and volatilization refer to the movement of pollutants from a region of high concentration towards a region of lower concentration (minus sign in equation VO-1). Thus, in soils, when a "slug" of highly concentrated pollutant is introduced into a volume of soil (soil, soil moisture, air), it will "spread" out (diffuse) and will occupy a greater volume and at a lower concentration. (Figure VO-1.) Within the soil compartment, this spreading is called diffusion. When the pollutant spreads from the soil column to the atmosphere, the process is called volatilization. Therefore, diffusion and volatilization are the two processes contributing to the continuous movement of a pollutant from its point of release into the soil compartment to the atmosphere.

2.3 Partitioning/Distribution

A soil environment consists of three media: air, water and soil. (Figure VO-2.) Therefore, a compound incorporated into a soil matrix will be partitioned, and the pollutant will be present in all three phases: (1) mixed in soil air, (2) dissolved in soil moisture, and (3) sorbed on soil particles. The concentrations of the compound in each medium can be related to equilibrium partitioning coefficients (frequently constant parameters or isotherms) as discussed in Appendix AD (Adsorption) and in Appendix PT (Pollutant Transport).

The three main distribution pathways involved in the diffusion/volatilization process of a compound incorporated in a soil matrix can be summarized as:

- Compound on soil particles ↔ compound in solution
- Compound in solution ↔ compound in vapor phase (in soil air)
- Compound in vapor phase → compound into atmosphere (volatilization)

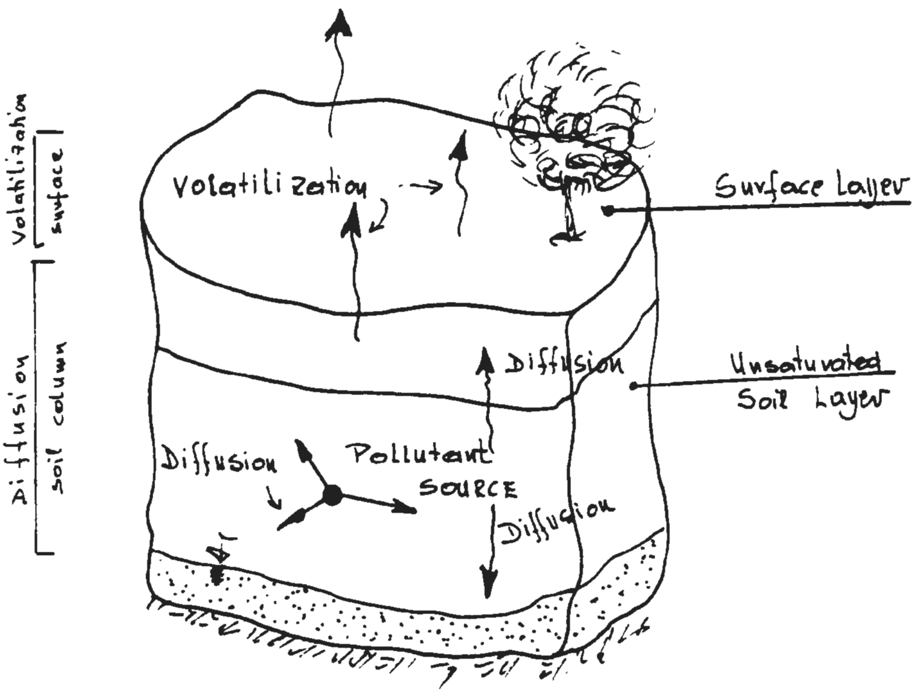


FIGURE VO-1

SCHEMATIC PRESENTATION OF DIFFUSION AND VOLATILIZATION

Total matrix volume: $V_T = V_a + V_w + V_s$
moisture content : $\theta = V_w / V_T$
air-soil content (air-porosity) : $n_{air} = V_a / V_T$
porosity (total) : $n = (V_a + V_w) / V_T$

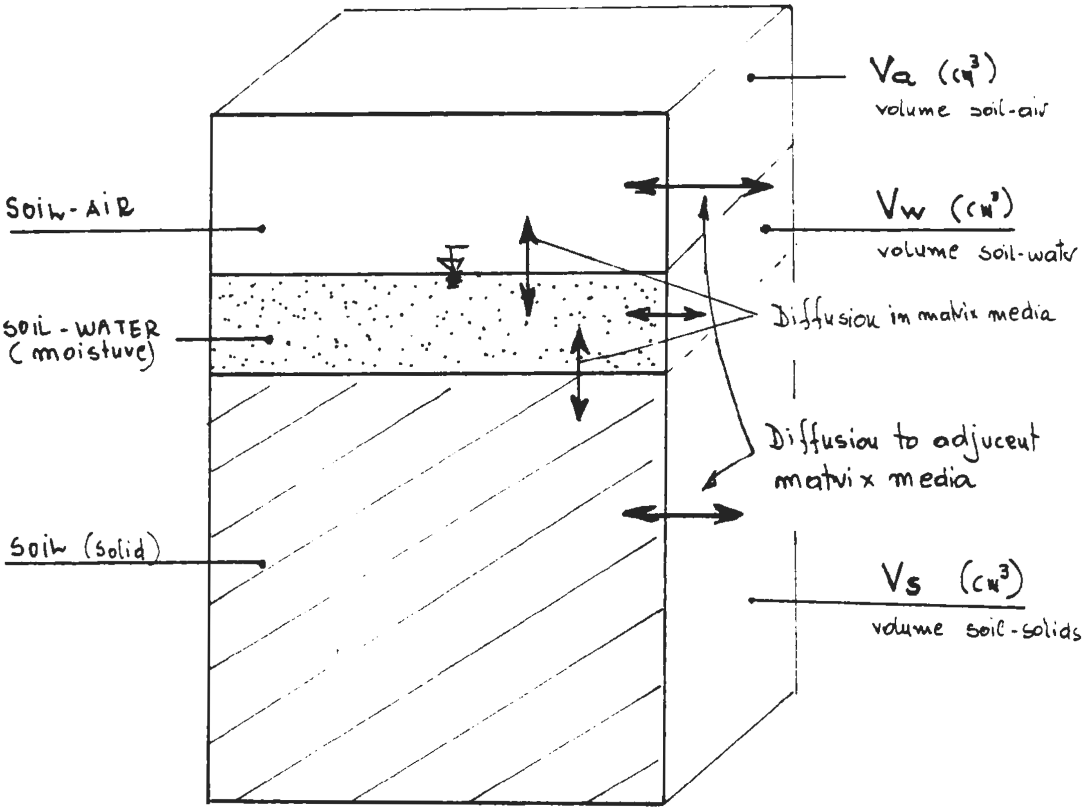


FIGURE VO-2

SOIL MATRIX PARTITIONING

Diffusion occurs in all three media of the soil environment; however, it takes place most rapidly in air and least rapidly in solids. Diffusion in the vapor phase (air) occurs 10^4 times faster than in water. Diffusion in the solid phase is extremely slow compared to other pollutant transport processes, therefore, it is neglected by most pollutant models.

Volatilization at the soil surface can also occur from all three phases. However, volatilization from every phase is much faster than diffusion. Thus, diffusion is the rate-controlling process in the movement of chemicals from a soil layer, to a soil surface, and then into the atmosphere.

Due to the interaction of diffusion within a phase with partitioning among phases, the rate of volatilization depends on both diffusion rates and partitioning behavior. Therefore, any factor which causes a small change in the distribution of a compound among the soil, soil-water, soil-air, and atmosphere can have a large effect on the rate of volatilization of that compound. For example, when a pollutant is in a soil to which it is strongly adsorbed, very little pollutant will be in the soil-air or the soil-water. Since diffusion in solids is slow, only small amounts of pollutant will be available to volatilize. When this (same) pollutant is in a slightly less adsorbant soil, soil-air concentrations can become significant, and the faster air diffusion process will contribute large amounts of pollutant to the soil surface. In the latter case, volatilization releases can be quite high.

2.4 Factors Affecting Volatilization

Chemical, soil and general environmental properties affect volatilization. Some of the physicochemical properties of a compound which can affect volatilization are vapor pressure, solubility in water, adsorption behavior, and diffusion coefficients in air and water. Some soil properties which influence volatilization behavior include moisture content, density, porosity, organic carbon content, clay content, and soil diffusion characteristics. Typical environmental factors impacting volatilization can be wind speed at the surface, humidity, temperature, pH, surface cover, and hydrology at the site (e.g., infiltration, capillarity).

The impact on volatilization rates of many of the above factors is not quantifiable yet. Therefore, to formulate mathematical models, assumptions have been made by researchers by limiting the factors included in their equations. As of now, no one general model is available to estimate volatilization rates in all situations, but effective and promising research is underway. The SESOIL model is designed to employ existing volatilization models; therefore, as more knowledge and information become available regarding the process, refined volatilization models might be implemented by SESOIL.

3.0 MATHEMATICAL MODELING

3.1 General

Volatilization modeling encompasses the

(1) Selection of a model most applicable to a user's needs (e.g., problem to be simulated, data availability);

(2) Estimation of the diffusion and other coefficients for the model selected.

Generally speaking, there exist two types of models for estimating volatilization rates

(1) Theoretical models based upon Fick's first and second laws;

(2) Experimental models based upon laboratory or field experimental data and statistically derived equations.

Fick's first law describes the steady state mass flux of a pollutant due to diffusion. (See Section 2.2.) Fick's second law is obtained from Fick's first law and the equation of continuity and describes the nonsteady state mass flux of a pollutant due to diffusion. Fick's second law is also known in the literature as the diffusion equation of solutes in porous media (air, water, soil).

Fick's first law in one direction z is expressed as

$$F = -D\,(dc/dz) \qquad \text{(VO-2)}$$

Fick's second law is expressed as

$$dc/dt = D^{*}\,(d^2c/dz^2) \qquad \text{(VO-3)}$$

where

$$D^{*} = k \cdot D \qquad \text{(VO-4)}$$

in which

F = mass flux across a surface; ($\mu g/cm^2 \cdot s$)

D = aqueous diffusion coefficient of compound; (cm^2/s)

c = solute concentration of compound in soil moisture; (ug/mL)

z = distance (depth) normal to diffusing direction; (cm)

t = time; (s)

D^* = apparent diffusion coefficient of compound in soil matrix; (cm^2/s)

k = proportionality coefficient, to correct for soil matrix effects; (-)

Diffusion coefficient (D, D*) definitions and other issues are discussed in the following section.

No scientist can argue that theoretical models are better or worse than experimental models since each type has its own strengths. In the first category are the models of Mayer et al (1973), Jury et al (1979), and Farmer et al (1980). In the second category are the models of Hartley (1969), Hamaker (1972), and Dow (1979). Each model cannot be applied to all situations. One model might be appropriate for pollutant applied on surface, another model might be more appropriate for a chemical incorporated into an upper soil layer, and a third one the most appropriate for a buried compound. Some of these models are presented in subsequent sections.

3.2 Diffusion Coefficients

Fick's law applies to all environmental media--air, water, and soil. Therefore, for a particular compound, we may have its diffusion coefficients in air (D_a), in water (D_w), in soil (D_s), in soil-air (D_{sa}), in soil-moisture (D_{sm}), and overall apparent coefficients (D^*) in all above media.

In the second Fick's law, the diffusion coefficient of ions is characterized as an "apparent" diffusion coefficient, D^*, which in soil systems is smaller than that in water bodies, because in porous media the ions follow longer paths of diffusion caused by the presence of the particles in the solid matrix and because of adsorption on the solids. In laboratory studies of diffusion of nonadsorbed ions in porous materials, k values between 0.5 and 0.01 are commonly observed (Freeze and Cherry 1979). No specific definition of an apparent coefficient can be made. Estimation of this apparent diffusion coefficient D^* is equation- and chemical-specific, and such issues are discussed in the following sections with the work of each individual researcher.

Most of the volatilization equations require as input a chemical-specific diffusion coefficient, primarily in air or water, in units of cm/s. It is worth mentioning at this point a few ways of obtaining this parameter since this information will facilitate readers to better understand the correct way of applying the various volatilization equations or models that will be presented in the subsequent sections.

Diffusion coefficients in the air (D_a) are available in the literature for some chemicals (e.g., Weast et al 1978). Diffusion coefficients in water (D_w) are also available in the literature or have been estimated by researchers individually (Bode et al 1973). Nelken (1981) gives some estimation techniques for both air and water diffusion coefficients.

3.2.1 Molecular Weight Effects

Air diffusion coefficients of two similar compounds 1 and 2 can be related by the expression

$$D_{a_1}/D_{a_2} = (M_2/M_1)^{1/2} \qquad \text{(VO-5)}$$

where

D_a = vapor phase (air) diffusion coefficient; (cm^2/s)

M = molecular weight of compound; (g/mol)

3.2.2 Porosity Effects

Millington and Quirk (1961) have proposed a correcting relationship for relating the apparent diffusion coefficient of a compound in the soil-air (D^*_{sa}) to the diffusion coefficient of the same compound in the air to (D_a).

$$D^*_{sa} = D_a\,(n_{air}^{10/3}/n^2) \qquad \text{(VO-6)}$$

where

D^*_{sa} = apparent diffusion coefficient of compound in soil-air; (cm^2/s)

D_a = diffusion coefficient of compound in vapor (air); (cm^2/s)

n_{air} = soil air-filled porosity; (cm^3/cm^3); (mL/mL)

n = soil (total) porosity; (mL/mL)

Frequently, it has been assumed in model applications that $D^*_{sa} = D_{sa}$; where, D^*_{sa}, the apparent diffusion coefficient of the compound in the soil-air and D_{sa} the "real" coefficient of the compound is the soil-air. This is done because of the difficulty in defining the meaning of the "apparent" diffusion coefficient.

The soil air-filled porosity in equation VO-6 can be estimated from

(a) either the (total) soil porosity (n) and the soil moisture content (θ)

$$n_{air} = n - \theta \qquad \text{(VO-7)}$$

(b) or the soil bulk density (ρ_b) and the soil particle density (ρ)

$$n = 1-\rho_b/\rho \quad \text{(VO-8)}$$

where

ρ_b = soil bulk density; (g/cm^3)

ρ = particle density; (g/cm^3)

The particle density can be measured, but for most soil minerals, materials it usually equals 2.65 g/cm^3.

3.2.3 Temperature Effects

Temperature affects values of an air diffusion coefficient according to (Farner et al 1980)

$$D_{a2} = D_{a1} (T_2/T_1)^{1/2} \quad \text{(VO-9)}$$

where

D_{a2}, D_{a1} = air diffusion coefficients of a compound at T_2 and T_1; (cm^2/s)

T_2, T_1 = temperatures; (^{o}K)

According to Hamaker (1972), vapor-phase (air) diffusion coefficients of the same compound and at different temperatures may be related by

$$D_{a1}/D_{a2} = p_2/p_1 (T_1/T_2)^m \quad \text{(VO-10)}$$

where

p = ambient total pressure; (consistent units)

T = temperature; (^{o}K)

m = experimental coefficient; (-)

3.3 Concentrations of Compound

Volatilization equations have to be employed with <u>care</u> because of diffusion and the concentration definitions. Some equations, for example, account for the total concentration of the pollutant in the soil c_o, other equations account only for the solute concentration c and others only for the pollutant concentration in the soil-air c_{sa}.

The total concentration of a chemical in the soil matrix can be expressed (Jury et al 1980) as

$$c_o = (\rho_b \cdot s + \theta \cdot c + n_{air} \cdot c_{sa}) \qquad \text{(VO-10)}$$

where

c_o = overall (total) concentration in soil matrix; (ug/cm^3 soil)

ρ_b = soil bulk density; (g/cm^3)

s = adsorbed concentration on soil particles (ug/g of soil)

θ = volumetric soil moisture content; (mL/mL)

c = solute concentration (in liquid phase) of compound; (ug/mL)

n_{air} = soil-air content or air-filled porosity; (mL/mL)

c_{sa} = concentration of compound in the soil-air; (ug/mL)

The solute concentration c of a compound can be related to its soil-air concentration c_{sa} via Henry's law.

$$c_{sa} = c \cdot H/R(T+273) \qquad \text{(VO-12)}$$

where

c_{sa} = concentration in soil-air; (ug/mL)

c = concentration in soil moisture; (ug/mL)

H = Henry's law constant; ($m^3 \cdot$atm/mol)

R = gas constant; (8.2×10^{-5} $m^3 \cdot$atm/mol$\cdot$°K)

T = temperature; (°C)

°K = °C+273

The solute concentration c of a compound can be related to its adsorbed concentration s on soil particles via adsorption isotherms, the latter being described in Appendix AD (Adsorption). Two well known isotherms are Freundlich and Langmuir.

3.4 Theoretical Models

The following sections present only a general overview of available mathematical volatilization models. Discussions are tailored to the needs of this appendix.

3.4.1 Farmer, Yang, Letey

A simple volatilization model to study the steady state rate of volatilization of hexachlorobenzene (HCB) wastes <u>in soil through a soil cover</u> is developed by Farmer et al (1980).

This model is based on a discretized version of Fick's first law (equation VO-2) over space, and assumes vapor phase diffusion being the rate controlling processes. The volatilization rate of HCB from the landfill, equals

$$P = -D^{*}_{sa} \, (c_{atm} - c_{sa})/L \qquad \text{(VO-13)}$$

where

P = pollultant flux across soil cover; ($ug/cm^2 \cdot s$)

D^{*}_{sa} = apparent steady diffusion coefficient in soil-air; (cm^2/s)

c_{atm} = concentration of the volatilizing compound in the atmosphere at the surface of the soil layer; (ug/mL)

c_{sa} = concentration of compound in the soil-air; (ug/mL)

L = depth of covering soil layer; (cm)

Expression VO-3 is known also as the Stephen equation. Farmer et al employed equations VO-6 and VO-7 for the estimation of the apparent diffusion coefficient. When employing this model, the concentration of a compound in the soil-air can be estimated from the concentration of the compound in the soil moisture via equation VO-11 and vice versa. The resulting equation is

$$P = D_a \cdot [(n-\theta)^{10/3}/n^2][H \cdot c/R(T+273) \cdot L] \qquad \text{(VO-14)}$$

and $P_o = P \cdot \Delta t$

where

P = pollutant flux across soil surface; (ug/cm$^2\cdot$s)

P_o = total pollutant flux/loss across soil surface; (ug/cm^2)

D_a = diffusion coefficient of compound in air; (cm^2/s)

H = Henry's law constant; (m$^3\cdot$atm/mol)

R = gas constant; ($8.2\cdot10^{-5}$ m$^3\cdot$atm/mol$\cdot{}^oK$)

T = temperature; (^{o}C)

c = concentration of compound in soil moisture; (ug/mL)

n = soil porosity; (fraction)

θ = soil moisture; (fraction)

Δt = length of simulation time step; (s)

This Farmer et al (1980) model is employed by the current version of SESOIL.

3.4.2 Jury, Grover, Spencer and Farmer

Jury et al (1980) account in their work for the total concentration of the chemical in the soil matrix (equation VO-11). By employing Fick's second law, Henry's law, linear adsorption isotherms and the moisture continuity equation in porous media, they derived the expression

$$P_o = 2(c_o-g)(D^*\cdot t/\pi\cdot e)^{1/2} \qquad \text{(VO-15)}$$

where

P_o = volatilized (total) chemical mass per unit area after time t; (ug/cm^2)

c_o = total initial concentration of compound in soil; (ug/g soil)

D^* = apparent diffusion coefficient; (cm^2/s)

π = 3.14

e = derived coefficient by Jury et al; (mL/mL)

g = derived coefficient by Jury et al; (ug/cm^3)

The above information is obtained from Thomas (1981); therefore, interested readers should refer to the original publication. The Jury et al model is not incorporated (coded) in the present version of SESOIL since its employment has not be mandated by a particular application.

3.4.3 Mayer, Letey and Farmer

Mayer et al (1974) applied Fick's second law (equation VO-3) to the mathematical description of the movement chemicals <u>in soils</u>. Diffusion is assumed to be the only mechanism transporting chemicals to the soil surface; therefore, this model may underestimate volatilization rates. (Thomas 1981.)

Depending upon the boundary conditions employed to solve the diffusion equation, Mayer et al presented five different solutions (models) of the form

$$c(z,t) = c(c_{to}, D^*, t, L, R_o) \qquad \text{(VO-16)}$$

$$P_o = f[c(z,t)]$$

where

$c(z,t)$ = solute concentration or concentration in soil-air of a compound; (ug/mL)

P_o = total volatilizing mass of compound; (ug/s·cm^2)

c_{to} = initial (t=0) concentration in soil moisture or as indicated; (ug/mL)

z = direction

t = time; (s)

D^* = apparent diffusion coefficient; (cm^2/s)

L = soil layer depth; (cm)

R_o = isotherm coefficients or Henry's law constant

As an example of Mayer's et al work, two solutions of equation VO-16 are presented below. This information is obtained from Thomas (1981); therefore, interested readers should refer to the original publication.

(1) Simplified solution of equation VO-3 for a compound that is removed rapidly from the soil surface; upward diffusion only.

$$c(z,t) = c_{to} \cdot \mathrm{erf}[z/2(D \cdot t)^{1/2}] \qquad \text{(VO-17)}$$

$$P_o = c_{to}(D/\pi \cdot t)^{1/2}$$

(2) Solution of previous problem; diffusion downwards has been accounted.

$$\begin{aligned} c(z,t) &= 0.5c_{to}[2\mathrm{erf}(A)-\mathrm{erf}(A-B)-\mathrm{erf}(A+B)] \\ P_o &= D \cdot c_{to}/(\pi Dt)^{1/2} \\ A &= z/2(D \cdot t)^{1/2} \\ B &= L/2(Dt)^{1/2} \end{aligned} \qquad \text{(VO-18)}$$

Adams et al (1976) indicated that equation VO-17 gives dependable estimates when

$$t \leqq z^2/14.4 \cdot D^* \qquad \text{(VO-19)}$$

From equation VO-19, it also follows that the time to reach a half concentration of a chemical, $c_o/2$, occurs when $\mathrm{erf}(x)=0.5$, or when $z/2(D^* \cdot t)^{1/2} \simeq 0.477$, from which we obtain

$$t_{1/2} = 0.91D^*/z^2 \qquad \text{(VO-20)}$$

The Mayer et al model is not incorporated (coded) into the present version of SESOIL since its employment has not been mandated by a particular application.

3.5 Experimental Models

Experimental and application specific models are based on field and laboratory sampling programs and on statistical data analyses. Two known models are of Dow and Hamaker. (Thomas 1981.)

3.5.1 Dow

Researchers at Dow Chemical Company (1979) have performed experiments to establish the relationship between the volatilization rate of a chemical applied to a soil surface and the chemical properties of vapor pressure, water solubility, and adsorption coefficient. The rate constant of volatilization for chemicals applied or spilled on the soil surface was found to equal

$$k_v = 4.4 \times 10^7 \cdot (P_{vp}/K_{oc} \cdot SL) \qquad \text{(VO-21)}$$

and $$c = c_o e^{-k_v \cdot t}$$

where

k_v = rate constant for volatilization; (day^{-1})

K_{oc} = soil adsorption coefficient (soil/water) based on organic carbon content; (ug/g)/(ug/mL)

SL = solubility of the compound; (ug/mL)

P_{vp} = vapor pressure of chemical; (mm Hg)

c_o, c = concentration of chemical; initial, after time t; (ug/mL)

t = time; (day)

3.5.2 Hamaker

Hamaker (1972) proposed a relationship for estimating the volatilization rates of chemicals that are strongly adsorbed on soil particles. The impregnated soil layer is assumed to be semi-infinite and the expression derived is

$$P_o = 2c_o \cdot (D^* \cdot t/\pi)^{1/2} \qquad \text{(VO-22)}$$

where

P_o = loss (total) of chemical per unit area after time t; (ug/cm^2)

c_o = total initial concentration of chemical in the soil; (ug/cm^3)

D^* = apparent diffusion coefficient in soil-air; (cm^2/sec)

t = time; (sec)

π = 3.14

The total initial concentration of chemical in the soil is given by equation VO-11. Other equations required together with VO-11 are the adsorption isotherm (e.g., equation AD-7, Freundlich), the porosity equation VO-7 and Henry's law equation VO-12.

3.6 The SESOIL Diffusion/Volatilization Models

3.6.1 Diffusion Model

The diffusion equation VO-1 (Fick's first law) is employed by the volatilization routine of SESOIL to estimate upward mass flow in the soil column and to the air. Upward diffusion is omitted since it is accounted explicitly via the volatilization model of the pollutant transport routine. Downward diffusion is omitted (as a diffusion term) since the pollutant transport routine accounts for diffusion (partitioning of phases; see Appendix PT) in the soil matrix explicitly. In that respect, downward diffusion is also accounted in a different way.

3.6.2 Volatilization Models

The selection of the appropriate volatilization model is entrusted to the user. Needs of certain simulations performed mandated the employment of two models, one of which is coded in Subroutines VOLA and VOLM. (See Appendix FC.) Only minor changes to the code are necessary to add other volatilization models. The following two sections describe models the developers of SESOIL have tested.

3.6.2.1 Farmer, Yang, Letey

The Farmer et al (1980) model, applied to HCBs (see Section 3.4.1), accounts for the Stephan equation which describes pollutant loss via volatilization of a pollutant that is buried under a layer of clean soil (cover). According to Farmer et al, this is an appropriate model to describe pollutant movement through soils where air diffusion is the rate controlling process of volatilization.

For convenience to SESOIL users, the model (equations)--applied over a simulation time step t--and its input parameters are summarized in a table. (Table VO-1.) The chemical-specific parameters (Henry's law and diffusion constants) are available from handbooks or may be estimated according to methods presented by Lyman et al (1981). The soil porosity values are available from the SESOIL documentation (Appendix ID), soil handbooks (USDA, USGS), or from experimental data. Temperature values for a site-specific area are obtained from NOAA reports. The compartment geometry parameters are chosen according to the needs of the investigation. Upward mass flux is accounted in SESOIL only by the existence of a concentration gradient (Fick's law).

3.6.2.2 Hamaker

The Hamaker (1972) experimental model which estimates time dependent volatilization fluxes of pollutants mixed in an upper soil layer was coded in the past in volatilization subroutine VOLATA of SESOIL. Information of this model is presented in Section 3.6.2. The diffusion coefficient of the model was obtained from handbooks. Other coefficients were estimated on-line by SESOIL. The code accompanying this version of SESOIL, however, does not contain the Hamaker model for various reasons.

TABLE VO-1

THE FARMER et al MODEL IN SESOIL

Governing Equation

$$P_o = D_a[(n-\theta)^{10/3}/n^2][c\cdot H/(R\cdot(273+T)\cdot L)]\cdot\Delta t \qquad \text{(VO-14)}$$

Derived by employing

The Stephan equation VO-13, Henry's law equation VO-12, the Millington and Quick (1961) equation VO-6, and the porosity convecting equation VO-7 which are given below.

St.eq : $P = -D^*_{sa}(c_{atm}-c_{sa})/L$ (VO-13)

H.law : $c_{sa} = c\cdot H/R(T+273)$ (VO-12)

MQ.eq : $D^*_{sa} = D_a(n_{air}^{10/3}/n^2)$ (VO-6)

Po.eq : $n_{air} = n-\theta$ (VO-7)

where

			FORTRAN Variable
P_o	=	total pollutant flux across soil surface within time Δt; (ug/cm^2)	PVOL
D_a	=	diffusion coefficient of chemical in air; (cm^2/s)	D
n	=	soil (total) porosity; (fraction)	N
θ	=	soil moisture content; (fraction)	THA
c	=	concentration of compound in the soil moisture; (ug/mL)	C
H	=	Henry's law constant for compound; (m$^3\cdot$atm/mol)	H
R	=	gas constant; ($8.2\text{x}10^{-5}$m$^3\cdot$atm/mol ^{o}K)	R
T	=	temperature; (^{o}C)	T
L	=	thickness of covering soil layer; (cm)	L
D^*_{sa}	=	apparent diffusion coefficient of chemical in soil-air; (cm^2/s)	DA

TABLE VO-1 (continued)

		FORTRAN Variable
c_{atm} =	0.0; concentration of compound in the atmosphere; (ug/mL)	CATM
c_{sa} =	concentration of compound in the soil-air; (ug/mL)	CAIR
n_{air} =	air-filled porosity (fraction)	NAIR
Δt =	length of simulation time step; (s)	DT

Assumptions

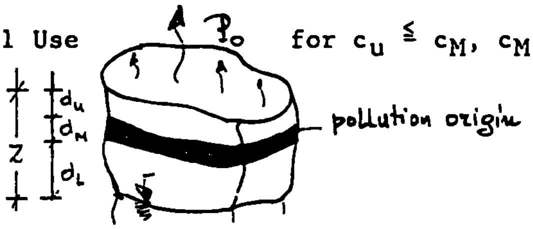
$c_{air} = 0.0$

Covering layer thickness (L) is equal to the length (depth) from the center of the SESOIL layer to the soil surface.

Input Parameters to SESOIL Subroutine

Parameters	Description	FORTRAN Variable
D_a	Diffusion coefficient of the pollutant in air; (cm^2/s)	DA
n	Porosity (total) of the soil; (-)	N
H	Henry's law constant of pollutant; ($m^3 \cdot atm/mol$)	H
T	Temperature; (°C)	TA
d_u, d_L	Soil depths; (cm)	DU, DL
z	Soil depth to groundwater; (m)	Z

Schematic of Model Use



for $c_u \leq c_M$, $c_M < c_L$

3.7 Numerical Example

Assuming trichloroethylene (TCE) as a chemical compound, in a sandy loam soil and constant environmental conditions as, for example

D_a = 0.072 cm^2/s

H = 0.060 $m^3 \cdot atm/mol$

R = 8.2×10^{-5} $m^3 \cdot atm/mol \cdot {}^oK$

n = 0.25

θ = 0.10

T = 14°C

L = 2.0 m = 200 cm

Δt = 1 month = $2.6 \times 10^6 s$

c = 10 ug/mL

We estimate (equation VO-14) the pollutant mass volatilized within a month through the soil cover to the atmosphere

$$P_o = 0.072[(0.25-0.10)^{10/3}/0.25^2][10 \cdot 0.060/8.2 \times 10^{-5}(14+273) \cdot 2.6 \times 10^6 =$$

$$= 685 \text{ ug/cm}^2$$

4.0 DISCUSSION

As repeated consistently throughout this Appendix, SESOIL users' volatilization equations must be employed with care because of both the diffusion and the concentration definitions employed by various researchers. Since input data to SESOIL are summarized in Table VO-1 together with the corresponding model employed, special attention has been given by the SESOIL model developers to facilitate use of this model and to prevent incorrect input data inserts. Therefore, input data are kept to a limited number and internal (on-line) model calculations (e.g., c_{sa} versus c partitioning) assist in accomplishing this objective. Users have to make sure to input the correct number only for an input parameter. (Table VO-1.)

5.0 NOMENCLATURE

Symbol	Description	Units
A	Function, Equation VO-18	-
B	Function, Equation VO-18	-
b	Soil bulk density	g/cm^3
^oC	Temperature in Celcius	^oC
c	Concentration of compound in soil moisture (solute concentration)	ug/mL
c_{atm}	Concentration of compound in atmosphere	ug/mL
c_{sa}	Concentration of compound in soil-air	ug/mL
c_{to}	Initial (t=0) concentration in soil moisture	ug/mL
c_o	Concentration (total) of compound in soil matrix	ug/g soil
d[]/dx	Gradient along x	-
D_a	Diffusion coefficient of compound in air	cm^2/s
D_w	Diffusion coefficient of compound in water	cm^2/s
D_s	Diffusion coefficient of compound in soil	cm^2/s
D_{sa}	Diffusion coefficient of compound in soil-air	cm^2/s
D_{sm}	Diffusion coefficient of compound in soil moisture	cm^2/s
D^*	Apparent diffusion coefficient of compound in various media	cm^2/s
e	Coefficient, Equation VO-15	mL/mL
erf[]	Error function	-

Symbol	Description	Units
F	Solute flux along a direction x, Equation VO-1	$ug/cm^2 \cdot s$
g	Coefficient, Equation VO-15	ug/cm^3
H	Henry's law constant	$m^3 \cdot atm/mol$
K_{oc}	Adsorption coefficient based on organic carbon content	(ug/g)/(ug/mL)
k	Proportionality coefficient to correct for soil matrix effects	-
^oK	Temperature (in Kelvin)	^oK
L	Depth of soil cover	cm
m	Exponent, Equation VO-10	-
M	Molecular weight of compound	g/mol
n	Soil porosity (total)	fraction
n_{air}	Soil-air filled porosity	fraction
P	Pollutant flux (volatilized) across soil cover	$ug/cm^2 \cdot s$
P_o	Volatilized (total) chemical mass after time t	ug/cm^2
P_d	Volatilized mass after Dow	ug/cm^2
P_{vp}	Vapor pressure of compound	mm Hg
R	Gas constant = $8.2x10^{-5}$	$m^3 \cdot atm/mol \cdot {}^oK$
R_o	Isotherm coefficient, Equation VO-16	-
SL	Solubility of compound	ug/mL
T	Temperature	^oC
t	Time	s
x	Direction	-

Symbol	Description	Units
z	Vertical distance/direction	cm
θ	Soil moisture content	fraction
ρ	Soil particle density	g/cm^3
ρ_b	Soil bulk density	g/cm^3
π	3.14	-

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AD - adsorption

APPENDIX AD

ADSORPTION AND DESORPTION

TABLE

1.0 INTRODUCTION

Adsorption is the adhesion of pollutant ions or molecules to the surface or soil solids, causing an increase in the pollutant concentration on the soil surface over the concentration present in the soil moisture. Adsorption occurs as a result of a variety of processes with a variety of mechanisms and some processes may cause an increase of pollutant concentration within the soil solids--not merely on the soil surface. Processes which can contribute to increased soil concentrations include ion exchange, physical sorption, specific adsorption, partitioning, fixation, and chemisorption. The general term sorption is often used to describe these phenomena, particularly when the adsorption mechanisms are not known. Most sorption processes are reversible; the reverse processes result in desorption.

Adsorption and desorption can drastically retard the migration of pollutants in soils, therefore, knowledge of this process is of importance when dealing with contaminant transport in soil moisture to groundwater. Sorption is usually considered to occur rapidly, relative to the rate of pollutant migration in the soil matrix due to the movement of soil moisture or groundwater flow. In addition, adsorption and desorption are usually considered to be in equilibrium--in mathematical modeling studies--and are modeled as one reversible process. This assumption facilitates modeling without substantially impacting overall long-term model estimates. Nonetheless, discrete adsorption and desorption modeling is always feasible.

Various scientists have carried out numerous experiments aimed at understanding the adsorption and desorption process, for example, Rifai, et al (1956), Day and Forsythe (1958), Biggow and Nielsen (1962), Kay and Elrick (1967) and Chiou, et al (1979). Their studies, however, do not always address questions of the nature of the chemical interactions occurring; they focus, rather, on the movement of pollutants in a soil column, from which estimates of the magnitude of pollutant involved in the sorption process.

This appendix is not intended to thoroughly describe the sorption process of pollutants in soil; rather, it provides background information on the nature of the adsorption, mathematical modeling issues and the way adsorption is modeled in SESOIL.

2.0 BACKGROUND

Background information contained in this section was obtained from the Encyclopedia of Soil Science, Part 1 (Fairbridge and Finke, 1979), and its chapter on adsorption phenomena authored by D.R. Kenney. Additional information is presented in the literature by Lyman (1981) and Dragun (1980).

In general terms, the sorption of pollutant refers to processes that result in a higher concentration of a particular component at the surface or within a solid phase than is present in bulk solution of soils and sediments. The general term sorption is frequently used instead of adsorption because the actual sorption mechanisms are not often known. Sorption is the major general retention mechanism for many organic compounds and metals, and the sorption and desorption phenomena play an important role in controling the availability of several plant nutrients, the rate of leaching to groundwater, volatilization from soil surface, or degradation of organic compounds such as pesticides. The sorption and desorption phenomena also protect water supplies by retaining numerous potential pollutants including nutrients, heavy metals, pesticides, and pathogens. Compounds or ions adsorbed on a soil particle surface are in equilibrium with the soil solution and are capable of desorption.

In the past the sorption of inorganic ions by soils was often thought to be due largely to precipitation reactions, i.e., the formation of a sparingly soluble solid phase. However, careful studies have shown that the solubility product principle will not account for the extremely low concentrations of phosphorus and many of the metals in the bulk solution of an aerated soil (Lindsay 1972). These studies have brought about the realization that precipitation generally dominates only at relatively high concentrations of the reactants.

Cation exchange, the interchange between a cation in solution and another cation on the surface of any surface-active material, is one important adsorption mechanism for cationic plant nutrients (potassium, calcium and magnesium) in soils. A similar type of anion exchange may be involved in the retention of nitrate and chloride in acid highly weathered soils carrying a net positive charge.

Physical sorption involves the attachment of the sorbent and sorbate through weak atomic and molecular interaction forces (van der Waal forces) that operate when the electron clouds of the atoms do not overlap sufficiently to cause strong attractive forces. The activation energy for this type of attraction is characteristically low, much lower than is normally observed for ions (e.g., orthophosphate) which are bound more strongly.

Most anions, as well as several heavy metals, exhibit a property termed specific adsorption. This property involves the exchange of the ion with surface ligands to form partly covalent bonds with lattice ions. The net result is that the amount of ion adsorbed is far greater than would be expected for nonspecifically adsorbed species that are adsorbed according to their relative abundance (Mott 1970).

Organic compounds, including materials such as proteins, enzymes, viruses, pesticides, and bacteria can be sorbed to soil particles (McLaren and Peterson 1965, Marshall 1971, Green 1974, Weed and Weber 1974). As with inorganic species, the mechanisms are extremely complex and are even more difficult to categorize because of differing chemical and physical characteristics of natural and synthesized organic materials.

In summary, sorption is the equilibrium association of pollutants by soil particles. If adsorption is the dominant process for pollutant behavior in soils, then pollutant migration to groundwater can be substantially "retarded." When no sorption occurs the pollutant can--theoretically--follow the soil moisture or the groundwater flow velocity. In general terms sorption processes mediate pollutant mass partitioning between the solute and adsorbed phase of a compound. This partitioning forms the concept of mathematical modeling presented in the following section.

3.0 MATHEMATICAL MODELING

3.1 General

Sorption models have been developed by various researchers by assuming the existence of a relationship between adsorbed and dissolved concentration of a compound in the soil matrix.

$$s = s(c) \qquad \text{(AD-1)}$$

where

s = adsorbed concentration of pollutant on soil particles; (ug/g soil)

c = dissolved concentration of pollutant in soil moisture; (ug/mL)

By differentiating the above equation with respect to time, we have

$$\partial s/\partial t = (ds/dc)\cdot(dc/dt) \qquad \text{(AD-2)}$$

in which ds/dc represents the partitioning of the contaminant between the solution and the solids. The temporal adsorbed concentration change of a pollutant may be estimated in two ways: from (1) tabulated values of ds/dc versus c, and (2) algebraic empirical formulas giving s as a function of c, known as adsorption isotherms. The latter approach is the most common in mathematical modeling and has been also employed in SESOIL.

Tabulated values of ds/dc versus c and algebraic formulas are derived from laboratory experiments. From these experiments, the partitioning of solutes between liquid and solid phases in a porous medium is expressed in two-ordinate graphical form, where the mass adsorbed per unit mass of dry solids is plotted against the concentration of the constituent in solution. These graphical relations of s versus c and their equivalent mathematical expressions are known as isotherms because they are derived from experiments conducted at constant (isothermic) temperature. (Freeze and Cherry 1979.)

Laboratory results of adsorption experiments are commonly plotted on double logarithmic paper. For solute species at low or moderate concentrations, straightline graphical relations are commonly obtained over large range of concentrations, a fact that can be expressed by

$$\log s = b\cdot\log c + \log K \qquad \text{(AD-3)}$$

or by

$$s = K\cdot c^b \qquad \text{(AD-4)}$$

For b=1, we have the linear solution

$$ds/dc = K \qquad \text{(AD-5)}$$

where

s = adsorbed concentration of pollutant; (ug/g soil)

c = dissolved concentration of pollutant; (ug/mL)

K = adsorption (partitioning) coefficient; (ug/g soil)/(ug/mL)

b = coefficient; (-)

K is a valid presentation of the partitioning between liquid and solids only if the reactions that cause the partitioning are fast and reversible and only if the isotherm is linear. Many contaminants meet this requirement.

Several mathematical descriptions of adsorption isotherms have been presented in the literature. The Freundlich and the Langmuir relations are widely used, and the literature provides numerous examples of experimental data to agree with these isotherms.

3.2 The Freundlich Model

The Freundlich sorptive model is expressed by

$$s = x/m = K \cdot c^{1/n} \qquad \text{(AD-6)}$$

where:

s = adsorbed concentration of contaminant on soil particles; (ug/g soil)

x = adsorbed pollutant mass on soil; (ug)

m = mass of soil; (g)

K = adsorption (partitioning) coefficient; (ug/g)/(ug/mL)

c = dissolved concentration of pollutant in soil moisture; (ug/mL)

n = Freundlich equation parameter; (-)

The Freundlich equation is frequently written as $x/m=K \cdot c^n$; therefore, care should be taken to determine the form of equation used before any value of n obtained from the literature is used. Values of 1/n in equation AD-6 are generally found to range from 0.7 to 1.1, although values as low as 0.3 and as high as 1.7 have been reported. (Hassett et al in press.) No methods are available for estimating n; therefore, in the absence of data, it is frequently assumed n=1.0. (Lyman et al 1981.)

The value of the adsorption coefficient K can be measured directly for many inorganic pollutants. For most organic pollutants, sorption (partitioning) occurs mainly on the organic portion of the soil particles. For these organic chemicals, a partitioning coefficient K_{oc} can be determined, which is the ratio of the amount of pollutant associated with the organic carbon of the soil to the pollutant remaining in solution. The adsorption coeffient K is related to K_{oc} by

$$K = K_{oc} \cdot (\%oc)/100 \qquad \text{(AD-7)}$$

where

K = adsorption coefficient of compound; (ug/g)/(ug/mL)

K_{oc} = adsorption coefficient of compound on organic carbon (oc) contained in soil; (ug/g oc)/(ug/mL)

$(\%oc)$= percentage of organic carbon contained in the soil or sediment; (-)

A discussion related to K_{oc} is presented by Miller (1980). Some investigators have related K_{oc} to the K of the soil on organic matter (K_{om}) rather than on soil-organic carbon.

$$K_{oc} = k \cdot K_{om} \qquad \text{(AD-8)}$$

where the value of k has been found in many studies to be approximately equal to 1.724. (Lyman et al 1981.)

Values of K_{oc} may range from <1 to 10^7. The existence of this chemical-specific adsorption parameter has an important bearing on assessments of the fate and transport of chemicals in soils and sediments. K_{oc} is commonly used in river models, runoff models, soil and groundwater models where the transport of a specific chemical is being investigated. The degree of adsorption may not only affect a chemical's mobility but may also be an important parameter in fate processes such as volatilization, photolysis, hydrolysis and biodegradation. (Lyman et al 1981.)

Methodologies to estimate K_{oc} and n values are proposed in the literature (Lyman 1981), but it is beyond the scope of this section to outline in detail other researchers' work. Briefly, all of the available methods for K_{oc} include empirical relationships with some other property of the chemical such as water solubility, octanol/water partition coefficient and bioconcentration. The relationships are regression equations obtained from various data sets and are usually expressed in log-log form. Some factors influencing the K and K_{oc} values are temperature, pH of soil and water, water salinity, particle size distribution and surface area. Regression equations for the estimation of K_{oc} are given in Table AD-1. The uncertainty in values of K_{oc}, K and x/m=s estimated from the equations presented, is related to a number of factors including estimation method errors, uncertainty in input data, variability in environmental factors, errors from extrapolating the linear isotherm equations and errors associated with the assumption of desorption. (Rao and Davidson 1980.)

3.3 The Langmuir Model

The Langmuir isotherm model was developed for single layer adsorption; however, it has been found to closely describe soil adsorption phenomena. (Novotny et al 1978.) It is based on the assumption that maximum adsorption corresponds to a saturated monolayer of solute molecules on the adsorbent surface, that the energy of adsorption is constant, and that there is no transmigration of adsorbate on the surface phase. The Langmuir model (Weber 1972) is described by

$$\begin{aligned} ds/dt &= K_{sw}\cdot(s_e - s) \\ s_e &= Q^o\cdot b\cdot c/(1+c) \end{aligned} \qquad \text{(AD-9)}$$

where

ds/dt= temporal variation of adsorbed concentration of compound on soil particles; (ug/(g soil)·s)

s = adsorbed concentration of compound on soil particles; (ug/g soil)

K_{sw} = Langmuir equilibrium soil-water adsorption kinetic coefficient; (s^{-1})

s_e = maximum soil adsorption capacity; (ug/g soil)

Q^o = number of moles (or mass) of solute adsorbed per unit weight of adsorbent (soil) during maximum saturation of soil; (ug/g soil)

b = adsorption partition coefficient; (ug/mL)

t = time; (s)

c = concentration of pollutant in soil moisture; (ug/mL)

Laboratory studies can provide the values of Q^o and b; however, for most modeling and pollutant transport studies, these variables can be estimated only roughly from a few routinely measured soil parameters. (Krenkel and Novotny 1980.) Several authors have correlated phosphate,

TABLE AD-1

REGRESSION EQUATIONS FOR THE ESTIMATION OF K_{oc}

Eq. No.	Equation[a]	No.[b]	r^2[c]	Chemical Classes Represented
4-5	$\log K_{oc} = -0.55 \log S + 3.64$ (S in mg/L)	106	0.71	Wide variety, mostly pesticides
4-6	$\log K_{oc} = -0.54 \log S + 0.44$ (S in mole fraction)	10	0.94	Mostly aromatic or polynuclear aromatics, two chlorinated
4-7[d]	$\log K_{oc} = -0.557 \log S + 4.277$ (S in μ moles/L)	15	0.99	Chlorinated hydrocarbons
4-8	$\log K_{oc} = 0.544 \log K_{ow} + 1.377$	45	0.74	Wide variety, mostly pesticides
4-9	$\log K_{oc} = 0.937 \log K_{ow} - 0.006$	19	0.95	Aromatics, polynuclear aromatics, triazines and dinitroaniline herbicides
4-10	$\log K_{oc} = 1.00 \log K_{ow} - 0.21$	10	1.00	Mostly aromatic or polynuclear aromatics, two chlorinated
4-11	$\log K_{oc} = 0.94 \log K_{ow} + 0.02$	9	e	s Triazines and dinitroaniline herbicides
4-12	$\log K_{oc} = 1.029 \log K_{ow} - 0.18$	13	0.91	Variety of insecticides, herbicides and fungicides
4-13[d]	$\log K_{oc} = 0.524 \log K_{ow} + 0.855$	30	0.84	Substituted phenylureas and alkyl N-phenylcarbamates
4-14[d,f]	$\log K_{oc} = 0.0067 (P - 45N) + 0.237$	29	0.69	Aromatic compounds ureas, 1,3,5 triazines, carbamates, and uracils
4-15	$\log K_{oc} = 0.681 \log BCF(f) + 1.963$	13	0.76	Wide variety, mostly pesticides
4-16	$\log K_{oc} = 0.681 \log BCF(t) + 1.886$	22	0.83	Wide variety, mostly pesticides

[a] K_{oc} = soil (or sediment) adsorption coefficient S = water solubility K_{ow} = octanol water partition coefficient BCF(f) = bioconcentration factor from flowing water tests BCF(t) = bioconcentration factor from model ecosystems, P = parachor, N = number of sites in molecule which can participate in the formation of a hydrogen bond

[b] No = number of chemicals used to obtain regression equation

[c] r^2 = correlation coefficient for regression equation

[d] Equation originally given in terms of K_{om} The relationship $K_{om} = K_{oc}/1.724$ was used to rewrite the equation in terms of K_{oc}

[e] Not available

[f] Specific chemicals used to obtain regression equation not specified

Source: Lyman et al (1981).

phosphorus and organic chemical sorpitivity to various soil parameters, including Novotny et al (1978), Chesters (1967), and Sanks et al (1976). For example, Novotny et al (1978) proposed

$$Q^o = a_1+e_1 \cdot 10^{-pH}+c_1(\%clay/100)+d_1(\%oc/100) \qquad \text{(AD-10)}$$

$$b = a_2+e_2 \cdot 10^{-pH}+c_2(\%clay/100)+d_2(\%oc/100) \qquad \text{(AD-11)}$$

where

a, e, c, d = coefficients; (-)

(%clay) = percent of soil clay content; (%)

(%oc) = percent of organic carbon content; (%)

3.4 The SESOIL Model Equation

The Langmuir isotherm is often preferred in simulation models because of the equation linearity, as contrasted to the Freundlich equation that is nonlinear and may require numerical trial and error solution algorithms. However, it has been determined that adsorption of most chemicals--and especially of organic chemicals--more nearly approximates the Freundlich isotherm. Because of this fact, more laboratory and other data are available for the Freundlich equation in the literature; therefore, the Freundlich equation is employed and coded in the version of SESOIL accompanying this documentation. Coding of the Langmuir equation into SESOIL is a minor task.

Table AD-2 presents a summary of the Freundlich model and the input parameters required for SESOIL.

TABLE AD-2

THE FREUNDLICH ADSORPTION MODEL IN SESOIL

Equation

$$P(t) = c(t) \cdot K^{1/n} \cdot \rho \cdot d_i \qquad \text{(AD-6)}$$

where

$K = K$ (overall adsorption)

or

$$K = K_{oc} \cdot (\%\ oc)/100 \qquad \text{(AD-7)}$$

in which

		FORTRAN Variable
$P(t)$	adsorbed pollutant mass at time t; ug	PADSU, PADSL
$c(t)$	dissolved pollutant concentration at time t; ug/uL	CUS, CUM, etc.
* K	overall adsorption coefficient; (ug/g)/(ug/mL)	KU, KM, KL
* K_{oc}	adsorption coefficient on organic carbon (oc); (ug/g oc)/(ug/mL)	KOC
* % oc	organic carbon content of soil; (%)	OC
* n	Freundlich parameter; (-)	FRN
* d_i	soil layer depth i (i=1,N); (cm)	DU, DM, DL
* ρ	soil specific weight; (g/cm^3)	RS

Note: The user has to input to the data file of the model, either K or the set (K_{oc},%oc), since these sets are mutually exclusive.

* = input variables to this adsorption model.

4.0 DISCUSSION

Equation AD-6 implies that desorption processes between two sequential time steps t and t+1 are also explicitly accounted by SESOIL because, as long as c(t+1) is greater than c(t), adsorbed transformation will take place in the soil matrix; otherwise, [when c(t+1) less than c(t)] desorption will take place.

Adsorption and desorption processes can be also studied by writing two separate equations for each phase, namely

$$s_A = K_A \cdot c^{1/nA} \text{ for } c(T+1) \geq c(t); \text{ adsorption} \qquad \text{(AD-12)}$$

and

$$s_D = K_D \cdot c^{1/nD} \text{ for } c(T+1) < c(5); \text{ desorption} \qquad \text{(AD-13)}$$

We believe that these mathematical manipulations of the Freundlich isotherm will not substantially improve the output of the model though more input data will be required to make the model run. Input data for equations AD-12 and AD-13 are not always available in the literature; therefore, the sorption equation AD-6 is assumed to be satisfactory for long-term simulations. Equation AD-6 might not be satisfactory for soil-chemical systems subject to extreme fluctuations and for micro-scale short-term simulations (e.g., fraction of a day) because of reaction time differences (i.e., fast adsorption reaction, slow desorption reaction), though no definite conclusions can be made at this point for the accuracy of the model output.

5.0 NOTATIONS

a,	coefficients; (-)
b	adsorption partition coefficient, equation AD-4; (ug/mL)
b	coefficient; (-)
c	dissolved concentration of pollutant in soil moisture; (ug/mL)
d	coefficient; (-)
e	coefficient; (-)
K	overall sorption (partitioning) coefficient; (ug/g)/(ug/mL)
K_A	adsorption coefficient, equation AD-12; (ug/g)/(ug/mL)
K_B	desorption coefficient, equation AD-13; (ug/g)/(ug/mL)
K_{oc}	adsorption coefficient of compound on organic carbon; (ug/g oc)/(ug/mL)
K_{om}	adsorption coefficient of compound on organic matter; (ug/g om)/(ug/mL)
K_{sw}	Langmuir equilibrium soil-water adsorption kinetic coefficient; (s^{-1})
m	mass of soil; (g)
n	Freundlich equation parameter; (-)
s, s_A	adsorbed concentration of pollutant on soil particles; (ug/mL)
s_D	desorbed concentration of pollutant on soil particles
s_e	maximum soil adsorption capacity; (ug/g soil)
t	time; (s^{-1})
Q^o	number of moles of solute adsorbed per unit of weight of adsorbent (soil) during maximum saturation of soil; (ug/g soil)
x	adsorbed pollutant mass on soil; (ug)
% clay	percent of soil clay; (%)
% oc	percentage of organic carbon contained in the soil or sediment; (%)

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DE - degradation

APPENDIX DE[*]

DEGRADATION AND DECAY

---

[*] Contribution by K. Scow

1.0 INTRODUCTION

Biodegradation is an important environmental process causing the breakdown of organic compounds. It is a significant loss mechanism in soil and aquatic systems contributing the mineralization process of organic compounds, that is their conversion to inorganic substances.

Biodegradation or decay (designated in the following paragraphs as degradation) of pollutants in the soil is a complex phenomenon involving a variety of mechanics. The quantification of these mechanics and the effects of environmental factors on the degradation rates of pollutants is an active research area.

This appendix is not intended to review and describe the biodegradation or decay process of chemical compounds in soil systems; rather it provides an overall background information on the nature of biodegradation and the way this chemical process is modeled. Alternative modeling approaches are also possible by SESOIL.

Detailed information regarding the biodegradation process, constant estimates and data availability has been presented in the literature by K. Scow (1981).

2.0 BACKGROUND

Several definitions of biodegradation have been proposed in the literature such as primary, ultimate and acceptable biodegradation. In this chapter biodegradation is defined as the primary degradation of organic compounds, namely any structural transformation in the parent compound that changes its identity.

Microorganisms are the most significant group of organisms involved in biodegradation. Although higher organisms, both plant and animal, are capable of metabolizing numerous compounds, microorganisms may convert to inorganic substances (H_2O, CO_2, mineral salts) many organic molecules that higher organisms are unable to metabolize.

The most important natural habitats for microorganisms in relation to environmental biodegradation are soil and water. In both environments, microorganisms are essentially aquatic organisms, and certain characteristics are shared by all species (Stotzky 1979).

Soil environments have a diverse microbial population, because they offer a large variety of food sources and habitats (Hamaker 1972). The mobility of microorganisms is decreased in soil, however, because of physical barriers (such as clay aggregates) and particularly distribution of supportive microhabitats (Scow 1981).

The parameters that influence the rate of biodegradation can be grouped into two general categories:

(1) those that determine the availability and concentration of the compound to be degraded or that affect the microbial population size and activity (eg. population interactions) and

(2) those that directly control the reaction rate itself (eg. population size, temperature).

Both direct and indirect variables can be classified as substrate-related, organism-related or environmental-related. Because of considerable variation in species, habitat, and chemical environment, not all variables will influence all situations in the same way. For example, low pH is likely to decrease metabolic activity in most bacteria but it favors activity in fungi (Scow 1981).

Important environmental and other parameters affecting biodegradation can be pH, temperature, moisture content in soil, adsorption, oxygen pressure (aerobic, anaerobic reactions), salinity, solute concentration of the substance in soil etc.; however, all these parameters are lumped in one quantified constant describing total loss over time. This is the biodegradation rate constant discussed in the following section.

3.0 MATHEMATICAL ANALYSIS

The process of biological degradation of pollutants is limited to microbial metabolism of the compound under aerobic conditions. Degradation is defined as any structural alteration in the parent compound at which point it disappears from the soil. Metabolic products as new chemicals would re-enter a new model run as biotic input to soil.

The equation describing biodegradation requires input of a first-order rate constant determined for the particular pollutant being modelled. It should be measured in a soil culture test under conditions similar to the site being simulated and complying with state-of-the-art technology.

Pollutant losses in soil moisture due to biological degradation is estimated by:

$$dc/dt = -K_{DE} \cdot c^n \qquad \text{(DE-1)}$$

c = dissolved concentration of pollutant in soil moisture (ug/mL)

K_{DE} = rate of degradation; (day^{-1})

n = order of the reaction; ($n=1$; first order)

Although soil moisture content, temperature and other environmental parameters strongly influence biological activity, the present SESOIL routine does not describe their influence on the rate of degradation. Expansion of the equation to account for these factors is possible assuming that enough general or chemical-specific data are available to define the limits they set on degradation rates.

Equation (DE-1) has a general application in all soil zones of the soil compartment (see Appendix PT), and is employed as a first order reaction, n=1 to express loss/transformation of pollutants from the moisture content of the unsaturated soil zone.

The total pollutant mass decayed over a short period Δt in a soil compartment (layer i) can be finally expressed by

$$P_{DE} = K_{DE} \cdot \Theta \cdot c \cdot d_i \cdot \Delta t$$

where

P_{DE} = decayed chemical mass within Δt; (ug/cm^2)

K_{DE} = biodegradation rate; (day^{-1})

Θ = soil moisture content; (fraction)

c = solute concentration of pollutant in soil moisture; (ug/mL)

d_i = soil layer depth; (cm)

Δ_t = time step; (day)

4.0 REFERENCES

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HD - hydrolysis

APPENDIX HD*

HYDROLYSIS OF ORGANIC COMPOUNDS

---

*Contribution by W. Lyman, Ph.D.

Dec. 1981

1.0 INTRODUCTION

Organic chemicals may undergo a variety of reactions with water. One family of reactions that leads to an ultimate transformation of the organic molecule is called hydrolysis. Some chemical classes (e.g., hydrocarbons) are known to be generally resistant to hydrolysis while others (e.g., alkyl halides, carbamates) are potentially susceptible. The relative importance of the hydrolysis degradation pathway is enhanced in the soil/groundwater compartment--especially at depths of approximately one meter below ground surface--since other degradation and loss pathways (e.g., photolysis, biodegradation, and volatilization) are eliminated or minimized. Other reactions involving organic molecules and water do occur, but these processes are not included in this chapter. These other reactions include reversible reactions (e.g., acid-base reactions and hydration) and additional reactions which require reaction conditions that are unlikely to occur in the environment.

The hydrolysis subroutine of SESOIL allows the user to simulate neutral, base-catalyzed and/or acid- or base-catalyzed hydrolysis reactions. The current hydrolysis subroutine is based upon the assumption that both dissolved and adsorbed organics are equally susceptible to hydrolysis. Existing experimental data regarding this assumption is contradictory, although some data show that rates of hydrolysis are not significantly affected by the presence of moderate amounts of suspended solids in aqueous systems.

The following sections provide additional background on hydrolysis reactions, the mathematical equations involved and the limitations the user should be aware of. For additional information, model users are referred to the work of Harris (1981), since much of the information presented in this appendix is a summary of a more detailed investigation presented by this author.

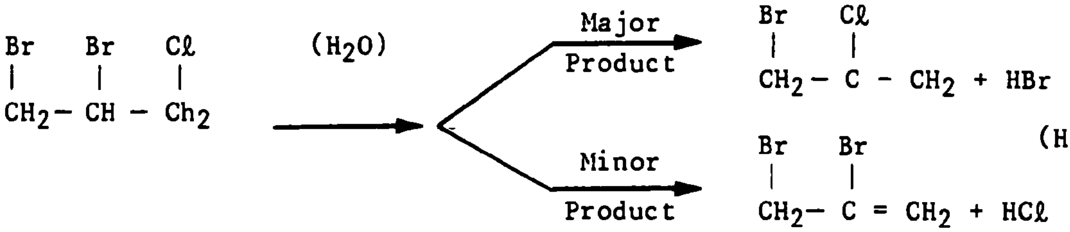
This appendix is <u>not</u> intended to thoroughly describe the hydrolysis process of organic compounds in soils; rather it provides background information on the nature of hydrolysis and the way this chemical process is modeled. Alternative modeling approaches are also possible by SESOIL.

2.0 BACKGROUND

Hydrolysis is a chemical transformation process in which an organic molecule, RX, reacts with water, forming a new molecule. By the normal definition of hydrolysis this involves the formation of a new carbon-oxygen bond and the cleaving of the carbon-X bond in the original molecule:

$$R\text{-}X \xrightarrow{H_2O} R\text{-}OH + X^- + H^+ \qquad \text{(HD-1)}$$

Other reactions involving water may result in the elimination of a hydrogen (H) and a leaving group (X) from neighboring carbons. This mechanism is apparently favored, for example, in the hydrolysis of Nemagon®:

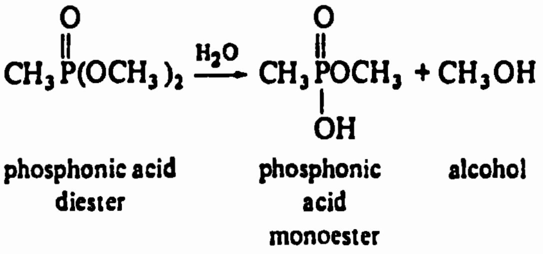


$$\overset{Br}{\overset{|}{CH_2}}-\overset{Br}{\overset{|}{CH}}-\overset{C\ell}{\overset{|}{Ch_2}} \xrightarrow{(H_2O)} \begin{cases} \xrightarrow[\text{Product}]{\text{Major}} \overset{Br}{\overset{|}{CH_2}}-\overset{C\ell}{\overset{|}{C}}-CH_2 + HBr \\ \xrightarrow[\text{Product}]{\text{Minor}} \overset{Br}{\overset{|}{CH_2}}-\overset{Br}{\overset{|}{C}}=CH_2 + HC\ell \end{cases} \qquad \text{(HD-2)}$$

Equations (HD-3) through (HD-8) illustrate some additional hydrolysis ractions, in which the identity of the original molecule is destroyed, although complete degradation is not implied. The initial products of hydrolysis may show wide variability in their susceptibility to subsequent degradation.

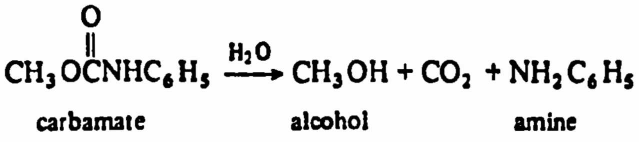
Certain types of hydrolysis reactions may be catalyzed by the presence of hydrogen ions, H^+, and/or hydroxide ions, OH^-. The concentration of these species in water is obtained from the pH of the water. Under certain conditions the model user may desire to account for these acid- or base-catalyzed reactions by specifying second-order rate constants for the catalyzed reactions.

The rate of hydrolysis of various organic chemicals, under environmental conditions, can range over more than 14 orders of magnitude, with associated half-lives (time for one half of the material to disappear) as low as a few seconds and as high as 10^6 years. Since the time resolution of SESOIL are on the order of a month to a few years, this subroutine should <u>not</u> be used for chemicals that hydrolyze extremely fast (e.g., $t_{1/2}$ less than 1 day) and need not be considered in modeling chemicals that hydrolyze extremely slowly (e.g., $t_{1/2}$ greater than 100 yrs).



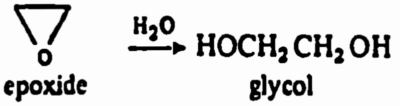
$$CH_3\overset{\overset{\displaystyle O}{\|}}{P}(OCH_3)_2 \xrightarrow{H_2O} CH_3\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle OH}{|}}{P}}OCH_3 + CH_3OH$$

(HD-3)

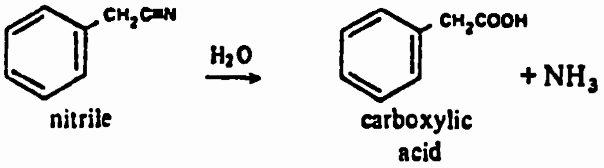


$$CH_3O\overset{\overset{\displaystyle O}{\|}}{C}NHC_6H_5 \xrightarrow{H_2O} CH_3OH + CO_2 + NH_2C_6H_5$$

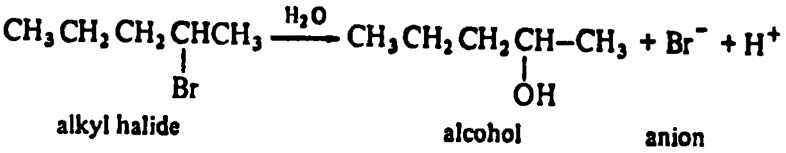
(HD-4)



(HD-5)

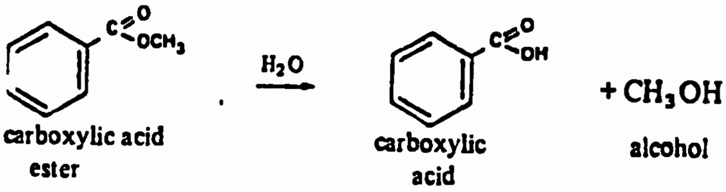


(HD-6)



$$CH_3CH_2CH_2\underset{\underset{\displaystyle Br}{|}}{C}HCH_3 \xrightarrow{H_2O} CH_3CH_2CH_2\underset{\underset{\displaystyle OH}{|}}{C}H{-}CH_3 + Br^- + H^+$$

(HD-7)



(HD-8)

Source: Lyman et al (1981).

Rates of hydrolysis are usually measured under controlled laboratory conditions that include constant temperature and may include the use of buffered solutions and solvating agents. Extrapolation of such data to environmental conditions involves considerable uncertainty, particularly with regard to the influence of temperature, solution ionic strength, adsorption on soils, and the possibility of catalytic action by either dissolved material (e.g., heavy metal cations) or solid surfaces. If uncorrected laboratory data are used in SESOIL--and this may often be the only choice--then model predicted pollutant concentrations should be considered as rough approximations only. Harris (1981) provides instructions for estimating hydrolysis rate constants for certain classes of chemicals.

It may be possible for a user to employ rate constants (k) that have been corrected for the difference between the temperature used for the measured (or estimated) value, and the temperature of the soil system. For example, if the activation energy (E_A) for the reaction is known, then extrapolation from a reported value of k_1, at temperature T_1, to an adjusted value of k_2 at temperature T_2 is given by:

$$k_2 = k_1 \exp - [\frac{E_A}{R} (\frac{1}{T_2} - \frac{1}{T_1})] \qquad \text{(HD-9)}$$

where:

k_2 = extrapolated hydrolosis rate constant of the compound at T_2; (sec^{-1})

k_1 = given hydrolysis rate constant of compound at T_1; (sec^{-1})

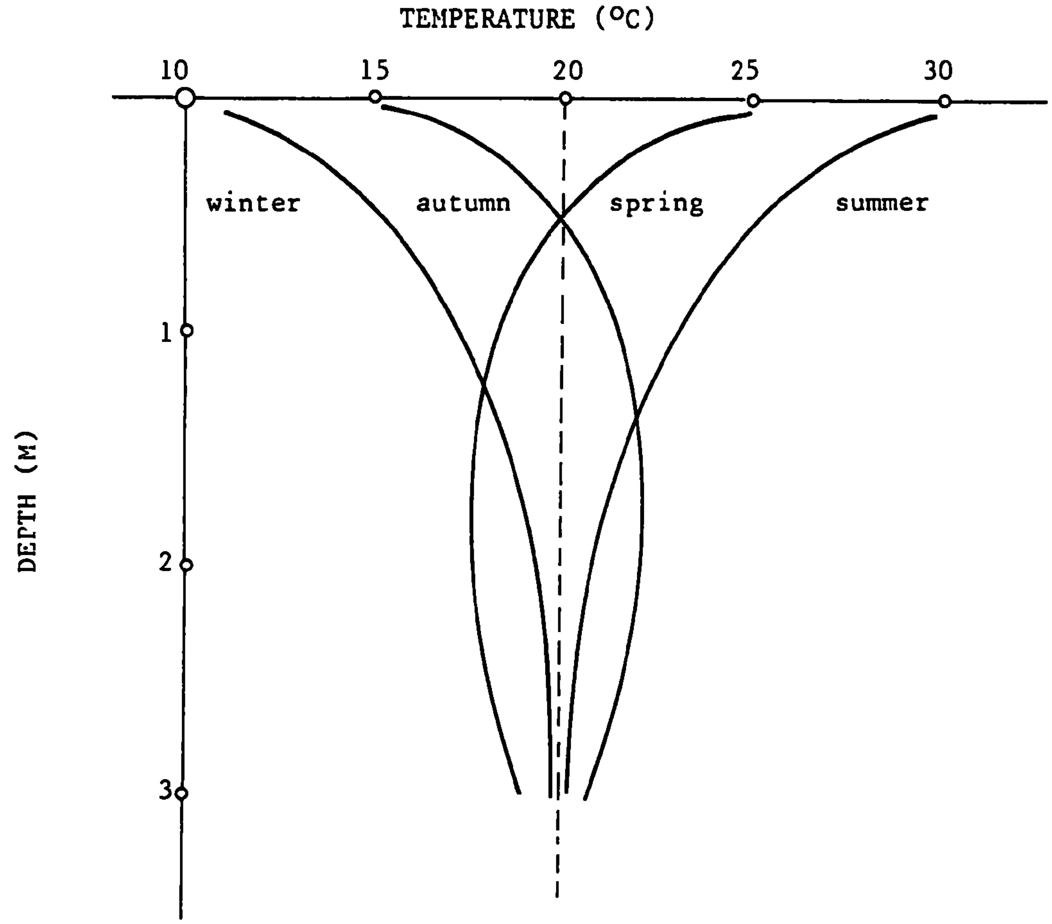
E_A = activation energy of reaction; (cal/mol)

R = gas constant of compound; (=1.987 cal/mol·K)

T_1, T_2 = temperature; (°Kelvin)

If a measured value of E_A is not available, a value of 17,500 cal/mole may be assumed (Harris 1981).

Soil temperature is generally a complex function of various parameters, such as geographic location, soil nature (including water content), soil depth, air temperature, and heat flow from below. For SESOIL, the diurnal variations in soil temperature (important for approximate the top meter of soil) can be ignored because of the longer time scales used by the model. Seasonal and depth variations, however, may be important and the user should seek to correct the estimated hydrolysis rate constants to the appropriate temperature. A typical soil-temperature profile as it might vary from season to season in a frost-free region is shown in Figure HD-1.



Source: Hillel 1980.

FIGURE HD-1

TYPICAL SEASONAL VARIATION OF SOIL TEMPERATURE PROFILE

3.0 MATHEMATICAL MODELING

3.1 Governing Equations

It is generally observed that hydrolysis of organic chemicals in water follows a first-order kinetic law, that is, the rate of its disappearance is proportional to the concentration of the compound:

$$-d[RX]/dt = k_T[RX] \tag{HD-10}$$

or by approximating the differential to a difference, by:

$$-\Delta[RX]/\Delta t = k_T[RX] \tag{HD-11}$$

where:

$[\ ]$ = concentration of organic compound RX; (mol/mL)

$d[] \approx \Delta[]$ = differential

k_T = hydrolysis rate constant; (day^{-1})

Δt = time, step in units compatible with k_T; (days)

The rate constant in equation (HD-10) is an oversimplification for most organic hydrolysis reactions. It is often appropriate to consider k_T as having contributions from neutral, acid-catalyzed and base-catalyzed reactions:

$$k_T = k_O + k_H[H^+] + k_{OH}[OH^-] \tag{HD-12}$$

where:

k_O = rate constant for neutral hydrolysis; ($days^{-1}$)

k_{OH} = rate constant for base-catalyzed hydrolysis; ($days^{-1}$ $mol^{-1} \cdot L$)

k_H = rate constant for acid-catalyzed hydrolysis; ($days^{-1}$ $mol^{-1} \cdot L$)

$[H^+]$ = hydrogen ion concentration = 10^{-pH}; (mol/L)

$[OH^-]$ = hydroxyl ion concentration = 10^{pH-14}; (mol/L)

The neutral rate constant (k_0) has units of (time^{-1}), while k_{OH} and k_H have units of (time^{-1}) · ($\text{concentration}^{-1}$). The user of the model must determine and input the values of k_0, k_{OH} and k_H; if no values are given a value of zero will be assumed. If k_H and k_{OH} are non-zero, then the pH of the soil water must also be input. This may require that some average pH and temperature be considered since SESOIL does not predict the variation in these parameters in the soil column.

For the SESOIL simulations, it is assumed that dissolved and adsorbed organic species are <u>equally</u> susceptible to hydrolysis, therefore, the total pollutant mass (M) degrated by hydrolysis during a simulation time step will be:

$$M_{total} = M_{H_2O} + M_{soil} \tag{HD-13}$$

By considering equations (HD-11) and (HD-13), we have:

$$M_{H_2O} = k_T \, [RX]_{H_2O} \cdot \Delta t \cdot V_{H_2O} \tag{HD-14}$$

$$M_{soil} = k_T \, [RX]_{soil} \cdot \Delta t \cdot V_{soil} \tag{HD-15}$$

or by employing the SESOIL designations and symbols:

$$M_{H_2O} = k_T \cdot c(t) \cdot \Delta t \cdot \theta(t) \cdot d_i \cdot AR \tag{HD-16}$$

$$M_{soil} = k_T \cdot s(t) \cdot \Delta t \cdot \rho \cdot d_i \cdot AR \tag{HD-17}$$

where:

M_{H_2O} = pollutant mass in soil moisture degrated by hydrolysis; (ug)

M_{soil} = pollutant mass on soil particles degrated by hydrolysis; (ug)

k_T = hydrolysis rate constant; (day^{-1})

$[RX]_{H_2O} = c(t)$ = dissolved concentration of pollutant at time t; (ug/ml)

$[RX]_{soil} = s(t)$ = adsorbed concentration of pollutant at time t; (ug/g of soil)

t = time; (days)

Δt = simulation time step; (days)

$\theta(t)$ = soil moisture at time t; (fraction)

d_i = depth of soil layer i; (cm)

ρ = soil density; (g/cm^3)

V_{H_2O} = volume of water in the compartment; (cm^3)

V_{soil} = volume of soil in the compartment; (cm^3)

AR = surface area of soil compartment; (cm^2)

3.2 Numerical Example

Calculate the mass of ethyl acetate hydrolyzed after one month in contact with a wet soil given: (1) an initial concentration of 100 ug/ml; (2) a soil temperature of 10°C; (3) hydrolysis rate constants at 25°C of 1.1×10^{-4} L/mol·s for k_H, 1.5×10^{-10} s^{-1} for k_0 and 1.1×10^{-4} L/mol·s for k_{OH}; (4) a soil moisture pH of 8.0; (4) no pollutant adsorbed on soil; (5) a soil moisture volume of 10 mL.

(1) To correct the rate constants from 25°C (298 K) to 10°C (283 K), use equation (HD-13) with an assumed value of 17,500 cal/mol for E_A.

$$k_2/k_1 = \exp\left[-\frac{17{,}500}{1.987}\left(\frac{1}{283} - \frac{1}{298}\right)\right] = 0.209$$

Thus, $k_H\ (10^oC) = 0.209 \cdot 1.1 \times 10^{-4} = 2.3 \times 10^{-5}$ L/mol·s

$k_0\ (10^oC) = 0.209 \cdot 1.5 \times 10^{-10} = 3.1 \times 10^{-11}\ s^{-1}$

$k_{OH}\ (10^oC) = 0.209 \cdot 1.1 \times 10^{-1} = 2.3 \times 10^{-2}$ L/mol·s

These corrected values (as well as pH) would be the user's input into SESOIL which would then carry out the following calculations.

(2) From equation (HD-12):

$$k_T = 3.1 \times 10^{-11} + 2.3 \times 10^{-5} \cdot 10^{-8} + 2.3 \times 10^{-2} \cdot 10^{-(8-14)} =$$

$$= 2.3 \times 10^{-8}\ s^{-1} = 1.99 \times 10^{-3}\ day^{-1}$$

(3) From equation (HD-14) with Δt = 30 days:

M_{H_2O} = Mass hydrolyzed=$1.99 \times 10^{-3} day^{-1} \cdot 100 ug/mL \cdot 30 days \cdot 10 mL = 59.7 ug$

3.3 Input Parameters

The input parameters to the hydrolysis routine are presented in Table HD-1. The chemical specific parameters (k, k_H, k_{OH}) can be obtained from handbooks (e.g., Lyman 1981). Site specific parameters must satisfy the needs of a site specific simulation and study.

TABLE HD-1

INPUT PARAMETERS TO THE HYDROLYSIS ROUTINE

	Parameter	Units	FORTRAN Variable
k_O	Neutral hydrolysis rate constant	day^{-1}	KNH
k_H	Acid catalyzed rate constant	$day^{-1} \cdot mol^{-1} \cdot L$	KAH
k_{OH}	Base catalyzed rate	$day^{-1} \cdot mol^{-1} \cdot L$	KBH
ρ	Soil density	g/cm^3	RS
d_i	Compartment depths	cm	DU, DM, Z
A	Compartment area	cm^2	AR
pH	pH of soil	-	PH

4.0 DISCUSSION

It is worth emphasizing again the assumptions made for the development of the hydrolysis subroutine in SESOIL.

- First, the calculations assume that dissolved and adsorbed organic species are equally susceptible to hydrolysis. If subsequent experiments show this to be a serious error, then the computer code would have to be modified to account only for an "available" fraction of pollutant.

- Second, the calculations consider only simple hydrolysis reactions (neutral, acid-catalyzed and base-catalyzed) and do not follow for general catalysis by other diverse acids, bases, cations or solids. The model does not consider effects of ionic strength or the presence of other dissolved organics, nor the variation of pH in the soil compartment, or temperature along the soil column.

- Third, the model assumes that the hydrolysis rate constants that are entered have been previously corrected to the correct soil temperature for the simulation.

The above assumptions imply that the model user should not "blindly" use just any laboratory-measured (or estimated) rate constants, but should give some considerations to the soil system modeled and the corrections that might have to be undertaken for the input data.

5.0 REFERENCES

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CE - cation exchange

APPENDIX CE*

CATION EXCHANGE

---

*Contribution by W. Lyman, Ph.D.

1.0 INTRODUCTION

Cation exchange is a mechanism by which cations in solution may be adsorbed on soil and thus removed from the mobile aqueous phase; charged species (cations) may exchange with various minerals and/or other soil constituents. The process of cation exchange is complex; for several ions--particularly metal cations--and under certain conditions, the cation exchange capacity of the soil is strongly correlated with the adsorption of the ion, as discussed in the next section.

The cation exchange subroutine of SESOIL is designed as an optional way of considering adsorption. Therefore, if this routine is used, the adsorption equation in SESOIL should not be used unless the user has selected the model inputs (cation exchange capacity and adsorption parameters) in a way to avoid any "double counting" for adsorption.

It is incumbent upon the user to insure that cation exchange is the predominant adsorption mechanism at the site being modeled. This may require considerations of the leachate characteristics (pH, ionic strength, concentration of major cations), metal speciation and soil characteristics.

This appendix is not intended to thoroughly describe the cation exchange chemistry of species in soils; rather it provides background information on the nature of cation exchange and the way this chemical process is modeled. Alternative modeling approaches are also possible by SESOIL.

2.0 BACKGROUND

The cation exchange capacity (CEC) of a soil is usually defined as the number of milliequivalents (m.e.) of the ion that can be exchanged (adsorbed) per 100 g (dry weight) of soil. The process is viewed as an exchange with some other cation that initially occupies the adsorption site on the solid. With clays, the exchanged ion is often calcium:

$$M^{++} + [\mathrm{Clay}] \cdot \mathrm{Ca} \rightleftharpoons \mathrm{Ca}^{++} + [\mathrm{Clay}] \cdot M \qquad \text{(CE-1)}$$

Among soils, clays tend to have the highest CEC values, although materials other than clay may contribute. Brady (1974) lists, for example, the following typical CEC values (m.e./100 g) for various materials: humus, 200; monomorillonite, 100; vermiculite, 150; hydrous mica and chlorites, 30; kaolimite, 8; and hydrous oxides, 4. He also provides data showing a range of CEC values in soils of 2-60 m.e./100g. This range is somewhat larger than the 2-37 m.e./100 g range associated with 11 soils studied by Fuller (1978), which in turn is larger than the 0-4.2 m.e./100 g range given by Wang et al (1975) for 30 soils in Rhode Island. The cation exchange capacity of a soil is not an invariable property of the soil; in most soils the exchange capacity increases with pH (Brady 1974).

The actual cation exchange reation--equation (CM-1)--is probably fast and is also reversible. One cation with a high affinity for an exchange site may displace the cation previously at the site if the latter has a lower affinity. This is called the "mass action" effect. The relative strengths of soil-cation interactions are seldom available from the literature; therefore, they are not modeled in SESOIL. Furthermore, very high concentrations of certain cations (e.g., the common Ca^{++}, Na^{+}, Fe^{++}, and K^{+}) may so overwhelm the exchange capacity of a soil that low concentrations of other cations--including those with higher affinities--will not be significantly adsorbed. Landfill leachates and aqueous industrial wastes often have very high concentrations of total dissolved solids (including Na^{+}, Ca^{++}, etc.) and one would expect the major cations in these wastes to effectively block the adsorption (by cation exchange) of other trace cations for some significant time and distance in the migration through the soil/groundwater system.

Without some laboratory data, it is difficult to predict when cation exchange will be important and for what cations. This is not to say that some situations have not been modeled. They have, but the models usually require the use of equilibrium constants, the consideration of the "mass action" and pH effects, and also require detailed knowledge about the nature of the soil and the constitutents (e.g., other major cations and anions) of the leachate. This information will seldom be easy to assemble. Griffin and Shimp (1978) give examples of cases in which cation exchange is likely to be important for Pb, Cu, Zn, Cd, Na, K, Mg, and NH_4. For the heavy metals, cation exchange is unlikely to play a significant role if the leachate pH is above 7; above this pH, precipitation may be the controlling factor in mobility.

It should be mentioned that the present version of SESOIL does not specifically consider the process of fixation for pollutants in the leachate. Fixation is a process whereby the pollutant (e.g., a metal cation) diffuses into the small pores or interstitial layers of the soil matrix and, following some form of chemisorption or bonding, becomes permanently bound (fixed) to the soil. Fixation can be a very important removal process for heavy metals in some situations. The fixation process might be simulated for SESOIL, however, by appropriate use of the adsorption or cation exchange routines that are available.

3.0 MATHEMATICAL MODELING

3.1 Governing Equations

The SESOIL subroutine for cation exchange is optional and when used will presumably obviate the need for any other adsorption subroutine. For modeling purposes, the process is considered to be "irreversible." The calculation of the pollutant mass immobilized by cation exchange is given by:

$$MECM = a \cdot CEC \cdot MWT/VAL \qquad (CE-2)$$

where:

MECM = maximum pollutant mass immobilized (cation exchanged) by the soil; (ug/g soil)

a = 10.0; units coefficient; (-)

CEC = cation exchange capacity of soil; (m.e./100g of dry wt. soil)

MWT = pollutant molecular (or atomic) weight; (g/mol)

VAL = valence of cation; (-)

Example:

Pollutant: Pb^{++} (MWT = 207, VAL=2)

Soil with: CEC = 3 m.e./100 g (of dry soil)

MCEC = 10.3.207/2 = 3100 ug/g soil

Once the maximum capacity of the soil has been reached in a given soil element, SESOIL will assume that no further adsorption takes place unless another adsorption subroutine has also been employed (e.g., for fixation modeling). Cation exchange is assumed to be instantaneous; therefore, it is modeled as proceeding to completion before the start of all other processes. These assumptions must be made in order to model a cation exchange process that is general to many situations. When more specific data are available, modifications to this routine can be made.

3.2 Input Parameters

The input parameters to the cation exchange routine are presented in Table CE-1. Data are available from soil and chemical handbooks.

TABLE CE-1

INPUT PARAMETERS TO CATION EXCHANGE ROUTINE

Parameter	Units	FORTRAN Variable
Cation exchange capacity of the soil	(ug/100 g dry soil)	CEC
Molecular or atomic weight of pollutant	(g/mol)	MWT
Valance of pollutant	(-)	VAL

4.0 DISCUSSION

It is incumbent upon the user to determine when it will be appropriate to use the cation exchange subroutine. This may require, as mentioned above, a consideration of the "speciation" of the pollutant, the soil pH, the presence of other cations, and the nature of the soil. For most metals the speciation can be predicted with models such as REDEQL (Ingle et al 1980). In general, no other adsorption routine should be used when the cation exchange routine is employed. The calculations in SESOIL assume a fast, irreversible removal of the cations from solution, no competition with other ions, and a higher priority than any other process in competition for the cation in solution.

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CM - complexation

APPENDIX CM[*]

COMPLEXATION OF METALS IN SOLUTION BY ORGANIC LIGANDS

TABLES

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[*] Contribution from W. Lyman, Ph.D.

1.0 INTRODUCTION

Complexation (or chelation) is the process by which metal ions and organic or other nonmetallic molecules (called ligands) can combine to form stable metal-ligand complexes.

It is well known that a number of organic materials, of both natural and anthropogenic origin, are capable of complexing with several heavy metals including (but not limited to) Cu, Pb, Fe, Zn, Cd and Ag. The complex that is formed will generally prevent the metal from undergoing other reactions or interactions that the free metal cation would.

The current level of understanding of this process is not very advanced (less so for interactions in groundwater and leachates than in surface waters) and the available information has not been shown to be particularly useful to quantitative chemical modeling (Jenne 1979; McCrady and Chapman 1979). However, complexation can have a significant effect on the behavior of metals and soils; therefore, a simplified representation of the complexation process is incorporated in SESOIL. As the process (and factors that affect it) becomes better understood and quantifiable, this routine can be improved to reflect the new knowledge.

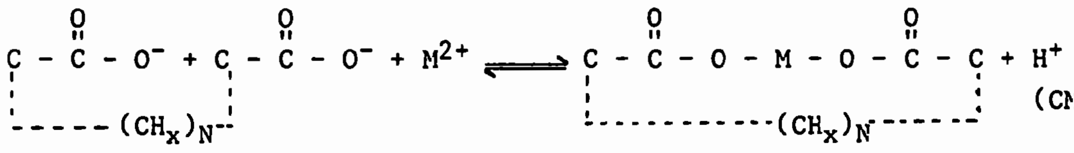
The current complexation subroutine of SESOIL allows the user to consider only a process in which a metal ion in solution is complexed by an organic ligand resulting in the formation of a soluble complex. It is incumbent upon the model user to determine if such a process is likely in the situation being modeled and to supply the appropriate stability constant, ligand concentration and mole ratio of metal to ligand in the complex.

This appendix is <u>not</u> intended to fully describe the complexation process of metals in solution by organic ligands; rather, it provides background information on the nature of complexation and one way this chemical process is modeled. Alternative modeling approaches in SESOIL <u>are</u> possible.

2.0 BACKGROUND

It is believed that metals bind to humic and fulvic acids through three possible types of bonds as shown in equations (CM-1), (CM-2) and (CM-3). (Giesy and Alberts 1981.)

$$R-\overset{O}{\overset{\|}{C}}-O^- + M^{2+} + H_2O \longrightarrow R-\overset{O}{\overset{\|}{C}}-O-M-OH+H^+ \qquad \text{(CM-1)}$$



$$\underbrace{C-\overset{O}{\overset{\|}{C}}-O^- + C}_{(CH_x)_N}-\overset{O}{\overset{\|}{C}}-O^- + M^{2+} \rightleftharpoons \underbrace{C-\overset{O}{\overset{\|}{C}}-O-M-O-\overset{O}{\overset{\|}{C}}-C}_{(CH_x)_N} + H^+ \qquad \text{(CM-2)}$$

$$\underbrace{C-\overset{O}{\overset{\|}{C}}-O^- + C}_{(CH_x)_N}\cdot OH + M^{2+} \rightleftharpoons \underbrace{C-\overset{O}{\overset{\|}{C}}-O-M-O-C}_{(CH_x)_N} + H^+ \qquad \text{(CM-3)}$$

Similar reactions may be involved in complexation with low molecular weight carboxylic acids such as those commonly found in landfill leachate. A general equation for this type of complexation reaction can be written as:

$$M^{x+} + bL^{y-} \rightleftharpoons (ML_b)^{x-by} \qquad \text{(CM-4)}$$

where one mole of a metal cation (M) with a change of x+ reacts with b moles of an organic ligand (L) with a charge of y- to yield one mole of the organo-metal complex (ML_b) with charge x-by. The stability (or dissociation) constant, K, for the complex is:

$$K = \frac{[ML_b{}^{x-by}]}{[M^{x+}][L^{y-}]^b} \qquad \text{(CM-5)}$$

where the brackets indicate molar concentration of the species. Values of K are a function of pH, ionic strength, and temperature. In some cases, the metal and ligand will form 1:1 complexes (in which case b=1) but certain ligands such as the humic and fulvic acids may have more than one effective binding site per equivalent.

A significant fraction of the humic and fulvic acids in surface waters is probably present in macromolecular or colloidal form (Gachter et al

1978; Giesy et al 1978) and in soils this material would likely be associated with the solid matrix of the soil. Low concentrations of these materials will be in solution although complexation with metals may cause some precipitation (Saar and Weber 1980) and adsorption of a soluble complex by soil is certainly possible. The complexation subroutine in SESOIL is only intended to model the situation where a soluble ligand reacts with a metal ion to form a soluble, nonadsorbable complex. Complexation by materials in the solid phase of the soil may be modeled (in some cases) by the cation exchange subroutine.

Considerably more information appears to be available on metal complexation in surface waters than in ground waters. Reports covering complexation in soils, sediments, groundwaters and/or leachates that may be useful to the reader include the works of Saar and Weber (1980), Kuo and Baker (1980), Davis and Leckie (1978), Knox and Jones (1979), Nriagu and Coker (1980), Oakley et al (1980), Oakley et al (1981), Pagenkopf (1978), Griffin and Shimp (1978), and Khalid et al (1977); papers by Fuller et al (1980) and O'Donnell et al (1980) report, in part, on the inverse correlation between metal mobility in soils and the total organic carbon content of the carrier fluid (leachate). The organic material in the leachate presumably contains low molecular weight carboxylic acids and higher molecular weight acids, including humic and fulvic acids, which complex the metals to form a complex that is less mobile than the free metal due to increased adsorption of the complex and/or to hindered movement of large molecules in the small pores of the soil. More general infomration on complexation may be found in the works of Geisy and Alberts (1981), Brinkman and Bellama (1978), and Sposito (1981).

In sediments, and presumably in soils, some studies (Pagenkopf 1978; Griffin and Shimp 1978) have shown that metals may be solubilized (desorbed) by the presence of complexing agents. However, just which metals can be solubilized, to what degree, and under what conditions is not predictable. If the user of SESOIL selects both the cation exchange and complexation subroutines, the model will assume that cation exchange takes precedence (i.e., happens first) and that ions involved in cation exchange are unavailable for complexation. (See Appendix CE). Other adsorption processes (e.g., via Langmuir or Freudlich equations) are modeled as being competitive with complexation. There is no clear justification for this order of operations and revisions of the subroutine are desirable as new data and better understanding are obtained.

In summary, agents or ligands can "pull" metals off the soil in certain cases, but when and how this occurs is unknown. Hence, in modeling cation exchange (see Appendix CE), we do not allow solubilization. The other sorption processes are modeled as being fully reversible, and thus complexation and adsorption will be competitive for available pollutant. However, complexation is not modeled as having an active role in the desorption of pollutant.

As with cation exchange, competition from other metal ions is an important consideration in complexation. A variety of metal cations may be complexed and a particular metal ion that is complexed may be displaced by a cation (present in equal concentrations) of higher affinity or by a cation of lower affinity if the latter is present in greater concentrations. In landfill leachate, competition with iron for complexation sites may be the most important consideration (Knox and Jones 1979). The present complexation subroutine in SESOIL does <u>not</u> consider such competition.

The complexation reaction is relatively fast compared to the simulation time steps of SESOIL although equilibrium partitioning in some cases may not be achieved for a few days (Oakley et al 1980). Values of the stability constant appear to range from about 10^2 to 10^{16} for the complexation of some common heavy metals (Cn, Cd, Zn, Fe, Co, Ni, Pb, Hg) with humic and fulvic acids (Pagenkopf 1978). Significantly higher values (10^5 to 10^{21}) are associated with some of the manmade chelating agents such as NTA, EDTA, HEDTA and CDTA (Drake et al 1976). As mentioned previously, the values of K are a function of pH and ionic strength. In general, K increases with increasing pH, and decreases with increasing ionic strength (Khalid et al 1977).

3.0 MATHEMATICAL MODELING

The mathematical expressions employed to model the complexation process and their corresponding input parameters are discussed in the following sections.

3.1 Mathematical Expressions

The mathematical modeling of complexation in SESOIL is based upon equation (CM-5) and the constraint of conservation of mass. Thus for either of the uncomplexed species,the concentration of the free species is equal to the total input (T) of that species minus the amount complexed (c):

$$[M^{x+}] = [M_T] - [M]_c \qquad \text{(CM-6)}$$

$$[L^{y-}] = [L_T] - [L]_c \qquad \text{(CM-7)}$$

The equilibrium constant (equation CM-5) has been written so that the each mole of complex includes one mole of metal and b moles of ligand.

$$[M]_c = [ML] \qquad \text{(CM-8)}$$

$$[L]_c = b[ML] \qquad \text{(CM-9)}$$

By combining equations (CM-5) through (CM-9) and omitting the designation of charges we have:

$$[ML] = K\,([M_T] - [ML])\,([L]_T - b[ML])^b$$

where:

$[M_T]$ = total concentration of metal in solution; (mol/mL)

$[ML]$ = complexed concentration of metal (with organic ligand) in solution; (mol/mL)

K = stability (or dissociation) constant of the complex; (-)

$[L_T]$ = total concentration of organic ligand in solution; (mol/mL)

b = number of moles of organic ligand reacting with one mole of metal cation (M); (-)

This equation is a non-linear equation (b does not necessarily = 1) and must be solved numerically. This numerically solution is performed for the monthly routines in subroutine COMP which used the same iterative procedure as used to the pollutant cycle (see appendix PT).

For the annual routines, which require an analytic solution, the ligand input concentration is assumed to be large compared to the amount of ligand complexed:

$$[L]_T > [L]_c \quad \text{therefore}$$

$$[L^y] = [L_T] - [L_c] \approx [L_T].$$

In this case equation CM-10 reduces to

$$[ML] = \frac{K[L]^b[M_T]}{1 + K[L_T]^b}$$

The masses of free and complexed species can be obtained from the concentrations by multiplying the concentration of the complex by the volume of the subcompartment:

$$P_{ML} = a \cdot [ML] \cdot V_{H2}O \qquad \text{(CM-8)}$$

where:

P_{ML} = pollutant mass complexed during time step of simulation (mol)

a = 1 conversion units factor (mL/cm^3)

$[ML]$ = complexed concentration of metal in solution; (mol/ml)

V_{H_2O} = $\theta \cdot d \cdot A$; volume of water (moisture) in soil subcompartment; (cm^3)

θ = volumetric moisture content of soil subcompartment; (fraction)

d = depth of soil layer; (cm)

A = cross sectional area of soil compartment; (cm^2)

In SESOIL, pollutant (i.e., metal) masses are expressed in units of micrograms (ug), in contrast to the previous expressions which are expressed in moles (mol). To convert from moles to micrograms, the molecular weight of the compound can be used as follows:

$$P \text{ (in ug)} = \frac{P\text{(in mole)}}{MWT \cdot f} \qquad \text{(CM-9)}$$

where:

P = pollutant mass

MWT = molecular weight of pollutant; (g/mol)

f = units conversion factor; (10^6 ug/g)

The expressions used in SESOIL for obtaining the mass of pollutant complexed are shown in Table CM-1. Note that the engineering designations of concentration ([M]) have been changed, so that the pollutant concentration at the step t is not designated as c(t).

3.2 Input Parameters

Input parameters to the complexation routine are presented in Table CM-2.

Compartment depths and input masses are chosen according to the needs of the simulation. Chemical/ligand specific constants are available from handbooks and laboratory studies.

Laboratory data sometime imply non-integer values for b. These non-integer values are accepted and used by SESOIL. For example, studies of the complexation of cadmium in landfill leachate by Knox and Jones (1979) indicated b values were in the range of 0.7 to 1.5 with an average of about 1.1.

For further information about input parameters and formats, see the user's manual section.

TABLE CM-1

EQUATION DESCRIBING THE COMPLEXATION CONCEPT IN SESOIL

Annual Routines (LEVEL 0, 1):

$$[L] = LIG_i/(\Theta \cdot d_i)$$

$$P[ML] = \frac{K([L]/MWT_L \cdot 10^6)^b (c(t)/MWT_M \cdot 10^6)}{1 + K([L]/MWT_L \cdot 10^6)} \cdot MWT \cdot \theta(t) \cdot d_i \cdot 10^6 \qquad \text{(CM-10)}$$

Monthly Routines:

$$\left.\begin{aligned} [L] &= LIG_i/(\Theta \cdot d_i) \\ [ML] &= K \cdot ([M_T] - [ML])\ ([L]_T - b[ML])^b \\ P[ML] &= [ML] \cdot \Theta(t) \cdot MWT \cdot 10^6 \cdot d_i \\ [L]_F &= [ML] \cdot \Theta(t) \cdot b \cdot MWT_L \cdot 10^6 \cdot d_i \end{aligned}\right\} \text{(solved iteratively)}$$

Parameter		Parameter Description	Units	FORTRAN Code
P[ML]	=	pollutant mass complexed during time step of simulation	(ug/cm^2)	PCOM
K	=	stability constant of the complex	(-)	SK
[L]	=	concentration of organic ligand in solution	(ug/mL)	LIGCU, LIGCL
MWT_L	=	molecular weight of L	(g/mol)	MWTLIG
c(t)	=	concentration of pollutant in solution	(ug/mL)	CUM, CMM, CLM
MWT_M	=	molecular weight of pollutant	(g/mol)	MWT

TABLE CM-1 (Continued)

EQUATION DESCRIBING THE COMPLEXATION CONCEPT IN SESOIL

b	=	number of moles of organic ligand reacting with one mole of the metal cation	(-)	B
$\theta(t)$	=	volumetric soil moisture content of soil	(-)	THA, THM
t	=	time of simulation		DT
d_i	=	depth of soil layer i	(cm)	DN, DM, DR
LIG_i	=	input mass of ligand	ug/cm^2	LIGU, LIGL
$[L]_F$	=	free ligand concentration	ug/mL	LIGUF, LIGLF

TABLE CM-2

INPUT PARAMETERS FOR COMPLEXATION ALGORITHMS

Parameter			FORTRAN Variable
Name	Designation	Units	
Soil Compartment Depths	d	cm; m	DL (upper), DM (middle) DL (lower)
Complexation Stability Constant	K	-	SK
Input Mass of Ligand	LIG_i	ug	LIGIN
Input Mass of Pollutant	-	ug	POLIN
Ratio: Moles Ligand/ Mole of Complex	b	-	B
Molecular Weight of Metal	MWT	g/mol	MWT
Molecular Weight of Ligand	MWT_L	g/mol	MWTLIG

4.0 DISCUSSION

As discussed in the previous sections, the subroutine calculations for complexation in SESOIL:

(1) are primarily for heavy metal cations in solution;

(2) do not consider competition with other ions or the effect of pH and ionic strength;

(3) assume equilibrium exists at all times;

(4) assume that complexation is fully reversible and competes with all other processes (except cation exchange); and

(5) assume that the complex formed is soluble, does not adsorb on the soil, and does not migrate from zone to zone.

(6) assume (for annual routines only) that the total ligand mass input is large compared to the ligand mass involved in complexation. This assumption is not made in the monthly routines.

It is incumbent upon the user to use this routine in the appropriate manner for environmental conditions where complexation is known to be a dominant factor in the mobility of the metal ions.

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CE - cation exchange

APPENDIX PH

PHOTOLYSIS

Photolysis of pollutant on soil surface layers might be another mechanism of pollutant loss. This process -- important for certain compounds -- will be incorporated in another SESOIL version.

FX - fixation

APPENDIX FX

FIXATION

Fixation is an important transformation process for certain compounds. It has been suggested by many scientists who are interested in SESOIL's modeling to incorporate into the model this process in the near future.

APPENDIX BI

BIOLOGIC ACTIVITIES

SESOIL is structured in a way that may allow the modeling of processes dealing with biologic activities in the soil. Although no definite plans are made by the developers regarding these issues, they believe that a SESOIL expansion in this area would lead to quite a useful tool for studying biologic soil activity due to manmade actions, as for example, POTW disposal actions on land.

NU - nutrient cycle

APPENDIX NU[*]

NUTRIENT CYCLE[**]

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[*] This subroutine is not operational; therefore, no great emphasis has been placed in its accurate documentation.

[**] Contribution from Joo Hooi Ong.

1.0 INTRODUCTION

1.1 General

Certain elements are essential for the growth of plants. These elements are called nutrients and are obtained from air and from water in the soil. Carbon, oxygen, and sometimes nitrogen (e.g. legumes can use gaseous nitrogen) are obtained from air. Of the nutrients required from soil, nitrogen, phosphorus, potassium, calcium, magnesium and sulfur are needed in relatively large quantities. Essential elements used in small amounts, i.e. trace elements include iron, manganese, boron, molybdenum, copper, zinc, chlorine, and cobalt. Nitrogen and phosphorus will be considered in the model because they are the principal nutrient pollutants.

In agricultural applications, nitrogen and phosphorus are usually supplied to the soil in the form of manure and commercial fertilizers. Nitrogen is commonly applied in the form of ammonium and nitrate salts and as urea. Other major ways by which nitrogen becomes available to plants are through fixation of gaseous nitrogen by bacteria, and through nitrogen dissolved in precipitation. These latter ways are especially important in natural ecosystems. Phosphorus is mostly applied as phosphates.

Nutrients in the soil are subject to various fate processes. They are absorbed by plant roots, transformed from one chemical form to another, adsorbed onto organic matter and clays, transported from the soil surface in runoff, or leached into the groundwater zone. Environmental quality is related to nutrient fate, for example, when nitrogen or phosphorus is transported from land into waterways and lakes, eutrophication and fish kills may result. If nitrates migrate into the groundwater zone and into drinking water supplies, health effects may result from ingestion of these supplies. A form of anemia called methaemoglobanaemia which predominantly affects children is caused by ingestion of nitrates. The use of fertilizers to increase productivity in agricultural areas must therefore by managed to minimize adverse environmental effects. A tool to predict nutrient concentrations in runoff, in the soil column, and in groundwater would be an important part of this management process.

The nutrient cycle module of SESOIL simulates the transport, transformation, and storages of nitrogen and phosphorus in the soil column. The nitrogen and phosphorus cycles in the environment and the nature of the microbial and chemical reactions involved in these cycles are described in the following sections. Following this background information, the mathematical formulation of these processes and the solution technique are explained.

1.2 Literature Review

A pioneering work in modeling nutrient cycling in soils is presented in the Agricultural Runoff Management (ARM) model (Donigian, *et al.*, 1977). The same subroutines, together with some extensions have later been incorporated into the Hydrological Simulation Program - Fortran (HSPF) model (Johanson, *et al.*, 1979). Both the ARM and the HSPF models simulate nitrogen and phosphorus transport and transformations in the soil column, and nutrient content in sediments and runoff from small agricultural watersheds. The soil column is divided into four zones in the ARM and HSPF models: (1) surface zone, (2) upper zone, (3) lower zone, and (4) groundwater zone. The transformations of the nutrient species are described by first order kinetics with a temperature correction using the Arrhenius equation. ARM uses regression equations for estimating soil temperatures from air temperatures. The ARM model simulates plant uptake of nitrate and phosphate by using monthly rate constants. HSPF includes uptake of ammonium by plants. It varies plant uptake on a monthly basis and distributes the uptake rate of nitrogen between nitrate-N and ammonium-N by factors, the sum of which is 1.0. The effect of moisture content on nutrient transformations is taken into account by discontinuing all transformations at very low moisture values. On the surface zone, transformations do not occur except during storm events since ARM assumes that the surface zone is dry except when runoff is occurring.

Another model which simulates nutrient transport and transformation is the CREAMS model (Knisel, 1980). This model is to be applied to field size areas and gives as output, the average concentrations of soluble nitrogen and phosphorus in runoff, the amount of nitrate leached and its average concentration, and the amounts of nitrogen and phosphorus associated with sediments. Phosphorus compounds are not simulated in the soil column, i.e., no phosphorus is assumed to leach into the soil. The soluble nitrogen compounds leached into the soil are assumed to be nitrate or compounds that are quickly converted to nitrate and are added to the nitrate pool in the soil. The soil column in CREAMS is divided into the surface layer and the root zone. On the surface, nutrients (soluble nitrogen and phosphorus) are removed with runoff and with the sediments. In the root zone, mineralization and denitrification are simulated using first order kinetics. Plant uptake and percolation of nitrate also occur at the root zone. Two options are available for calculating plant uptake: (1) plant growth as a function of plant water use and nitrogen uptake as a function of plant nitrogen content, and (2) by assuming that nitrogen uptake follows a normal probability curve. The denitrification rate is modified by the moisture content of the soil by assuming that the rate constant is only positive when the moisture content exceeds field capacity.

The nutrient cycle module in SESOIL simulates nitrogen and phosphorus transport and transformations in the soil column, and the concentrations in sediments and in runoff. SESOIL is not limited by the size of the watershed modeled and it does not need to be calibrated.

Many of the principles in the ARM model are used in the nutrient cycle module in SESOIL. The differences between the two models are:

(1) SESOIL uses monthly temperature inputs for each soil zone while ARM uses regression equations for estimating soil temperatures. The advantage of having user-input temperatures is that the model does not have to be calibrated to each site.

(2) SESOIL includes plant uptake of ammonium-N whereas ARM only has an uptake rate for nitrate-N. HSPF does however include plant uptake of ammonium-N. Since uptake of ammonium-N is a major nitrogen uptake path in most applications, it would be more accurate to include it.

CREAMS is useful in applications when nitrate leaching, availability of nitrogen to plants, and nutrient concentrations in runoff and sediments are the primary interests. Since it does not simulate storages of any other species except nitrate in the soil column, it cannot be used to predict nutrient concentrations in soils. The nutrient cycle module in SESOIL would, therefore, have a wider application than the CREAMS since the soil column is modeled in SESOIL.

2.0 BACKGROUND

Both the nitrogen and phosphorus cycles consist of many physical, chemical and biological processes, and very often combinations of these processes. Because of the difficulty involved in defining precisely which mechanism is involved in each phenomenon, this section provides only background information about the nitrogen and phosphorus cycles. Detailed descriptions are not given here of the process mechanisms and dependencies on environmental factors, such as temperature, organic carbon content, oxygen content, soil moisture content, and pH. Quantitative knowledge of these relationships are generally lacking. A comprehensive qualitative source for understanding the nitrogen cycle in soils is Bartholomew (1965). Similarly, Larsen (1967) provides a review of the phosphorus cycle. Other sources used in writing the following sections are Brady (1974) and Odum (1971).

2.1 Physical, Chemical and Biological Processes

Physical, chemical and biological processes all play a role in the nitrogen and phosphorus environmental cycles. A physical process is one that does not alter the nature of the chemical species involved. Chemical processes generally involve reactions in which there is a transformation of chemical species without the aid of any organisms. Biological processes are biochemical transformations of chemical species by microbial metabolism. In the natural environment it is very difficult to define in a clear-cut fashion whether a phenomenon is due to an individual, or more likely, a combination of physical, chemical, or biochemical processes. For example, adsorption is usually considered a physical process but chemisorption contributes to the concentration of the adsorbed species.

The factors which affect the growth of bacteria are important in determining the rates of transformation of the nutrient species. Some processes (e.g. mineralization) involve primarily bacteria requiring oxygen gas, or aerobic bacteria. Other processes (e.g. denitrification) involve anaerobic bacteria using mostly combined oxygen. Bacteria which can use either of the two oxygen forms are called facultative bacteria. Soil moisture affects bacterial growth in two ways: water is needed by bacterial metabolic activities, and the moisture content in soil affects the diffusion rate of oxygen through the soil. The temperature range at which most bacterial activity is optimal is between 20°C and 40°C, with the optimum temperature at around 35°C. Under ordinary soil temperature extremes (e.g. in winter) however, bacterial activity seldom halts. Organic matter is used as the energy source for the majority of bacteria. The amount and nature of the soil organic matter determines to a certain degree the types of bacteria present in the soil and their growth rates. Under conditions of high calcium, the pH of the soil column is usually between 6 and 8 which is generally best for most bacteria, although certain bacteria species are adapted for low pH and others at high pH. The calcium content and the pH values play a role in determining the specific bacteria present.

2.2 The Nitrogen Cycle

Figure NU-1 shows the nitrogen cycle in nature with some typical magnitudes of the transformations. In arable soils, nitrogen is acquired by soil primarily in three ways: through nitrogen fixation, additions through precipitation, and application of nitrogen in fertilizers and manures. Atmospheric nitrogen is fixed by bacteria in symbiosis with legumes. Depending on the soil conditions and the crop, the amount of nitrogen fixed can range from 50-250 lbs/acre-year (Brady, 1974). Soil conditions required are good aeration, drainage, moisture, optimal pH, and a certain amount of active calcium. The nitrogen added in this way is used by the host plant and also passed into the soil itself. Certain organisms in symbiosis with non-legumes, mostly angiosperms can also fix atmospheric nitrogen under conditions of low soil nitrogen. Free-living organisms that are not directly associated with higher plants, for example, several groups of bacteria, blue-green algae and fungi, are also capable of nonsymbiotic or free fixation of atmospheric nitrogen. The rate of fixation is assumed to be low. Direct addition of nitrogen through rain and snow is variable with season and location. In a humid temperate

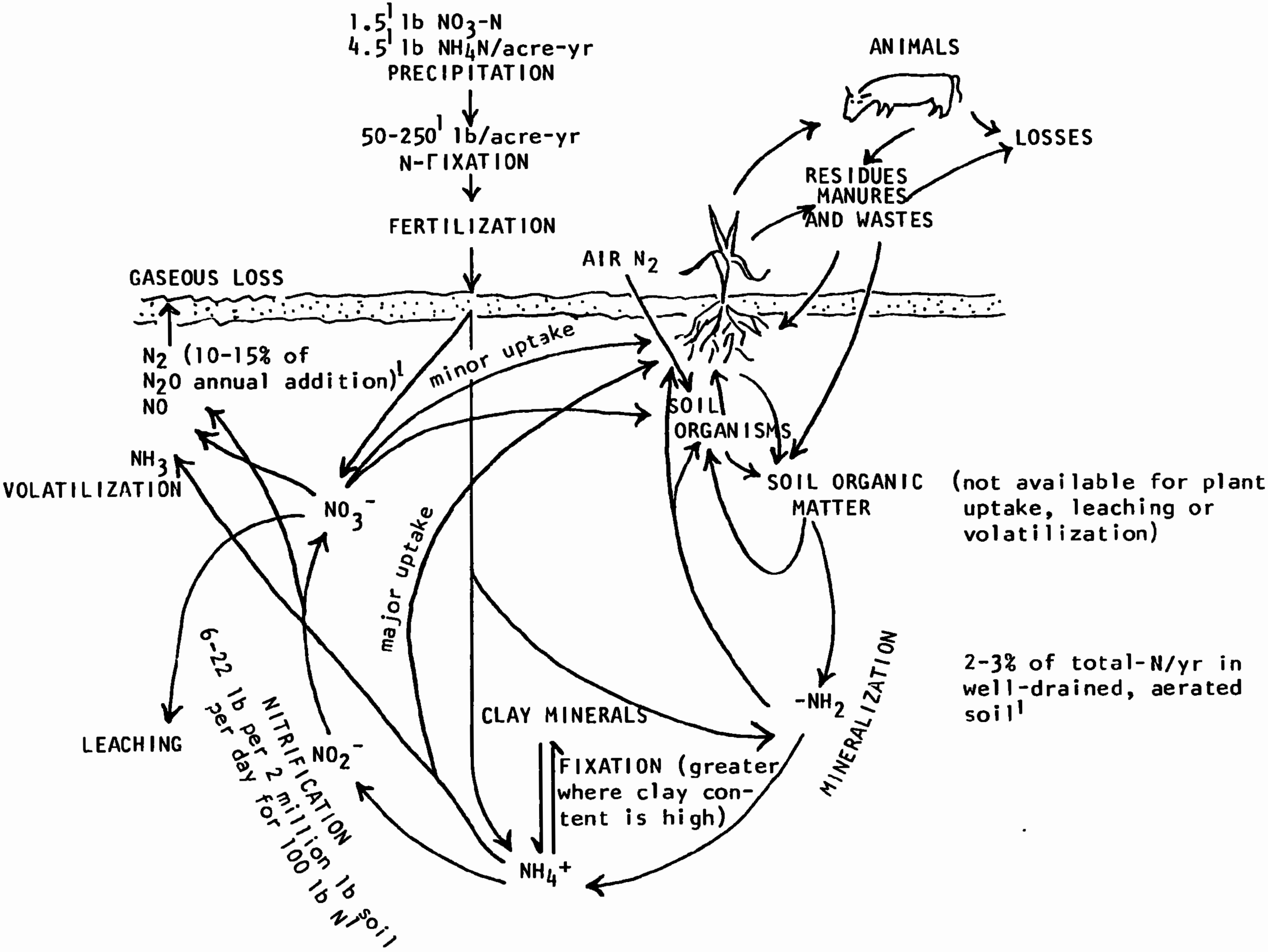

FIGURE NU-1: MAIN PORTIONS OF THE NITROGEN CYCLE

Source: Brady (1974)

Obtained from Brady (194).

climate, it is estimated that additions to soil average around 4.5 lbs of NH_4-N and 1.5 lbs of NO_3-N for every acre per year (Brady, 1974). In agricultural lands, the nitrogen additions in fertilizer is probably the largest component of the three contributions. The forms added are nitrate, ammonia and urea. The amount of nitrogen added depends on the kind of crop to be grown, the chemical condition of the soil, and the physical state of the soil. Application rates range from less then 100 lbs of nitrogen per acre to 300 lbs of nitrogen per acre.

Nitrogen is depleted from the soil in crop removal, drainage, erosion, and volatilization of the gaseous form. In an arable situation, crop removal is the most significant way by which nitrogen is removed. Gaseous losses are usually small but can become significant under anaerobic conditions, such as in water-logged soils.

2.2.1 Forms of Soil Nitrogen

There are basically three forms of soil nitrogen: (1) organic nitrogen associated with the soil humus, (2) ammonium fixed by certain clay minerals, and (3) soluble inorganic ammonium and nitrate compounds. Most of the nitrogen is associated with organic matter. A very small percentage (2-3%) of this organic-N is converted to inorganic forms a year (Brady, 1974). Mineral surface soils contain from 0.4 to 10% of organic matter (Brady, 1974). Typical soils contain around 4% of organic matter. Subsoils generally contain much less organic matter. Up to 8% of the total-N is fixed by clay (Brady, 1974). The soluble ammonium and nitrate compounds in soils seldom form more than 1-2% of the total-N present (Brady, 1974).

2.2.2 Nitrogen Transformations in the Soil Column

Mineralization

Mineralization is a biological process whereby organic nitrogen forms are converted to inorganic forms, usually to ammonium. Soil organisms attack the organic nitrogen compounds by enzymic digestion converting the more complex proteins to ammonium. Using the example of an amino combination, the reaction is as follows:

$$\left.\begin{array}{l} R\text{-}NH_2 + HOH \xrightarrow[\text{hydrolysis}]{\text{enzymic}} R\text{-}OH + NH_3 + \text{energy} \\ 2NH_3 + H_2CO_3 \longrightarrow (NH_4)_2\ CO_3 \rightleftarrows 2NH_4{}^+ + CO_3{}^{2-} \end{array}\right\} \qquad (NU\text{-}1)$$

In general the overall reactions are described by:

$$\text{organic-N} \longrightarrow \text{ammonium-N} \qquad (NU\text{-}2)$$

This transformation proceeds best in well-drained aerated soils but will take place to some extent under almost any conditions because of the diverse species capable of this process. Annually, only 2-3% of organic-N may be expected to be mineralized (Brady, 1974). Mineralization is a very slow process relative to the other soil reactions.

Immobilization

This phenomenon is the conversion of inorganic species to organic forms and may be regarded as the reverse of the mineralization process. Soil microbes or plants take up soluble nutrient species for growth, converting these to organic compounds which are released to the soil upon death and cell decay. Immobilization may be represented as:

$$\left.\begin{array}{l} NH_4\text{-}N \\ NO_3\text{-}N \end{array}\right\} \longrightarrow \text{org-N} \qquad (NU\text{-}3)$$

The rate constants for these transformations are dependent on those factors affecting mineralization. Suboptimum temperature and soil mositure slow down the rate of immobilization. Anaerobic conditions may also have an important effect on slowing down the rate; however, there is a possibility of adaptation of different microbial species across a range of oxygen concentration. The sensitivity of different microbes to ranges in pH could also affect the rate constants for these reactions. Immobilization is a fast process relative to mineralization.

Nitrification

Nitrification is a process of enzymic oxidation of ammonium. It takes place in two steps due to the activity of two separate groups of bacteria. The first step is the production of nitrous acid and the second step is the oxidation of the nitrite form to nitrate. The group of bacteria primarily responsible for the first step is the Nitrosomonas bacteria and for the second, Nitrobacter bacteria.

$$\left.\begin{array}{l} 2NH_4 + 3O_2 \xrightarrow[\underline{\text{Nitrosomonas}}]{\text{enzymic oxidation}} 2NO_2^- + 2H_2O + 4H^+ + \text{energy} \\ \\ 2NO_2^- + O_2 \xrightarrow[\underline{\text{Nitrobacter}}]{\text{enzymic oxidation}} 2NO_3^- + \text{energy} \end{array}\right\} \text{(NU-4)}$$

Other bacterial species are also able to oxidize and produce nitrate products but it is uncertain whether they are significant contributors of nitrate to soil. Soil conditions affecting nitrification are soil oxygen content, temperature, moisture, pH, fertilizer salts, and the nitrogen-carbon ratio. The temperature range under which nitrification occurs is between 0°C and 52°C. The most favorable temperatures are between 27-32°C (Brady, 1974). Nitrification is slow at very low or very high moisture content although it is known to proceed appreciably under very dry conditions. The most favorable soil moisture content is similar to that for growth of higher plants. Nitrification is low at low pH values but acidity itself is not significant when adequate exchangeable bases are present. Under ideal temperature, soil and moisture conditions, nitrification is a very fast process. Daily rates from 6 to 22 lbs of nitrogen per 2 million lbs of soil when 100 lbs of ammonium-N was added have been observed (Brady, 1974).

Denitrification

Denitrification is a reduction of nitrate-N to gaseous compounds. Facultative anaerobic baceria which prefer free oxygen use the combined oxygen in nitrate-N. The exact mechanisms are not known and may be chemical as well as biochemical. One way to describe it is as in reaction (b), which is basically respiration using nitrate instead of free oxygen as an oxygen source. The reactions could be adequately described in several ways:

$$\left.\begin{aligned}
&(a)\quad \underset{\text{nitrates}}{2NHO_3} \xrightarrow{-2[O]} \underset{\text{nitrates}}{2NHO_2} \xrightarrow[-H_2O]{-2[O]} \underset{\text{nitrous oxide}}{N_2O} \xrightarrow{-[O]} \underset{\text{elemental nitrogen}}{N_2} \\
&(b)\quad C_6H_{12}O_6 + 4NO_3^- \longrightarrow 6CO_2 + 6H_2O + 2N_2
\end{aligned}\right\} \text{biochemical reduction} \quad \text{(NU-5)}$$

$$\left.(c)\quad \underset{\text{nitrite}}{2HNO_2} + \underset{\text{urea}}{CO(NH_2)} \longrightarrow CO_2 + 3H_2O + 2N_2\right\} \text{chemical reduction}$$

In general, the process may be described as:

$$NO_3^- \longrightarrow NO_2^- \longrightarrow N_2$$

The rate of disappearance of NO_3-N is dependent on soil oxygen content, and the presence of reducing agents and organic matter. The pH, temperature and moisture content are important factors as well. The rate of denitrification is slow under acidic conditions and high under alkaline conditions. Higher soil moisture content also increases the rate of denitrification possibly by indirectly affecting oxygen diffusion in the soil column (Bartholomew, 1965). Denitrification is most likely to occur in poorly drained soils and in acidic soils containing nitrates. Poor aeration enhances denitrification. Under conditions of poor drainage and aeration, loss of nitrogen through denitrification can be substantial.

Plant Uptake

Nitrogen is taken up by plants mostly in the forms of ammonium or nitrate. The form that is taken up depends on the conditions of the soil, the kind of plant and the stage of plant growth. Factors which influence plant uptake of nitrogen are biomass or root surface area of plants, temperature, soil moisture, soil oxygen content, season of the year, among others. When the plants are harvested, a large fraction of nitrogen is removed from the immediate location.

Adsorption-Desorption

Ammonium-N is adsorbed by clay minerals. Colloidal clay particles ordinarily carry negative charges. Positively charged ions are attracted to the colloidal crystal and are held in a non-exchangeable form. This non-exchangeable or fixed ammonium is released slowly.

$$\underset{\text{(soil solution)}}{NH_4^+} \rightleftarrows \underset{\text{(exchangeable)}}{NH_4^+} \rightleftarrows \underset{\text{(fixed)}}{NH_4^+} \qquad \text{(NU-6)}$$

Ammonium fixation by clay minerals is greater in subsoils than in topsoil because of the higher clay content in subsoils. Organic matter or humus in soil also behaves like clay colloid particles in that ammonium-N can be fixed by these particles as well. The exact mechanism is unknown but it could be a chemical reaction by which compounds are formed between the soil organic matter and ammonium. This latter fixation is most favorable in the presence of oxygen and at high pH.

2.3 The Phosphorus Cycle

Figure NU-2 shows the phosphorus cycle in nature. Phosphorus is added to soils mostly in the form of fertilizers, especially in agricultural applications. Phosphorus is depleted from the soil in crop removal, drainage, and erosion.

2.3.1 Forms of Soil Phosphorus

In most soils, more than 50 percent of the total soil phosphorus is organic, present either as specific organic phosphorus compounds or as organic compounds linked with inorganic phosphorus groups (Larsen, 1967). Inorganic phosphorus forms present in soils depend on the pH of the soil. Under alkaline conditions, the HPO_4^{2-} ion is dominant. At low pH values, the $H_2PO_4^-$ ion is prevalent. Both these ions prevail at intermediate pH values.

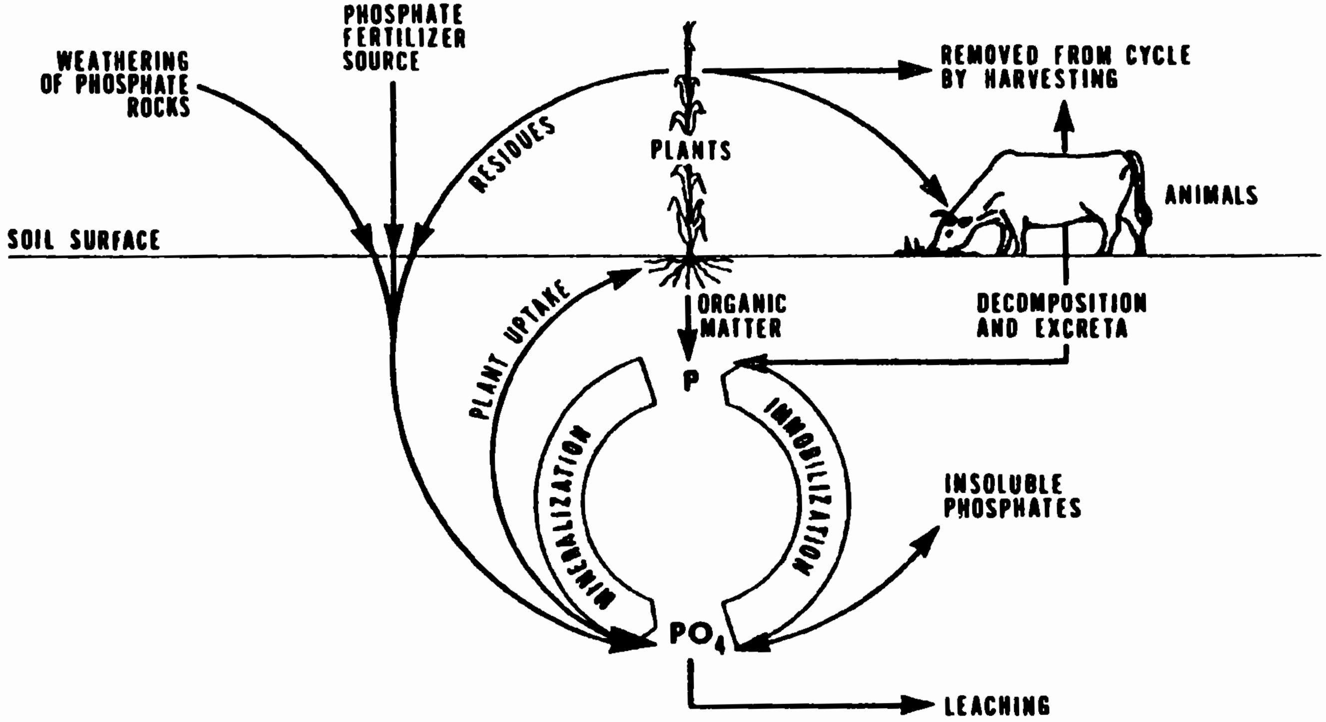

FIGURE NU-2: MAIN PORTIONS OF THE PHOSPHORUS CYCLE

Source: Donigian, Beyerlein, Davis, and Crawford, 1977

2.3.2 Phosphorus Transformations in the Soil Column

Mineralization

Organic forms of phosphorus are converted to inorganic forms by bacteria in a process called mineralization similar to that of the mineralization of organic-N.

$$\text{organic-P} \longrightarrow \text{phosphate-P} \qquad \text{(NU-7)}$$

The same conditions which affect nitrogen mineralization regulate phosphorus mineralization.

Immobilization

Inorganic phosphorus is transformed to organic phosphorus through the process of immobilization. Soil organisms and plants take up soluble inorganic phosphorus for growth, converting these to organic forms which are released to the soil upon death.

$$\text{phosphate-P} \longrightarrow \text{organic-P} \qquad \text{(NU-8)}$$

Plant Uptake

Both the phosphate forms, HPO_4^{2-} and $H_2PO_4^-$ are adsorbed by higher plants. The forms available depend on the pH of the soil. Organic phosphorus cannot be used to any extent directly by higher plants but only after mineralization. Plant uptake of phosphorus is influenced by biomass or root surface area, temperature, soil moisture, soil oxygen content, season of the year, among others.

Adsorption-Desorption

The mechanism by which inorganic phosphorus ions are fixed by soil particles is not a simple adsorption mechanism. In acid soils, phosphates are precipitated by iron, aluminium, and manganese ions, and fixed by hydrous oxides and by silicate clays. At high pH values, phosphates are precipitated by calcium compounds. Therefore, it is more accurate to assume the process as a combination of precipitation and adsorption-desorption.

2.4 Summary of Background of Nutrient Cycles

Table NU-1 shows typical dominant pathways in a soil column and transformations that may be expected in each soil zone. It must be emphasized that the relative rates vary with climate, soil type, vegetation, among other factors.

TABLE NU-1: DOMINANT NUTRIENT PATHWAYS IN EACH SOIL ZONE

	Ammonium-N in Solution	Ammonium-N Adsorbed	Nitrate-N in Solution	Organic-N in Solution	Inorganic-P Adsorbed	Inorganic-P Adsorbed	Organic-P in Solution
Surface	Runoff Leaching Volatilization	Loss in Sediments	Runoff Leaching	Runoff Leaching	Runoff Leaching	Loss in Sediments	Runoff Leaching
	Plant Uptake Adsorption-Desorption Immobilization Mineralization Nitrification	Adsorption-Desorption	Plant Uptake Immobilization Nitrification	Immobilization Mineralization	Plant Uptake Adsorption-Desorption Immobilization Mineralization	Adsorption-Desorption	Immobilization Mineralization
Upper Unsaturated	Leaching		Leaching	Leaching	Leaching		Leaching
	Plant Uptake Adsorption-Desorption Immobilization Mineralization Nitrification	Adsorption-Desorption	Plant Uptake Immobilization Nitrification Denitrification	Immobilization Mineralization	Plant Uptake Adsorption-Desorption Immobilization Mineralization	Adsorption-Desorption	Immobilization Mineralization
Lower Unsaturated	Leaching		Leaching	Leaching	Leaching		Leaching
	Plant Uptake Adsorption-Desorption Immobilization	Adsorption-Desorption	Plant Uptake Immobilization Dentrification	Immobilization	Plant Uptake Adsorption-Desorption Immobilization	Adsortpion-Desorption	Immobilization

3.0 MATHEMATICAL FORMULATION

3.1 General

The important nutrient species included in this modeling effort are: organic nitrogen in soil solution (org-N), ammonium in soil solution (NH_4-N(s)), ammonium adsorbed on soil particles (NH_4-N(a)), nitrate in soil solution (NO_3-N), organic phosphorus in soil solution (org-P), orthophosphate in soil solution (PO_4-P(s)), and orthophosphate adsorbed on soil particles (PO_4-P(a)). These are the dominant species in a soil column. Each of the organic nutrient species is considered as a group because they are insufficiently characterized and because data are usually available for the organic nitrogen and organic phosphorus as individual groups. Nitrite (NO_2-N) is not considered as a separate species by itself since it is unstable and usually exists at concentrations that are orders of magnitude less than nitrate-N. The fluxes in and out of the NO_2-N pool are expected to be high; the storage capacity is very small.

Schematic diagrams of the nitrogen and phosphorus cycles modeled by the nutrient module of SESOIL are shown in Figures NU-3 and NU-4 respectively. These models are simplified representations of the cycles in nature.

Table NU-1 gives the processes in the soil column that affect transport and transformation of nutrient species in each soil zone. The physical processes of losses in runoff, sediments, leaching, and volatilization are modeled by the pollutant transport routine in SESOIL and will not be repeated here. The pollutant transport routine is called by the executive program of the model.

3.2 Nutrient Transformations

Each of the nutrient transformations is modeled as a first order reaction. Assuming that the soil being modeled is microbially active, at the low nutrient concentrations normally present in soils, first order kinetics best estimates what happens in the soil column. Since the Freundlich, the Langmuir and an overall adsorption equation are modeled by the

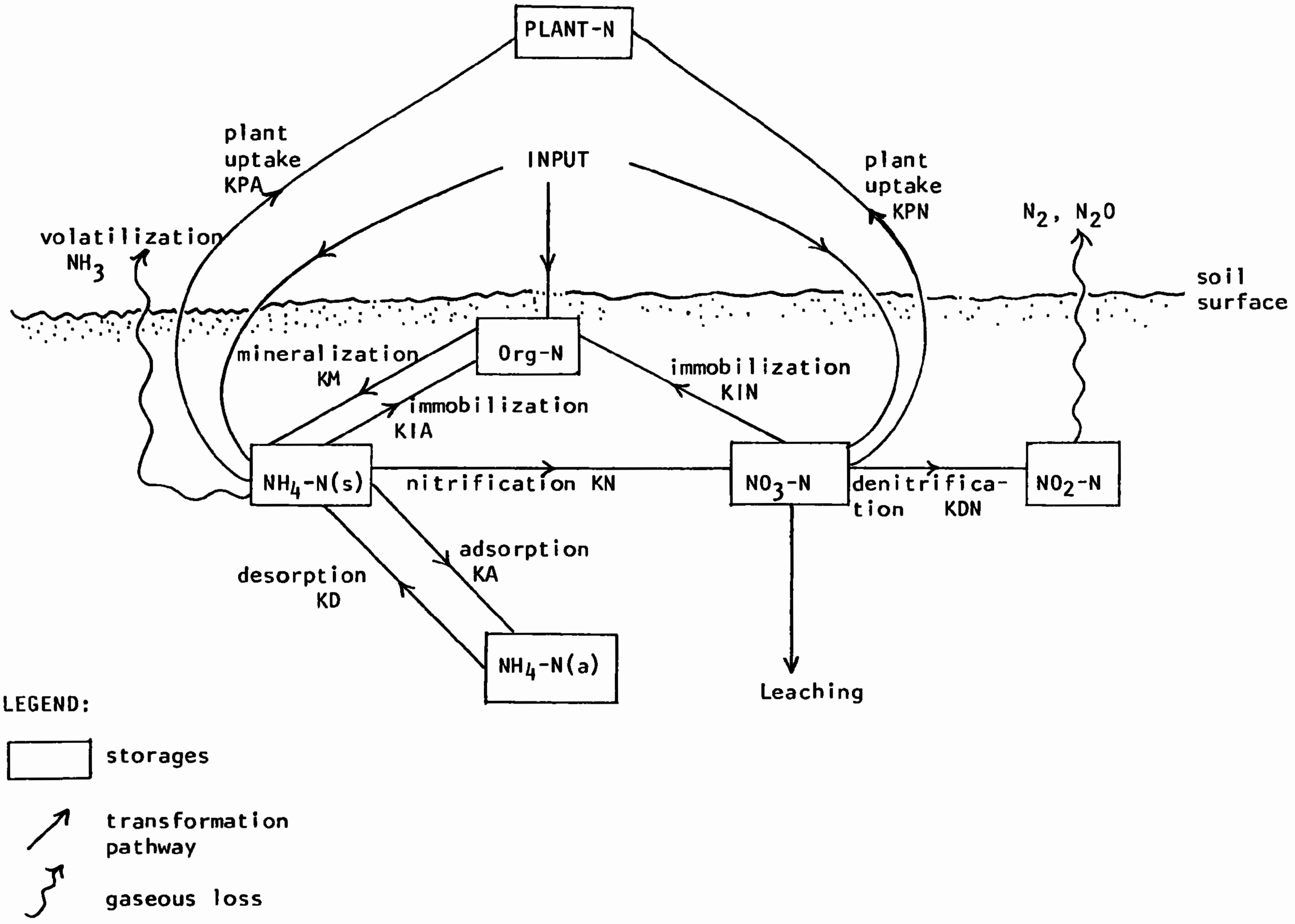

FIGURE NU-3: SCHEMATIC DIAGRAM OF NITROGEN CYCLE MODELED

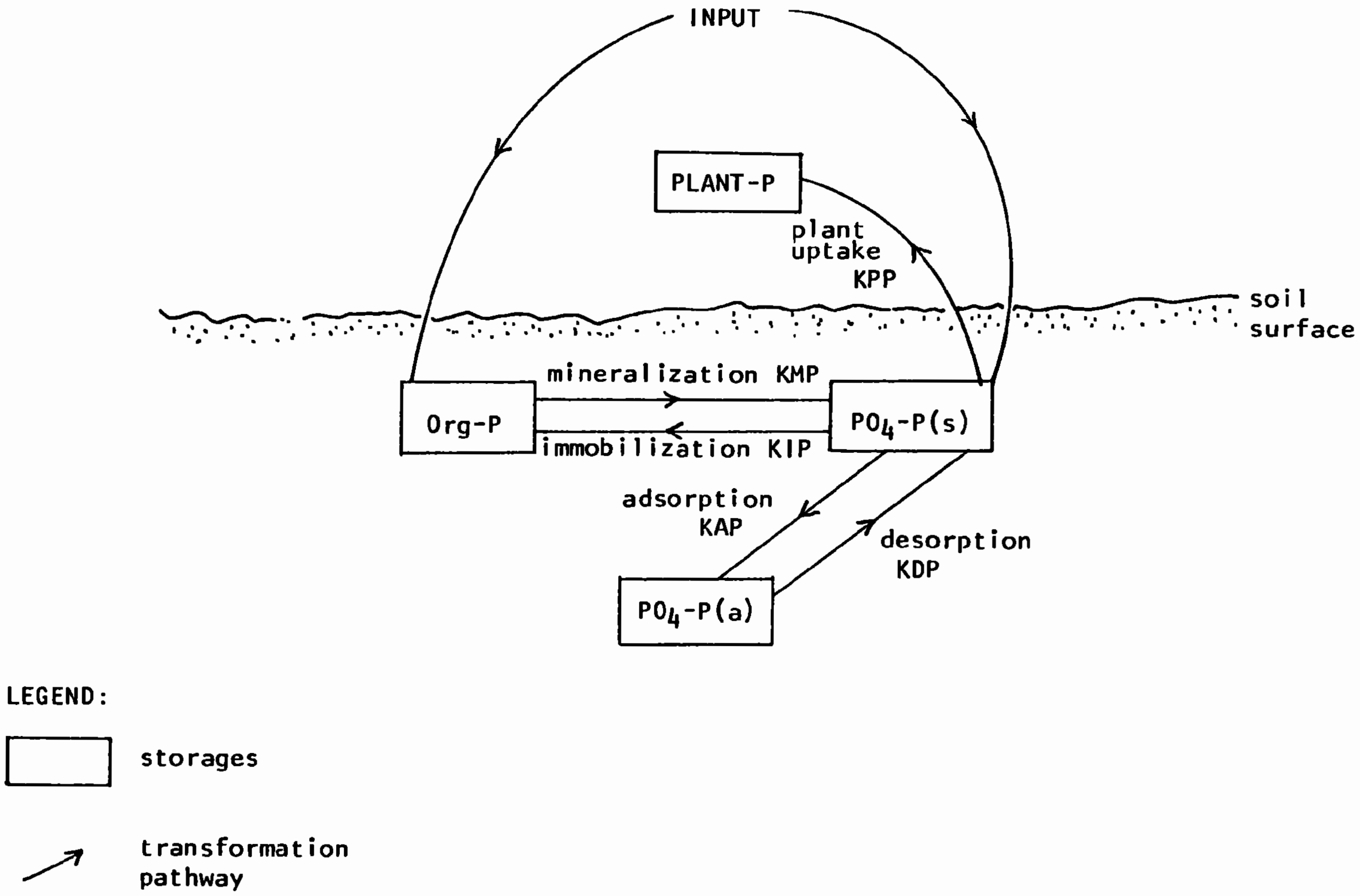

FIGURE NU-4: SCHEMATIC DIAGRAM OF PHOSPHORUS CYCLE MODELED adsorption-desorption routine of SESOIL, a choice is given to the user depending on the data availability and other factors.

3.3 Rate Constants

Table NU-2 shows the rate constants used in the model to describe the transformations in the soil column. These are first order rate constants to be specified by the user for each reaction and for each soil zone being modeled. The dependency of the rate constant on temperature is described by the Arrhenius equation.

$$K_T = K_{35°C} \quad \gamma^{(T-35)}$$

where:

K_T = rate constant at T°C (day^{-1})

$K_{35°C}$ = optimum K at 35°C (day^{-1})

γ = temperature coefficient (constant)

T = temperature (°C)

The temperature coefficients for the nutrient transformations are shown in Table NU-2. The user has to input the values of rate constants at 35°C and the temperature coefficient for each of the rate constants. Some typical values of rate constants and temperature coefficients are given in Table NU-3.

3.4 System of Equations

The system of equations governing the nitrogen and phosphorus transformations in soil is given in Table NU-4. The transformations are based on nutrient mass per mass of soil or soil water in each zone, i.e., mass-based concentrations. The ammonium desorption rate KD, the nitrogen mineralization rate KM, the phosphate desorption rate KDP, and the phosphorus mineralization rate KMP are based on per soil mass. All the other rates are based on per soil water mass in each zone.

To calculate soil and water masses in each zone, soil bulk densities have to be specified for each zone, and soil moisture content has to be

TABLE NU-2: RATE CONSTANTS AND TEMPERATURE COEFFICIENTS

Rate Constant (day^{-1})	Temperature Coefficient	Transformation Process in Soil Column
Nitrogen		
KA	TKA	Adsorption of ammonium from solution to adsorbed phase
KD	TKD	Desorption of ammonium from adsorbed phase to solution
KN	TKN	Nitrification of ammonium in solution to nitrate
KDN	TKDN	Denitrification of nitrate to gaseous nitrogen
KIN	TKIN	Immobilization of nitrate to organic nitrogen
KIA	TKIA	Immobilization of ammonium in solution to organic nitrogen
KM	TKM	Mineralization of organic nitrogen to ammoniun in solution
KPA	TKPA	Plant uptake of ammonium in solution
KPN	TKPN	Plant uptake of nitrate
Phosphorus		
KAP	TKAP	Adsorption of phosphate from solution to adsorbed phase
KDP	TKDP	Desorption of phosphate from adsorbed phase to solution
KIP	TKIP	Immobilization of phosphate in solution to organic phosphorus
KMP	TKMP	Mineralization of organic phosphorus to phosphate in solution
KPP	TKPP	Plant uptake of phosphate in solution

TABLE NU-3: TYPICAL RATE CONSTANTS AND TEMPERATURE COEFFICIENT VALUES

PROCESS	RATE CONSTANT (day^{-1})	TEMPERATURE COEFFICIENT
Nitrogen:		
Mineralization		
org-N → NH_4-N	0.001 - 0.0078[1] (11 soils with wide range of properties)	1.07[2]
Immobilization		
NH_4-N → org-N	0.15[1] (Ontario loam)	1.07[2]
NO_3-N → org-N	0.15[1] (Ontario loam)	1.07[2]
Nitrification		
NH_4-N → NO_2-N	0.22[1] (Salinas clay)	1.07[2]
NO_2-N → NO_3-N	9.0[1] (Salinas clay)	1.07[2]
NH_4-N → NO_2-N	0.143[1] (Milville loam)	1.07[2]
NO_2-N → NO_3-N	9.0[1] (Milville loam)	
NH_4-N → NO_3-N	0.0033 - 1.11[1] (various loams)	1.07[2]
Denitrification		
NO_3-N → (N_2 + N_2O)	0.004 - 0.192[1] (various loams)	1.07[2]
Adsorption		
NH_4-N(s) → NH_4-N(a)	1.0000[3]	1.050[3]
Desorption		
NH_4-N(a) → NH_4-N(s)	1.0000[3]	1.050[3]
Plant Uptake[4]		
NO_3-N → Plant-N	0-0.0975[3]	1.070[3]
NH_4-N → Plant-N	0-0.0975[5]	1.070[5]
Phosphorus:		
Mineralization		
org-P → PO_4-P(s)	0.002 - 0.02[3]	1.070[3]

TABLE NU-3: (Continued)

PROCESS	RATE CONSTANT (day^{-1})	TEMPERATURE COEFFICIENT
Immobilization		
PO_4-P(s) $\longrightarrow$ org-P	0[3]	1.070[3]
Adsorption		
PO_4-P(s) $\longrightarrow$ PO_4-P(a)	1.0000[3]	1.050[3]
Desorption		
PO_4-P(a) $\longrightarrow$ PO_4-P(s)	0.0015 - 0.0150[3]	1.050[3]
Plant Uptake[4]		
PO_4-P(s) $\longrightarrow$ Plant-P	0 - 0.0525[3]	1.070[3]

---

1. Adapted from Knisel, Davidson, *et al.*, 1978. Laboratory values under various conditions.
2. Brady, 1974 gives a typical doubling of a rate constant for every 10°C increase in temperature, which would indicate a temperature coefficient of 1.07 for biochemical reactions.
3. Donigian, *et al.*, 1977. P-2 Watershed, Watkinsville, PA.
4. Range due to seasonal dependence.
5. Obtained by assuming equal uptake of NH_4-P and NO_3-N.

TABLE NU-4: DIFFERENTIAL EQUATIONS DESCRIBING NITROGEN AND PHOSPHORUS TRANSFORMATIONS

Organic Nitrogen

$$\frac{d}{dt}\left\{\text{org-N}\right\} = \text{KIA}\left\{NH_4\text{-N(s)}\right\} + \text{KIN}\left\{NO_3\text{-N}\right\} - \text{KM}\left\{\text{org-N}\right\}$$

Ammonium in Solution

$$\frac{d}{dt}\left\{NH_4\text{-N(s)}\right\} = \text{KM}\left\{\text{org-N}\right\} + \text{KD}\left\{NH_4\text{-N(a)}\right\} - (\text{KPA+KIA+KA+KN})\left\{NH_4\text{-N(s)}\right\}$$

Adsorbed Ammonium

$$\frac{d}{dt}\left\{NH_4\text{-N(a)}\right\} = \text{KA}\left\{NH_4\text{-N(s)}\right\} - \text{KD}\left\{NH_4\text{-N(a)}\right\}$$

Nitrate

$$\frac{d}{dt}\left\{NO_3\text{-N}\right\} = \text{KN}\left\{NH_4\text{-N(s)}\right\} - (\text{KIN+KDN+KPN})\left\{NO_3\text{-N}\right\}$$

Organic Phosphorus

$$\frac{d}{dt}\left\{\text{org-P}\right\} = \text{KIP}\left\{PO_4\text{-P(s)}\right\} - \text{KMP}\left\{\text{org-P}\right\}$$

Phosphate in Solution

$$\frac{d}{dt}\left\{PO_4\text{-P(s)}\right\} = \text{KMP}\left\{\text{org-P}\right\} + \text{KDP}\left\{PO_4\text{-P(a)}\right\} - (\text{KIP+KAP+KPP})\left\{PO_4\text{-P(s)}\right\}$$

Adsorbed Phosphate

$$\frac{d}{dt}\left\{PO_4\text{-P(a)}\right\} = \text{KAP}\left\{PO_4\text{-P(s)}\right\} - \text{KDP}\left\{PO_4\text{-P(a)}\right\}$$

obtained from the hydrologic cycle routine of SESOIL. Soil mass in each zone is the product of the bulk density and volume of the zone. Knowing soil mass and soil water mass, the nutrient concentrations may be calculated appropriately to be used in the transformation equations. NH_4-N(a), PO_4-P(a), org-N and org-P are therefore in the units of mass per soil mass and the other nutrient species are in the units per soil water mass.

3.5 Input/Output Parameters

The input and output parameters used in the nutrient cycle module of SESOIL are summarized in Table NU-5.

3.6 Numerical Solution Techniques of Equation Systems

Table NU-4 gives the nitrogen and phosphorus equations modeled by the nutrient subroutine of SESOIL. An analytical solution of first order differential equation systems might be possible (theoretically), but for practical reasons SESOIL employs numerical algorithms.

Various solution algorithms are available in the literature, such as the simple Euler integration technique employed by the Agricultural Runoff Management (ARM) model [Donigian, et al., 1977] and the Runge-Kutta techniques [Abramowitz and Segun , 1968]. SESOIL employs a second order and fourth order Runge-Kutta solution method for the annual and the monthly simulations respectively.

For a given system of two first order differential equations as an illustration:

$$\begin{aligned} y' &= f(x,y,z) \\ z' &= g(x,y,z) \end{aligned} \qquad \text{(NU-9)}$$

The "second order" Runge-Kutta discretized solution is obtained from:

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{2}(k_1 + k_2) + 0(h^3) \\ z_{n+1} &= z_n + \frac{1}{3}(l_1 + l_2) + 0(h^3) \end{aligned} \qquad \text{(NU-10)}$$

TABLE NU-5: INPUT/OUTPUT PARAMETERS

	PARAMETER	UNITS
INPUT		
1.	Loadings of: NH_4-N NO_3-N org-N PO_4-P	kg/m^2
2.	Times of applications of: NH_4-N NO_3-N org-N PO_4-P	historical dates
3.	Method of incorporation of loadings	
4.	Monthly rate constants (35°C) for nitrogen and phosphorus uptake by plants for each soil zone. KPA; KPN; KPP	day^{-1}
5.	Rate constants (35°C) for each transformation other than plant uptake for each soil zone. KA; KD; KN; KDN; KIN; KIA; KM; KAP; KDP; KIP, KMP	day^{-1}
6.	Temperature coefficients for each rate constant. TKA; TKD; TKN; TKDN; TKIN; TKIA; TKM; TKPA; TKPN; TKAP; TKDP; TKIP; TKMP; TKPP	(-)
7.	Monthly temperatures in each soil zone.	°C
8.	Volume of soil in each soil zone.	m^3
9.	Bulk density of each soil zone.	g/cm^3
10.	Soil moisture content (from hydrologic simulations).	(-)
11.	Time step of simulations.	month

TABLE NU-5: INPUT/OUTPUT PARAMETERS
(Continued)

PARAMETER	UNITS
OUTPUT	
1. Monthly concentrations of nutrient species in each soil zone.	
(A) NH_4-N(a)	$\frac{\text{mg}}{\text{kg of soil}}$
org-N	
PO_4-P(a)	
org-P	
(B) NH_4-N(s)	$\frac{\text{mg}}{\text{kg of soil water}}$
NO_3-N	
PO_4-P(s)	

where:

$$k_1=h\cdot f(x_n,y_n,z_n)$$

$$k_2=h\cdot f(x_n+h,y_n+k_1,z_n+k_1)$$

$$l_1=h\cdot g(x_n,y_n,z_n)$$

$$l_2=h\cdot g(x_n+h,y_n+k_1,z_n+l_1)$$

The "fourth order" Runge-Kutta discretized solution is obtained from:

$$y_{n+1}=y_n+\frac{1}{6}(k_1+2k_2+2k_3+k_4)+0(h^5),$$

$$z_{n+1}=z_n+\frac{1}{6}(l_1+2l_2+2l_3+l_4)+0(h^5)$$

where:

$$k_1=hf(x_n,y_n,z_n)$$

$$k_2=hf\left(x_n+\frac{1}{2}h,y_n+\frac{1}{2}k_1,z_n+\frac{1}{2}l_1\right)$$

$$k_3=hf\left(x_n+\frac{1}{2}h_1y_n+\frac{1}{2}k_2,z_n+\frac{1}{2}l_2\right)$$

$$k_4=hf(x_n+h,y_n+k_3,z_n+l_3)$$

$$l_1=hg(x_n,y_n,z_n)$$

$$l_2=hg\left(x_n+\frac{h}{2},y_n+\frac{k_1}{2},z_n+\frac{l_1}{2}\right)$$

$$l_3=hg\left(x_n+\frac{h}{2},y_n+\frac{k_2}{2},z_n+\frac{l_2}{2}\right)$$

$$l_4=hg(x_n+h,y_n+k_3,z_n+l_3)$$

The FORTRAN code of the Runge-Kutta solution techniques is presented in subroutine RUNGEK, Appendix FC.

4.0 CONCLUSIONS

The nutrient cycle of SESOIL simulates the transport, transformations and storages of nutrient species in soil and gives as an output the storages of each species in each zone of the soil column.

The accuracy of the nutrient cycle output depends on the accuracies of the hydrologic and pollutant transport simulations because it uses both these routines in its simulations. This module can be used in the management of agricultural runoff, nutrient residues in the soil column, and the contamination of groundwater by nutrients via leaching.

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PT - pollutant cycle

APPENDIX PT

POLLUTANT CYCLE

FIGURES

TABLES

1.0 INTRODUCTION

The ultimate fate or distribution of a pollutant in the SESOIL compartment is governed by the hydrologic cycle processes, the sediment cycle processes and the interaction of the various chemical fate processes related to the pollutant involved. The actual quantity or mass of a pollutant in any one process will depend at a particular time on the "competition" among all the processes for the available pollutant mass. This competition constitutes the basic philosophy of the pollutant-transport routine of SESOIL that will be described in the following sections.

The hydrologic cycle processes have been described in appendix HY. The sediment cycle processes have been outlined in appendices SW and SR. The individual chemical fate processes (diffusion, volatilization, sorption, etc) have been described separately in previous appendices. In SESOIL all these processes are considered interrelated and are combined under different equation systems -- depending on the level of SESOIL operation. The solutions of these systems determine the spatial and temporal distribution of a pollutant in the various subcompartments (soil-air, soil-moisture, soil, etc) of the SESOIL "environment." The mathematical routine/equation that combines all the previously described processes (from appendix HY to appendix NU) is designated as the "pollutant cycle" routine of SESOIL.

The processes of sedimentation, soil resuspension, photolysis, fixation, biologic activity and nutrient transportation are not modeled in this version (1981) of SESOIL. Such a modeling effort is anticipated by the model developers in the near future (maybe 1982) in connection with the watershed features of SESOIL.

This appendix presents the pollutant cycle routine of the model including: (a) a short literature review of previous modeling efforts; (b) the rationale governing the pollutant cycle equation structure and the actual equations employed; and (c) the numerical techniques developed for each level of SESOIL operation. Information regarding input data requirements to the pollutant cycle routine is presented in section 3.0, User's Manual, of this report. One of the model objectives has been to provide the literature with a "user friendly" package; therefore input parameters to this routine have been kept to a minimum by using many values that are estimated on-line by the model. Thus, although SESOIL models a complex system of many processes and interactions, it is intended to be relatively easy to use.

2.0 MODELING BACKGROUND

2.1 Literature Review

The watershed modeling features of SESOIL are not presented in this documentation; therefore the following literature review focuses only in the unsaturated soil zone modeling aspects of the soil environment.

Previous sophisticated pollutant transport modeling efforts have mainly employed the one- or two-dimensional time dependent diffusive, convective mass transport differential equation in homogeneous isotropic soils, which in a one-dimensional domain is written

$$\frac{\partial(\Theta c)}{\partial t} = \frac{\partial}{\partial t}\left(\Theta \cdot K_D^* \frac{\partial c}{\partial z}\right) - \frac{\partial (Vc)}{\partial z} - \rho\frac{\partial s}{\partial t} \pm \Sigma P \qquad \text{(PT-1)}$$

where Θ = soil moisture content, c = dissolved pollutant concentration in soil moisture, K_D^* = apparent diffusion coefficient of compound in soil-air, V = Darcy velocity of soil moisture, ρ = soil density, s = adsorbed concentration of compound on soil particles ΣP = sum of sources or sinks of the pollutant within the soil volume and z = depth.

The above equation has been solved principally: (a) numerically over a temporal and spatial discretized domain, via finite difference or finite element mathematical techniques (eg. Bonazountas et al 1979); and (b) analytically, by seeking exact solutions for simplified environmental conditions (eg. Enfield et al 1980). It must be pointed out that the theoretical derivation of the mass transport equation PT-1 is based upon a mass balance consideration of the pollutant in a representative soil element of volume dV=dxdydz.

The principal scientific deficiencies when modeling pollutant transport via equation PT-1 are: (1) only diffusion, convection, adsorption and possibly decay can be modeled, whereas other processes such as fixation or cation-exchange have to be neglected; (2) this equation is applicable mainly to pollutant transport of organics, whereas transport of metals which can be strongly affected by other processes cannot be directly modeled; (3) this equation can predict volatilization only implicitly via boundary diffusion constraints, however, experimental studies have frequently demonstrated an overestimation or underestimation of the theoretical volatilization rate; (4) no experimental or well accepted equation for a process (eg. volatilization) can be incorporated in PT-1, since the model has its own predictive mechanism; (5) pollutant concentrations are estimated only in the soil-moisture and on soil-particles, whereas pollutant concentrations in the soil-air are omitted; (6) the discretized version of the equation has a pre-set temporal and spatial discretization grid that results in high operational costs (professional time, computer time) of the model, since input data have to be entered into each node of the grid; and (7) it is difficult and costly to run above models for typical canonical environmental scenarios (soils, climates, pollutants) for reasons discussed in section 3.16 canonical environments, of the User's Manual.

In order to bypass the above and other deficiencies of the traditional mathematical modeling, the SESOIL model developers have designed -- based on their experience with the traditional modeling (Bonazountas et al 1979) -- a new pollutant transport routine, which is presented conceptually in the following section.

2.2 The SESOIL Pollutant Transport Routine Concept

In SESOIL, any soil subcompartment of irregular cross area A_i and of depth d_i is considered a "pollutant mass carrier," that can receive pollutant mass from other subcompartments, store pollutant mass and export pollutant mass to other subcompartments. Assuming, for example, that a compartment (Figure PT-1) contains originally a pollutant mass M_{orig} -- of a particular pollutant -- and receives during an infinitesimal time step $\Delta t=(t)-(t-1)$ an impulse of pollutant mass M_{input}, then for this subcompartment we can write the equation

$$M_{orig}(t) + M_{input}(t) = M_{trans}(t) + M_{rem}(t) + M_{out}(t) \qquad \text{(PT-2)}$$

where

$M_{orig}(t)$ = initially available pollutant mass in the soil compartment, at time t

$M_{input}(t)$ = input pollutant mass to the soil compartment in (Δt)

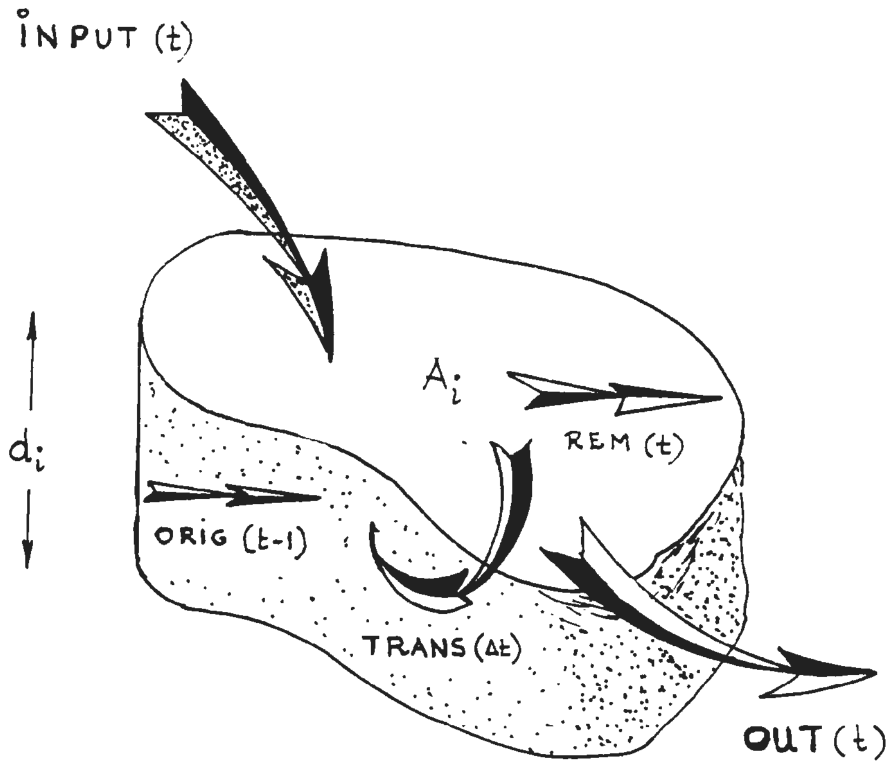
$M_{out}(t)$ = time dependent exported pollutant mass by the pollutant carrier

$M_{trans}(t)$ = time dependent pollutant transformation (or loss) within the compartment

$M_{rem}(t)$ = remained pollutant mass in the compartment due to various reasons.

Some of the processes of individual terms of equation PT-2 are time dependent over the infinitesimal time step Δt (eg. volatilization), others are assumed time independent (eg. adsorption). These issues are discussed in later sections.

The mass balance concept (above) has been applied in SESOIL to a soil matrix consisting of three phases: (a) solids (soil); (b) liquid (soil-moisture); and (c) gas (soil-air). Phases and subcompartments in SESOIL



input(t) = Pollutant mass introduced in a soil layer or in its subcompartments of soil-air, soil-moisture, at time (t).

orig(t-1) = Pollutant mass available in subcompartments of soil-air, soil-moisture, soil-solids at (t-1).

trans(t) = Pollutant mass transformation within the soil layer during the time step $\Delta t=(t)-(t-1)$.

out(t) = Pollutant mass exported by soil compartment at the end of time (t).

rem(t) = Remaining pollutant mass in the compartment at time (t).

FIGURE PT-1: CONCEPTUAL PRESENTATION OF THE SOIL-LAYER ACTING AS A "POLLUTANT MASS CARRIER" OVER TIME are interrelated (Figure PT-2). It is the pollutant cycle that simulates these interrelations by modeling both the chemical partitioning among the three phases, and transport between subcompartments i.

2.3 Chemical Partitioning

The soil environment consists in SESOIL of three media: (1) soil-air (gaseous phase); (2) soil-moisture (liquid phase); and (3) soil (solid phase). The fate (transport/transformation) of pollutants in the soil column -- and consequently their ultimate fate -- depends on the pollutant partitioning among these three phases. This partitioning is a function of various parameters such as the chemical-specific partition coefficients (eg. air/soil moisture) and rate constants.

In SESOIL, the three phases are assumed to be in equilibrium at all times. Thus once the concentration in one phase is known, the concentrations in the other phases can be calculated. In SESOIL, the pollutant cycle is based on the pollutant concentration in the soil-moisture. The concentration in the soil-air is then calculated by Henry's law, and the concentration in the soil is calculated from the adsorption, cation exchange, and other sorption processes included in the model. Henry's law and the sorption processes are briefly described below.

The solute (dissolved) concentration of a compound is related to its soil-air concentration via Henry's law (see equation VO-12).

$$c_{sa} = c \cdot H/R(T+273) \qquad \text{(PT-3)}$$

where

c_{sa} = pollutant concentration in soil-air; (ug/mL)

c = dissolved pollutant concentration; (ug/mL)

H = Henry's law constant; ($m^3 \cdot atm/mol$)

R = gas constant; (8.2×10^{-5} $m^3 \cdot atm/mol \cdot °K$)

T = temperature; (°C)

$°K = °C + 273$

In SESOIL, the pollutant concentration on the <u>soil</u> is determined from the <u>sum</u> of the concentrations of the pollutant adsorbed, cation-exchanged, and/or otherwise associated with the soil particles, eg. via adsorption isotherms as discussed in appendix AD (adsorption) and in appendix CE (cation exchange). One commonly used adsorption isotherm equation is the Freundich equation

$$s = K \cdot c^{1/n} \qquad \text{(PT-4)}$$

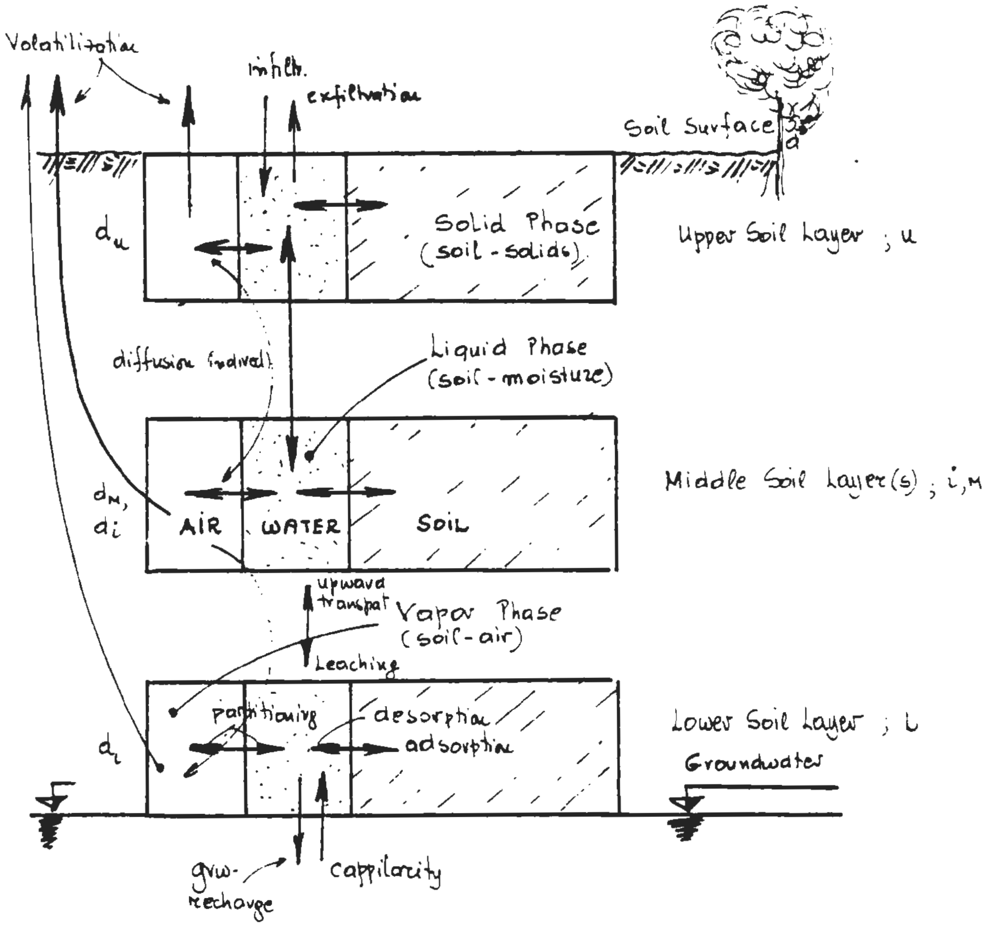


FIGURE PT-2: SCHEMATIC OF PHASES DESCRIBING THE SOIL MATRIX, AND INTERRELATION OF SOIL LAYERS where

s = absorbed concentration of compound; (ug/g soil)

K = partitioning coefficient; (ug/g soil)/(ug/mL)

c = dissolved concentration of compound; (ug/mL)

n = Freundich constant; (-)

All these sorption processes are -- and are expressed in SESOIL as -- a function of the dissolved concentration of the pollutant in the soil moisture.

The total concentration of a chemical in a soil matrix can be calculated from the concentration of the pollutant in each phase and the related volume of each phase (see also appendix VO) by

$$c_o = (n-\Theta)c_{sa} + (\Theta)c + (\rho_b)s \qquad \text{(PT-5)}$$

where

c_o = overall (total) concentration of pollutant in soil matrix; (ug/cm^3 soil)

n = soil (total) porosity; (mL/mL)

Θ = soil moisture content; (mL/mL)

$n-\Theta$ = n_{air}; soil-air content or soil-air filled porosity; (mL/mL)

c_{sa} = pollutant concentration in soil-air; (ug/mL)

c = pollutant concentration (dissolved) in soil-moisture; (ug/mL)

ρ_b = soil bulk density; (g/cm^3)

s = pollutant concentration on soil particles; (ug/g soil)

2.4 Pollutant Mass Balance

The pollutant concentration in the SESOIL compartment changes with both time and space due to the change of pollutant mass within the subcompartment of the soil column. According to the law of mass conservation for a representative element, the change of pollutant mass and over a small time step Δt in that element will equal

$$\Delta M = M_{in} - M_{out} - M_{trans} \qquad \text{(PT-6)}$$

where: ΔM = change in pollutant mass in the element; M_{in} = mass entered the element; M_{out} = mass left the element; and M_{trans} = mass transformed (ie. degraded) within the element.

Assuming that pollutant mass entered rapidly (instantaneously) at the beginning of the time step, and by discretizing equation PT-6 over the finite time step from, for example, t=0 to t=t (ie. Δt=t), we have

$$\left[\Delta M\right]_o^t = M_t - M_o = M_{in,o} - M_{out,t} - M_{trans,t} \qquad \text{(PT-7)}$$

where: M_t = pollutant mass in the element at time t; M_o = original pollutant mass in the element; $M_{in,o}$ = input pollutant mass at t=0; $M_{out,t}$ = pollutant mass lost in time t; and $M_{trans,t}$ = pollutant mass transformed in time t.

When the original (initial) mass in the element, and the input to the element are known, the fate of the pollutant at time t can then be determined by rearranging the terms of equation PT-7 and by expressing the right hand side of the equation as a function of unknown variables such as the dissolved, the adsorbed, and the vapor concentration of the pollutant, or

$$M_{in,o} + M_o = M_t(c,s,c_{sa},t) + M_{trans,t}(c,s,c_{sa},t) + M_{out,t}(c,s,c_{sa},t) \qquad \text{(PT-8)}$$

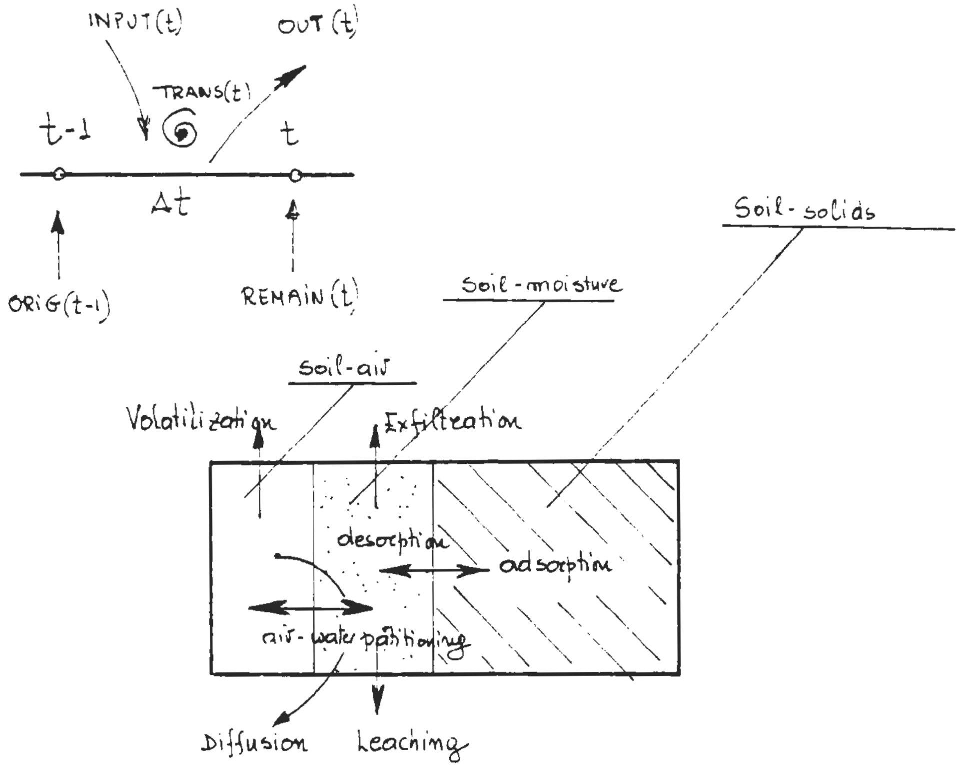
The above equation, which forms the basic philosophy of SESOIL, is consistent with a discretized version of equation PT-1 for a constant soil moisture content Θ:

$$\Theta(c_t - c_{t-1})/\Delta t = f(c,s,D^*,V,t) \qquad \text{(PT-9)}$$

however, in PT-8 pollutant mass balance (and not transport) is performed for all three pollutant phases (vapor, liquid, solid) as contrasted to PT-9 whose pollutant transport is studied only in the liquid and solid phase. Pollutant transport will result from the mass balance equation (PT-8) where the soil matrix is considered as a "pollutant carrier" as previously described and discussed below.

In addition, each of the terms of PT-8 is expressed in SESOIL as the weighted sum of the contributions (see equation PT-5) of various individual processes that cannot be accounted for by PT-9. For example, the term $M_{trans,t}$, the mass transformed during an infinitesimal time period Δt, is equal to the sum of the masses involved in hydrolysis from water (soil moisture), hydrolysis from soil solids and other degradation processes. This is a feature that cannot be studied via equation PT-9.

Finally, the SESOIL pollutant cycle equation is formulated for individual processes and for an infinitesimal time step Δt (Figure PT-3), and not



$$\underbrace{\text{INPUT}(t)} + \underbrace{\text{ORIG}(t-1)} = \underbrace{\text{OUT}(t)} + \underbrace{\text{TRANS}(t)} + \underbrace{\text{REMAIN}(t)}$$

- Total	- in soil-air	- to air = f(t) ↑ (volatilization)	- eg:	- in soil-air
- via Rain	- in soil moisture		- decay(t)	- in soil-moist
			- hydrolized (t)	
- Other	- on soil (adsorbed, cation exch, ...)	- Leaching/Exfil. ↕	- other(t)	- adsorbed
	- complexed	- other		- complexed

FIGURE PT-3: PARTITIONING AND OTHER TIME OR NON-TIME DEPENDENT PROCESSES WITHIN Δt.

for a differential time step $\Delta t=(t)-(t-1)$. This formulation allows SESOIL to easily prioritize strength of individual processes when necessary (eg. cation exchange takes precedence over all other processes, only that mass not able to be exchanged is available for other sorption processes) a modeling approach not followed before. This infinitesimal approach for interrelated soil subcompartment on soil layers, in each of which all pollutant phases are further interrelated, allows model developers to be able to employ more than one well accepted equation of the literature for one and the same process; for example, volatilization via Hamaker (1979), Farmer et al (1980), others -- see appendix VO.

The individual components of the SESOIL basic equation PT-8 are different depending on the number of soil layers considered/modeled, the nature of the process (eg. time-, non-time dependent), and the temporal resolution of the simulation. This results in the employment of different numerical procedures for solving the equation systems and in other scientific issues discussed in the following sections. Model users, however, need not be concerned with these issues which are handled internally (on-line) by the model.

2.5 Compartments

The mass balance equation PT-8 presented in the previous section was formulated for any representative soil element that was assumed to be homogenous and isotropic. The model calculated pollutant concentration for this element reflects an average over the entire compartment, which means that spatial variation within the selected compartment is ignored. However, the user can select a fine cross-sectional (areal) resolution of his compartment in order to increase areal-accuracy of his predictions as discussed at the end of this section.

To increase the depth dependent spatial resolution of the model, without incurring the numerical and computational difficulties of formulating and solving discretized partial differential equations, the SESOIL compartment has been treated as a series of interconnected layers. Each layer then has its own mass balance equation, and can both receive and release pollutant to and from other layers (above or below).

Presently, SESOIL can handle simulations with two or three soil zones (Figure PT-2). A top layer exposed to the atmosphere, a middle layer and a lower layer are of user specified depth. There is no optimal advice for the physical boundaries of these soil layers. In many cases, these layers can be used to simulate a shallow root zone of 5-25 cm; in other cases a wider depth may be used. However, the minimum depth is 1 cm, for mathematical reasons only.

Multiple soil layers (eg. N instead of 3) can be simulated even with this version of SESOIL; however, potential users should contact model developers (Bonazountas, Wagner) for this issue.

In SESOIL, a soil column can be specified to cover any area from 1 cm^2 (finite approach) to several km^2 (watershed approach). To simplify the mathematics and to avoid computer round-off errors, the hydrologic cycle, the sediment cycle and the pollutant cycle equations of SESOIL are normalized to an area of 1 cm^2. Pollutant fluxes across and within an element boundary have been simulated via equation PT-8 which has been formulated as

$$P_{in,o} + P_o = P_t + P_{out,t} + P_{transf,t} \qquad \text{(PT-10)}$$

where

$P_{in,o}$ = normalized (per cm^2) pollutant input flux; (ug/cm^2)

P_o = normalized original pollutant mass in compartment; (ug/cm^2)

P_t = normalized pollutant mass in compartment at time t; (ug/cm^2)

$P_{out,t}$ = normalized pollutant output flux; (ug/cm^2)

$P_{trans,t}$ = normalized pollutant mass transformed within time t; (ug/cm^2)

Equation PT-10 has been expanded to include various processes (hydrologic cycle, chemistry) taking place in the soil compartment. Time has become part of each individual processes within the time step of each simulation or level of operation. (Table PT-1).

TABLE PT-1

SUMMARY OF LEVEL FEATURES

LEVEL (#)	TIME Resolution	SPATIAL[3] Resolution	OTHER
0	Annual	2 soil layers	Hydrocycle is user input
1	Annual	2 soil layers	Hydrocycle is estimated [2]
2	Monthly[1]	2 soil layers	Hydrocycle is estimated [2]
3	Monthly[1]	3 soil layers	Hydrocycle is estimated [2]

[1] Provides annual averages of monthly estimates.

[2] Hydrocycle estimate infiltration and groundwater recharge participation for mass balance purposes.

[3] User should employ n+1 layers, where n is the user's needs. The +1 layer (next to groundwater) is for mass balance purposes.

3.0 POLLUTANT CYCLE ROUTINES

3.1 General

Currently SESOIL can be operated at four different levels -- LEVEL0, to LEVEL3 (Table PT-1) -- each level serving a different purpose and providing a different temporal and spatial resolution of processes simulated (eg. soil quality, pollutant mass to groundwater). LEVEL0 and LEVEL1 are associated with annual simulations and two soil layers, whereas LEVEL2 and LEVEL3 are associated with monthly simulations and either two soil layers (LEVEL2) or three soil layers (LEVEL3).

The SESOIL theory is structured around the temporal resolution of a simulation. The spatial resolution is separately studied within each temporal subset (sections 3.2 and 3.3 below). For information as to the appropriate level of model operation for a particular application, consult section 3.0, user's manual, of this document.

3.2 Annual Pollutant Cycle Routine (LEVEL0, LEVEL1)

3.2.1 General

Rough annual pollutant cycle simulations can be performed via LEVEL0 and LEVEL1 of SESOIL. These two levels differ only in the hydrologic cycle.

In LEVEL0, the hydrologic cycle components (soil moisture, infiltration, groundwater, runoff, etc) are <u>user</u> input to the model. In LEVEL1, these components are estimated by the model via its annual hydrologic cycle routine (HYDROA) and the site specific climatological (ie. NOAA) and soil data. The hydrologic cycle drives the pollutant cycle.

The same pollutant cycle routine (TRANSA) is used for both levels, LEVEL0 and LEVEL1. The routine design is based upon:

(1) a discretization of the soil compartment into two zones, upper unsaturated zone (watershed) exposed to the atmosphere and lower unsaturated zone which extends to the groundwater table; and

(2) the formulation of annual mass-balance equations PT-10 for each of the two soil layers.

The principal assumptions made for the formulation of the annual pollutant cycle equations are:

(1) the total pollution entering the subcompartment over the year is a "one-hit-event" which takes place at the start of the simulation;

(2) the total pollutant mass entering the subcompartment is instantaneously distributed throughout the subcompartment;

(3) the soil column is uncontaminated at the start of the simulation;

(4) the simulation is to be performed for only one year;

(5) the soil moisture content is represented by its long-term annual average value and does not vary with time within the year or spatially along the soil column.

LEVEL0 and LEVEL1 have specialized applications, for example: screening of a large number of chemicals that have to be compared for their environmental effects when released into a soil compartment. These levels should be employed with <u>care</u> (see also section 1.4 in the user's manual); therefore, if any of the previously given assumptions are not relevant to a particular application, the user has to select a higher level for his simulations, such as LEVEL2 or LEVEL3.

3.2.2 Governing Equations

Each of the two soil layers is considered a pollutant carrier with its own individual processes. The pollutant cycle equation system is solved analytically for reasons described in the following section and is coded in FORTRAN in subroutine TRANSA and in its related programmed functions -- eg. VOLA, ADSA. The equation system, formulated for an upper soil layer and a lower soil layer, is presented in Table PT-2.

3.2.3 Solution Procedure

The annual pollutant routine is designed for approximate studies, where the emphasis in both LEVEL0 and LEVEL1 is placed on the differences among predicted concentrations -- for various environments and chemicals -- and not on "accurate" values of the concentrations. Therefore, all processes in the annual routines are modeled as being of first-order, thus allowing a simple analytical solution of the systems to be obtained. A moisture penetration constraint is incorporated in both LEVEL0 and LEVEL1 simulations. This is discussed in detail in section 3.3.4 for all levels of SESOIL operations.

Because all of the individual fate processes/terms of the mass balance equation are linear functions of the pollutant concentration in the soil-moisture of each zone, the equations have been rearranged to give the pollutant concentrations in the soil-moisture directly as a function of the input parameters to the model (Table PT-3). The pollutant concentrations in the media of soil-air and soil-solids are calculated from the dissolved pollutant concentration, either via the partitioning equations presented in Section 2.3, or by dividing the pollutant masses previously calculated as being in each phase by the volume of that phase.

TABLE PT-2

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

All terms in paragraphs 1, 2, and 3 below are in units of $\mu g/cm^2$.

1. **General Mass Balance Equation** $P_{IN,i} + P_{O,i} = P_{REM,i} + P_{OUT,i} + P_{TRANS,i}$

2. **Individual Processes - Upper Zone**

Input mass: $P_{IN,U} = P_{INP,U} + P_{INF,U}$

Mass available at beginning of year: $P_{O,U} = 0.0$ (assumption 3, section 3.2.1)

Mass remaining at end of year: $P_{REM,U} = P_{MOI,U} + P_{ADS,U} + P_{CEC-F,U} + P_{COM,U} + P_{VAP,U}$

Mass out in year: $P_{OUT,U} = P_{RS} + P_{INF,L} + P_{VOL,U}$

Mass transformed within year: $P_{TRANS,U} = P_{HYD-H_2O,U} + P_{HYD-S,U} + P_{DEG,U}$

3. **Individual Processes - Lower Zone**

Input mass: $P_{IN,L} = P_{INP,L} + P_{INF,L}$

Mass available at beginning of year: $P_{O,L} = 0.0$ (assumption 3, section 3.2.1)

Mass remaining at end of year: $P_{REM,L} = P_{MOI,L} + P_{ADS,L} + P_{CEC-F,L} + P_{COM,L} + P_{VAP,L}$

Mass out in year: $P_{OUT,L} = P_{RG}$

Mass transformed within year: $P_{TRANS,L} = P_{HYD-H_2O,L} + P_{HYD-S,L} + P_{DEG,L}$

TABLE PT-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

Where:

i subscript for soil layer i

U subscript for the upper soil layer

L subscript for the lower soil layer

P_{IN} = pollutant mass input to soil compartment (total)

P_{O} = pollutant mass originally in soil compartment

P_{REM} = pollutant mass remaining in soil compartment

P_{OUT} = pollutant mass output from soil compartment

P_{INP} = pollutant mass directly input to soil compartment

P_{INF} = pollutant mass infiltrating to a zone

P_{MOI} = pollutant mass dissolved in soil moisture

P_{ADS} = pollutant mass adsorbed on soil particles

P_{CEC-F} = final pollutant mass cation exchanged

P_{COM} = pollutant mass complexed

P_{VAP} = pollutant mass in vapor phase (soil air)

TAB[illegible] T-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

P_{RS} = pollutant mass in surface runoff

P_{VOL} = pollutant mass volatilized

P_{TRANS} = pollutant mass transformed in the soil compartment

P_{HYD-H_2O} = pollutant mass hydrolyzed from soil moisture

P_{HYD-S} = pollutant mass hydrolyzed from soil solids

P_{DEG} = pollutant mass degraded (other than by hydrolysis)

P_{RG} = pollutant mass in groundwater recharge

TABLE PT-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

4. Individual Fate Process Equations

$P_{INP,i} = POLIN_i$

$P_{INF,U} = I_A \cdot a_{SL} \cdot SL$

$P_{INF,L} = c_U(A) \cdot I_{A,dU}$

$P_{MOI,i} = c_i(A) \cdot 0 \cdot d_i$

$$P_{COM,i} = \left(\frac{\left(c_i(A)/(MWT \cdot 10^6)\right) \cdot k_{eq} \cdot \left([L]_i/(MWT_{LIG} \cdot 10^6)\right)^b}{1 + (k_{eq} \cdot [L]_i/(MWT_{LIG} \cdot 10^6))^b}\right) \cdot MWT \cdot 10^6 \cdot 0 \cdot d_i$$

$P_{VAP,i} = c_i(A) \cdot \left(H/(R \cdot (T_a + 273))\right) \cdot (n - \theta) \cdot d_i$

$P_{ADS,i} = c_i(A) \cdot K_i \cdot \rho \cdot d_i$

$P_{CEC,i}$ = Calculated by comparing the total ion exchange capacity of the soil with the input mass

$$T_{CEC,i} = (CEC_i \cdot MWT/VAL) \cdot 10 \cdot \rho \cdot d_i$$

Case 1: All available pollutant is exchanged $P_{CEC,i} = P_{IN,i}$

Case 2: Exchange capacity of soil is exceeded $P_{CEC,i} = T_{CEC,i}$

$P_{RS} = c_U(A) \cdot R_{S,A} \cdot i_{RS,A}$

$$P_{VOL,U} = \left[c_u(A) \cdot (H/(R \cdot (T_a + 273) \cdot (d_u/2)))\right] \left[D_a \cdot ((n-\theta)^{10/3}/n^2)\right] \cdot (365 \cdot 86400)$$

TABLE PT-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

$P_{HYD-H_2O,i} = c_i(A) \cdot K_{T,i} \cdot \theta \cdot d_i \cdot 365$

$P_{HYD-S,i} = (c_i(A) \cdot K_i \cdot K_{T,i} \cdot \rho \cdot d_i \cdot 365) + (P_{CEC,i} \cdot K_{T,i} \cdot 365)$

$P_{DEG,i} = c_i(A) \cdot K_{DE,i} \cdot \theta \cdot d_i \cdot 365$

$P_{RG} = c_L(A) \cdot R_{G,A}$

5. <u>Supporting Equations</u>

$I_{A,d_U} = R_{G,A} + ((I_A - R_{G,A}) \cdot (d_L/Z))$

$MWT_{ML} = MWT + b \cdot MWT_{LIG}$

$K_i = K_{oc} \cdot (\%\ oc_i)/100$
(for organics)

$oc_L = oc_U \cdot a_{oc}$

$CEC_L = CEC_U \cdot a_{CEC}$

$K_{T,i} = K_N + K_H \cdot 10^{(-pH_i)} + K_{OH} \cdot 10^{-(14-pH_i)}$

$pH_L = pH_U \cdot a_{pH}$

$P_{CEC-F,i} = P_{CEC,i} - P_{CEC,i} \cdot K_{T,i} \cdot 365$

$[L]_i = LIG_i/(\theta \cdot d_i)$

$K_{DE,L} = K_{DE,U} \cdot a_{K_{DE}}$

TABLE PT-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

$$\text{DEPTH} = (I_A + R_{G,A})/(2 \cdot \theta \cdot n)$$

Where:

			Fortran Variables
U		subscript for upper soil layer	
L		subscript for lower soil layer	
i		subscript for any soil layer	
$POLIN_i$	=	annual direct pollutant input; ($\mu g/cm^2$)	POLINU,POLINL
I_A	=	annual rainfall infiltration; (cm)	IA
a_{SL}	=	concentration of pollutant in the rainfall infiltration as fraction of solubility; (-)	ASL
S_L	=	pollutant aqueous solubility; ($\mu g/mL$)	SL
$c_i(A)$	=	annual concentration of pollutant in soil moisture (layer i); ($\mu g/cm^2$)	CUA,CLA
I_{A,d_U}	=	annual infiltration at depth d_U; (cm)	IADU
d_i	=	depth of soil layer; (cm)	DU,DL
θ	=	average annual soil moisture content; (fractional)	THA

TABI 'T-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

			Fortran Variables
ρ	=	soil bulk density; (g/cm^3)	RSA
MWT	=	molecular weight of pollutant; (g/mol)	MWT
MWT_{LIG}	=	molecular weight of ligand; (g/mol)	MWTLIG
MWT_{ML}	=	molecular weight of pollutant-ligand complex; (g/mol)	MWTML
k_{eq}	=	stability constant of pollutant-ligand complex; (-)	SK
$[L]_i$	=	concentration of ligand in soil moisture; (μg/mL)	LIGCU,LIGCL
b	=	number of moles of ligand per mole of pollutant complexed; (-)	B
H	=	Henry's Law constant; $(m^3 \cdot atm/mol)$	H
R	=	gas constant; $(8.2 \times 10^{-5}\ m^3 \cdot atm/mol - {}^\circ K)$	R
T_a	=	temperature; (°C)	TA
n	=	soil effective porosity; (fractional)	N
K	=	adsorption coefficient on soil; [(μg/g)/(μg/mL)]	K
$T_{CEC,i}$	=	total compartment (i) cation exchange capacity; $(\mu g/cm^2)$	TCECU,TCECL
CEC,i	=	soil layer i cation exchange capacity; (milli equivalents/100g soil)	CECU,CECL
VAL	=	pollutant valence; (-)	VAL

TABLE PT-2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

			Fortran Variables
$R_{S,A}$	=	annual surface runoff; (cm)	RSA
$i_{RS,A}$	=	index (=0,1) of surface runoff participation in pollutant distribution; (-)	IRSA
D_A	=	diffusion coefficient of pollutant in air; (cm^2/S)	D
$K_{T,i}$	=	total hydrolysis rate constant; (day^{-1})	KTN
$K_{DE,i}$	=	degradation rate constant; (day^{-1})	KDE
$R_{G,A}$	=	annual groundwater recharge (cm)	RGA
Z	=	depth to groundwater; (cm - data input in m)	Z
K_{oc}	=	adsorption coefficient on organic carbon; [(μg/g OC)/(μg/mL)]	KOC
oc	=	soil organic carbon content; (%)	OC
a_{oc}	=	ratio soil organic carbon content lower: upper; (-)	AOC
a_{CEC}	=	ratio soil cation exchange capacity lower: upper; (-)	ACEC
K_N	=	neutral hydrolysis rate constant; (day^{-1})	KN
K_H	=	acid-catalyzed hydrolysis rate constant; ($day^{-1} . mol^{-1}/L^{-1}$)	KAH
K_{OH}	=	base catalyzed hydrolysis rate constant; ($day^{-1} . mol^{-1}/L^{-1}$)	KBH

TABLE 2 (Continued)

ANNUAL POLLUTANT CYCLE EQUATIONS - LEVELS 0,1

			Fortran Variables
pH_i	=	pH in layer i; (-)	PH
a_{pH}	=	ratio soil pH lower: upper; (-)	APH
$a_{K_{DE}}$	=	ratio degradation rate constant lower: upper; (-)	AKDE
$P_{CEC-F,i}$	=	final pollutant mass remaining cation exchanged; ($\mu g/cm^2$)	PCECU,PCECL
DEPTH	=	depth rain penetration since start of simulation; (cm)	DEPTH
LIG_i	=	ligand input mass	LIGU,LIGL

TABLE PT-3

SOLUTION TO POLLUTANT CYCLE EQUATIONS FOR LEVELS 0,1

Upper Zone:

$$C_U(A) = [P_{INP,U} + P_{CEC,U}]/[\theta \cdot d_U + k_U \cdot \rho \cdot d_U + H \cdot (n-\theta) \cdot d_U / R \cdot (T_a + 273) + R_{S,A} \cdot i_{RSA}$$

$$+ I_{A,d_U} + K_{T,U} \cdot \theta \cdot d_U \cdot 365 + K_{T,U} \cdot k_U \cdot \rho \cdot d_U \cdot 365 + k_{DE} \cdot \theta \cdot d_U \cdot 365 +$$

$$H/(R \cdot (T_a + 273) \cdot (d_U/2)) \cdot D_A \cdot (n-\theta)^{10/3} n^2 \cdot 86400 \cdot 365 + (1/(MWT \cdot 10^6)) \cdot k_{eq}$$

$$\cdot \left([L]_U / (MWT_{LIG} \cdot 10^6)\right)^b / \left(1 + (k_{eq} \cdot [L]_U/(MWT_{LIG} \cdot 10^6))^b\right) \cdot MWT \cdot 10^6 \cdot \theta \cdot d_U]$$

$$S_U(A) = (c_U(A) \cdot k_U \cdot \rho \cdot d_u + P_{CEC-F,u})/(\rho \cdot d_u)$$

$$C_{SA,U}(A) = C_U(A) \cdot H/ R \cdot (T_a + 273)$$

Lower Zone:

$$C_L(A) = [P_{INP,L} + P_{CEC,L}]/[\theta \cdot d_L + k_L \cdot \rho \cdot d_U + H \cdot (n-\theta) \cdot d_L / R \cdot (T_a + 273) + R_{GA} + K_{T,L}$$

$$\cdot \theta \cdot d_L \cdot 365 + K_{T,L} \cdot k_L \cdot \rho \cdot d_L \cdot 365 + k_{DE,L} \cdot \theta \cdot d_L \cdot 365 + (1/(MWT \cdot 10^6)) \cdot k_{eq}$$

$$\cdot \left([L]_L / (MWT_{LIG} \cdot 10^6)\right)^b / \left(1 + (k_{eq} \cdot [L]_L / (MWT_{LIG} \cdot 10^6))^b\right) \cdot MWT \cdot 10^6 \cdot \theta \cdot d_L]$$

$$S_L(A) = (C_L(A) \cdot k_L \cdot \rho \cdot d_L + P_{CEC-F,L})/ (\rho \cdot d_L)$$

$$C_{SA,L}(A) = c_{L(A)} \cdot H/ R \cdot (T_a + 273)$$

TABLE PT-3

SOLUTION TO POLLUTANT CYCLE EQUATIONS FOR LEVELS 0,1

Where:

$C_i(\Lambda)$ = pollutant concentration in moisture of zone i

$S_i(A)$ = pollutant concentration on soil of zone i

$C_{SA,i}(\Lambda)$ = pollutant concentration in soil-air of zone i

For other symbols and supporting equations, see table PT-2.

Because such a direct solution can be obtained only when all equation terms are linear with respect to the dissolved pollutant concentration, only the linear Freundlich adsorption isotherm (n=1) has been incorporated into these levels. In addition, the equations of the time dependent chemical processes are solved with an annual time step, which in fact causes numerical computational inaccuracies in the predicted pollutant concentrations. This is one of the reasons why these levels of operation should <u>not</u> be employed for site specific simulations.

3.3 Monthly Pollutant Cycle Routine (LEVEL2, LEVEL3)

3.3.1 General

Both LEVEL2 and LEVEL3 routines simulate monthly cycles. They differ only by the number of user specified layers that form the soil column. In LEVEL2, the soil column has been divided into two soil zones; the upper unsaturated soil zone and the lower unsaturated soil zone. LEVEL3 has three soil zones; the upper, the middle and the lower unsaturated zones. A monthly pollutant cycle subroutine has been formulated for each of the above layers.

The principal assumptions made for the formulation of the pollutant transport equations are:

(1) the total pollutant mass enters a subcompartment sequentially (at a user specified rate) during the simulation period;

(2) all physical phases of the subcompartment (soil, air, soil-moisture, soil-particles) are in equilibrium within a time step;

(3) the soil-moisture content is represented by its monthly long-term averaged value and does not vary over the course of the month or along the vertical of the soil column (an improved version of SESOIL is underway).

It is believed that these levels of SESOIL will cover a wide range of applications with predictive accuracies within expected limits and simultaneously offer great savings in user input data effort and computer time. For situations where the above assumptions are not considered satisfactory development (and use) of a fully discretized (over time and space) numerical version of SESOIL is necessary. Model developers (Bonazountas & Wagner) have planned for this level of operation -- LEVELN.

3.3.2 Governing Equations LEVEL2, LEVEL3

For each level, the individual pollutant carrying layers account for different sets of individual processes. Table PT-4 presents the derivation of the pollutant cycle equations for LEVEL2, Table PT-5 presents

TAB PT-4

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

All terms in paragraphs 1, 2, and 3 below are in units of $\mu g/cm^2$.

1. <u>General Mass Balance Equation</u>

$$P(t)_{IN,i} + P(t)_{0,i} = P(t)_{REM,i} + P(t)_{OUT,i} + P(t)_{TRAN,i}$$

2. <u>Individual Processes - Upper Zone</u>

Input mass: $P(t)_{IN,U} = P(t)_{INP,U} + P(t)_{INF,U}$

Mass available at beginning of time step: $P(t)_{0,U} = P(t-1)_{MOI,U} + P(t-1)_{SOIL,U} + P(t-1)_{COM,U} + P(t-1)_{VAP,U}$

Mass remaining at end of time step: $P(t)_{REM,U} = P(t)_{MOI,U} + P(t)_{ADS,U} + P(t)_{CEC-F,U} + P(t)_{COM,U} + P(t)_{VAP,U}$

Mass out in time step: $P(t)_{OUT,U} = P(t)_{RS} + P(t)_{INF,L} + P(t)_{VOL,U} + P(t)_{SINK,U}$

Mass transformed within time step: $P(t)_{TRAN,U} = P(t)_{HYD-H_2O,U} + P(t)_{HYD-S,U} + P(t)_{DEG,U} + P(t)_{TRANS,U} + P(t)_{HYD-C,U}$

3. <u>Individual Processes - Lower Zone</u>

Input mass: $P(t)_{IN,L} = P(t)_{INP,L} + P(t)_{INF,L}$

Mass available at beginning of time step: $P(t)_{0,L} = P(t-1)_{MOI,L} + P(t-1)_{SOIL,L} + P(t-1)_{COM,L} + P(t-1)_{VAP,L}$

Mass remaining at end of time step: $P(t)_{REM,L} = P(t)_{MOI,L} + P(t)_{ADS,L} + P(t)_{CEC-F,L} + P(t)_{COM,L} + P(t)_{VAP,L}$

Mass out in time step: $P(t)_{OUT,L} = P(t)_{RG} + P(t)_{VOL,L} + P(t)_{SINK,U}$

Mass transformed within time step: $P(t)_{TRAN,L} = P(t)_{HYD-H_2O,L} + P(t)_{HYD-S,L} + P(t)_{DEG,L} + P(t)_{TRANS,L} + P(t)_{HYD-C,L}$

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

Where:

i subscript for soil layer i

t indicates the current time step

$t-1$ indicates the previous time step

U subscript for the upper soil layer

L subscript for the lower soil layer

P_{IN} = pollutant mass input to soil compartment (total)

P_{O} = pollutant mass originally in soil compartment

P_{REM} = pollutant mass remaining in soil compartment

P_{OUT} = pollutant mass output from soil compartment

P_{TRAN} = pollutant mass transformed in the soil compartment

P_{INP} = pollutant mass directly input to soil compartment

P_{INF} = pollutant mass infiltrating to a zone

P_{MOI} = pollutant mass dissolved in soil moisture

P_{SOIL} = pollutant mass associated (adsorbed, exchanged) with soil

P_{COM} = pollutant mass complexed

TABLE -4 (Continued)
MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

P_{VAP} = pollutant mass in vapor phase (soil air)

P_{ADS} = pollutant mass adsorbed on soil particles

P_{CEC-F} = final pollutant mass cation exchanged

P_{RS} = pollutant mass in surface runoff

P_{VOL} = pollutant mass volatilized

P_{SINK} = pollutant mass in other sinks (e.g., sediment transport)

P_{HYD-H_2O} = pollutant mass hydrolyzed from soil moisture

P_{HYD-S} = pollutant mass hydrolyzed from adsorbed pollutant

P_{HYD-C} = pollutant mass hydrolyzed from exchanged pollutant

P_{DEG} = pollutant mass degraded (other than by hydrolysis)

P_{TRANS} = pollutant mass in other transformations (e.g., fixation)

P_{RG} = pollutant mass in groundwater recharge

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS – LEVEL 2

4. Individual Fate Process Equations

$$P(t)_{INP,i} = POLIN_i/NI$$

$$P(t)_{INF,U} = I_M \cdot a_{SL} \cdot SL/NI$$

$$P(t)_{INF,L} = c_U(t) \cdot I_{M,dU}/NI$$

$$P(t)_{MOI,i} = c_i(t) \cdot \theta(t) \cdot d_i$$

$$P(t)_{SOIL,i} = s_i(t) \cdot \rho \cdot d_i$$

$$P(t)_{VAP,i} = c_i(t) \cdot \Big(H/\big(R \cdot (T_a + 273)\big)\Big) \cdot \big(n - \theta(t)\big) \cdot d_i$$

$$P(t)_{ADS,i} = c_i(t)^{1/FRN} \cdot K_i \cdot \rho \cdot d_i$$

$P(t)_{CEC,i}$ = Calculated by comparing the total ion exchange capacity of the soil with the input mass

$$T_{CEC,i} = (CEC_i \cdot MWT/VAL) \cdot 10 \cdot \rho \cdot d_i$$

Case 1: All available pollutant is exchanged $P(t)_{CEC,i} = P(t)_{IN,i}$

Case 2: Exchange capacity of soil is exceeded $P(t)_{CEC,i} = T_{CEC,i}$

$$P(t)_{RS} = c_U(t) \cdot R_{S,M} \cdot i_{RS,M}/NI$$

$$P(t)_{VOL,U} = \Big[c_U(t) \cdot \Big(H/\big(R \cdot (T_a + 273) \cdot (d_U/2)\big)\Big)\Big] \Big[D_a \cdot \Big(\big(n-\theta(t)\big)^{10/3}/n^2\Big)\Big] \cdot \left(\frac{30 \cdot 86400}{NI}\right)$$

TABLE I (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

$P(t)_{VOL,L}$ = Calculated according to concentration gradient

Case 1: $c_U(t) < c_L(t)$ (Gradient is upward.)

$$P(t)_{VOL,L} = \left[c_L(t) \cdot \left(H/\left(R \cdot (T_a + 273) \cdot \left(\frac{d_U+d_L}{2}\right)\right)\right)\right]\left[D_A \cdot \left(\left(n-\theta(t)^{10/3}\right)/n^2\right)\right]\left(\frac{30 \cdot 86400}{NI}\right)$$

Case 2: $c_U(t) \geq c_L(t)$ (Gradient is downward or zero.)

$$P(t)_{VOL,L} = 0.0$$

$$P(t)_{SINK,i} = P_{SINK,i}/NI$$

$$P(t)_{HYD\text{-}H_2O,i} = c_i(t) \cdot K_{T,i} \cdot \theta(t) \cdot d_i \cdot (30/NI)$$

$$P(t)_{HYD\text{-}S,i} = (c_i(t)^{1/FRN} \cdot K_i \cdot K_{T,i} \cdot \rho \cdot d_i \cdot (30/NI))$$

$$P(t)_{DEG,i} = c_i(t) \cdot K_{DE,i} \cdot \theta(t) \cdot d_i \cdot (30/NI)$$

$$P(t)_{TRANS,i} = P_{TRANS,i}/NI$$

$$P(t)_{RG} = c_L(t) \cdot R_{G,M}/NI$$

$$P(t)_{HYD\text{-}C,i} = (P(t)_{CEC,i} \cdot K_{T,i} \cdot (30/NI))$$

$$P(t)_{COM,i} = [ML]_i \cdot MWT \cdot 10^6 \cdot \theta(t) \cdot d_i \quad SK = [ML]_i/\left[\left(\frac{C_i(t)}{MWT \cdot 10^6} - [ML]_i\right)\left(\frac{[L]_i}{MWT_{LIG} \cdot 10^6} - b[ML]_i\right)^b\right]^*$$

---

*Solved numerically in subroutine COMP

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

5. Supporting Equations

$$I_{M,d_U} = \left(R_{G,M} + (I_M - R_{G,M}) \cdot (d_L/Z)\right) \cdot \frac{k(1)_u}{k(1)_z}$$

$$k(1)_z = \frac{Z}{\frac{d_U}{k(1)_u} + \frac{d_L}{k(1)_L}}$$

$$MWT_{ML} = MWT + b \cdot MWT_{LIG}$$

$$K_i = K_{OC} \cdot (\%\ OC_i)/100$$

(for organics)

$$oc_L = oc_u \cdot a_{oc}$$

$$CEC_L = CEC_U \cdot a_{CEC}$$

$$K_{T,i} = K_N + K_H \cdot 10^{(-pH_i)} + K_{OH} \cdot 10^{-(14-pH_i)}$$

$$pH_L = pH_U \cdot a_{pH}$$

$$K_{DE,L} = K_{DE,U} \cdot a_{KDE}$$

$$P(t)_{CEC-F,i} = P(t)_{CEC,i} - P(t)_{CEC,i} \cdot K_{T,i} \cdot (30/NI)$$

$$S_i(t) = \left(p(t)_{ADS,i} + P(t)_{CEC-F,i}\right) / (\rho \cdot d_i)$$

$$DEPTH(t) = (I_M + R_{G,M})/(2 \cdot 0 \cdot n \cdot NI)$$

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

$$[L]_i = LIG_i / (\theta \cdot d_i)$$

$$[L]_{i,FREE} = \left([L]_i \cdot d_i \cdot \theta - B \cdot P_{COM} \cdot \left(\frac{MWTLIG}{MWT} \right) \right) / (d_i \cdot \theta)$$

$$c_{SA,i}(t) = c_i(t) \cdot H \; / (R \cdot (T_a + 273))$$

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

Where:

			Fortran Variables
t		indicates current time step	
$t-1$		indicates previous time step	
U		subscript for upper soil layer	
L		subscript for upper soil layer	
i		subscript for any soil layer	
$POLIN_i$	=	monthly direct pollutant input; ($\mu g/cm^2$)	POLINU,POLINL
NI	=	number of numerical iterations per month; (-1)	NI
I_M	=	monthly rainfall infiltration; (cm)	IM
a_{SL}	=	concentration of pollutant in the infiltration as fraction of solubility; (-)	ASL
S_L	=	pollutant aqueous solubility; ($\mu g/mL$)	SL
$c_i(t)$	=	concentration of pollutant in soil moisture (layer i); ($\mu g/cm^2$)	CUM,CLM
I_{M,d_U}	=	monthly infiltration at depth d_U; (cm)	IMOU
d_i	=	depth of soil layer; (cm)	DU,DL
θ	=	average soil moisture content; (fractional)	THA
$s_i(t)$	=	concentration of pollutant on soil solids (layer i); ($\mu g/g$ soil)	SUM,SLM

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

			Fortran Variables
ρ	=	soil bulk density; (g/cm^3)	RS
MWT	=	molecular weight of pollutant; (g/mol)	MWT
MWT_{LIG}	=	molecular weight of ligand; (g/mol)	MWTLIG
MWT_{ML}	=	molecular weight of pollutant-ligand complex; (g/mol)	MWTML
k_{eq}	=	stability constant of pollutant-ligand complex; (-)	SK
$[L]_i$	=	concentration of ligand in soil moisture; (ug/mL)	LIGCU,LIGCL
b	=	number of moles of ligand per mole of pollutant complexed; (-)	B
H	=	Henry's Law constant; (m^3 . atm/mol)	H
R	=	gas constant; (8.2 x 10^{-5} m^3 · atm/mol - °K)	R
T_a	=	temperature; (°C)	T
n	=	soil effective porosity; (fractional)	N
K	=	adsorption coefficient on soil; [(µg/g)/(µg/mL)]	K
FRN	=	Freundich exponant; (-)	FRN
$T_{CEC,i}$	=	total compartment cation exchange capacity; (µg/cm^2)	TCECU,TCECL
CEC,i	=	soil cation exchange capacity; (milli equivalents/100g soil)	CECU,CECL
VAL	=	pollutant valence; (-)	VAL

TABLE PT-4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

			Fortran Variables
$R_{S,M}$	=	monthly surface runoff; (cm)	RSM
$i_{RS,M}$	=	index (=0,1) of surface runoff participation in pollutant distribution; (-)	IRSM
D_A	=	diffusion coefficient of pollutant in air; (cm^2/S)	D
$P_{OUT,i}$	=	other pollutant sinks per month; $(\mu g/cm^2)$	POUTU,POUTL
$K_{T,i}$	=	total hydrolysis rate constant; (day^{-1})	KTN
K_{DE}	=	total degradation rate constant; (day^{-1})	KDE
$P_{TRANS,N}$	=	other pollutant transformations per month; $(\mu g/cm^2)$	PTRANU,PTRANL
R_G	=	monthly groundwater recharge	RGM
Z	=	depth to groundwater; (cm)	Z
K_{OC}	=	adsorption coefficient on organic carbon; $[(\mu g/g\ OC)/(\mu g/mL)]$	KOC
OC	=	soil organic carbon content; (o/o)	OC
a_{OC}	=	ratio soil organic carbon content lower: upper; (-)	AOC
a_{CEC}	=	ratio soil cation exchange capacity lower: upper; (-)	ACEC
K_N	=	neutral hydrolysis rate constant; (day^{-1})	KN

TABLE -4 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 2

			Fortran Variables
K_H	=	acid-catalyzed hydrolysis rate constant; $(day^{-1} \cdot mol^{-1}/L^{-1})$	KAH
K_{OH}	=	base catalyzed hydrolysis rate constant; $(day^{-1} \cdot mol^{-1}/L^{-1})$	KBH
pH_i	=	soil pH; (-)	PH
a_{pH}	=	ratio soil pH lower: upper; (-)	APH
a_{KDE}	=	ratio degradation rate constant lower: upper; (-)	AKDE
$P(t)_{CEC-F,i}$	=	final pollutant mass remaining cation exchanged; $(\mu g/cm^2)$	PCECU,PCECL
$k(1)_z$	=	average intrinsic soil permeability; (cm^2)	K1
$k(1)_i$	=	intrinsic permeability of soil zone i; (cm^2)	K1U,K1L
DEPTH	=	depth rain penetration since start of simulation; (cm)	DEPTH
C	=	pore disconnectedness index; (-)	C
K(1)	=	saturated hydraulic conductivity; (cm/day)	BK1
LIG_i	=	ligand input mass; $(\mu g/cm^2)$	LIGU,LIGL
$[L]_{i,FREE}$	=	free ligand concentration; $(\mu g/mL)$	LIGCUF,LIGCLF
$c_{Sa,i}(t)$	=	pollutant concentration in soil air; $(\mu g/cm^3)$	CUSA,CLSA
$[ML]$	=	concentration of ligand-pollutant complex (mol/mL)	MLC

the derivation of these equations for LEVEL3. The LEVEL2 equations are coded in FORTRAN in subroutine TRANSM, those of LEVEL3 are coded in subroutine TRANS3. Both subroutines call several functions containing individual fate equations (see appendix FC, FORTRAN code).

3.3.3 Numerical Solution Procedures

3.3.3.1 General

All of the individual fate processes which compose the SESOIL mass balance equation are -- and are expressed as -- functions of

(1) a variety of rate, partitioning and other constants; and

(2) the pollutant concentration in the moisture of each zone.

Some of the concentration terms are non-linear; therefore, these equations can not be solved directly as in the case of the annual cycle routines. An iterative solution procedure has been developed to solve this system efficiently.

The solution procedure involves the following steps for each layer -- starting at the surface of the soil column:

(1) an initial value c (t) = 0.0 is assumed;

(2) the mass balance equation PT-10 is solved iteratively

$$P_i = P_{in,i} + P_{o,i} - P_{a,i} - P_{out,i} - P_{transf,i}$$

by incrementally increasing the value of c(t) by Δc (Δc is large at the beginning) until P_i meets one of the five constraint criteria described in the next section;

(3) the incremental interval Δc is decreased to a new value $\Delta c1 < \Delta c$ and the system is resolved within a narrower numerical range by following again the above rationale.

(4) Above procedure is repeated until:

  (a) $P_n \leq \varepsilon$, where ε is a confidence limit presently specified as 0.01, or

  (b) the accuracy limits of the computer (machine) is reached (i.e. accumulation of round-off becomes significant).

TABL T-5

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

All terms in paragraphs 1-4 below are in units of $\mu g/cm^2$.

1. **General Mass Balance Equation** $P(t)_{IN,i} + P(t)_{REM,i} = P(t)_{A,i} + P(t)_{OUT,i} + P(t)_{TRAN,i}$

2. **Individual Processes - Upper Zone**

Input mass: $P(t)_{IN,U} = P(t)_{INP,U} + P(t)_{INF,U}$

Mass available at beginning of time step: $P(t)_{O,U} = P(t-1)_{MOI,U} + P(t-1)_{SOIL,U} + P(t-1)_{COM,U} + P(t-1)_{VAP,U}$

Mass remaining at end of time step: $P(t)_{REM,U} = P(t)_{MOI,U} + P(t)_{ADS,U} + P(t)_{CEC-F,U} + P(t)_{COM,U} + P(t)_{VAP,U}$

Mass out in time step: $P(t)_{OUT,U} = P(t)_{RS} + P(t)_{INF,M} + P(t)_{VOL,U} + P(t)_{SINK,U}$

Mass transformed within time step: $P(t)_{TRAN,U} = P(t)_{HYD-H_2O,U} + P(t)_{HYD-S,U} + P(t)_{DEG,U} + P(t)_{TRANS,U} + P(t)_{HYD-C,U}$

3. **Individual Processes - Middle Zone**

Input mass: $P(t)_{IN,M} = P(t)_{INP,M} + P(t)_{INF,M}$

Mass available at beginning of time step: $P(t)_{O,M} = P(t-1)_{MOI,M} + P(t-1)_{SOIL,M} + P(t-1)_{COM,M} + P(t-1)_{VAP,M}$

Mass remaining at end of time step: $P(t)_{REM,M} = P(t)_{MOI,M} + P(t)_{ADS,M} + P(t)_{CEC-F,M} + P(t)_{COM,M} + P(t)_{VAP,M}$

Mass out in time step: $P(t)_{OUT,M} = P(t)_{INF,L} + P(t)_{VOL,M} + P(t)_{SINK,M}$

Mass transformed within time step: $P(t)_{TRAN,M} = P(t)_{HYD-H_2O,M} + P(t)_{HYD-S,M} + P(t)_{DEG,M} + P(t)_{TRANS,M} + P(t)_{HYD-C,}$

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

4. Individual Processes - Lower Zone

Input mass: $P(t)_{IN,L} = P(t)_{INP,L} + P(t)_{INF,L}$

Mass available at beginning of time step: $P(t)_{O,L} = P(t-1)_{MOI,L} + P(t-1)_{SOIL,L} + P(t-1)_{COM,L} + P(t-1)_{VAP,L}$

Mass remaining at end of time step: $P(t)_{REM,L} = P(t)_{MOI,L} + P(t)_{ADS,L} + P(t)_{CEC,L} + P(t)_{COM,L} + P(t)_{VAP,L}$

Mass out in time step: $P(t)_{OUT,L} = P(t)_{RG} + P(t)_{VOL,L} + P(t)_{SINK,U}$

Mass transformed within time step: $P(t)_{TRAN,L} = P(t)_{HYD-H_2O,L} + P(t)_{HYD-S,L} + P(t)_{DEG,L} + P(t)_{TRANS,L} + P(t)_{HYD-C,L}$

TABLE [illegible]-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

Where:

i subscript for soil layer i

t indicates the current time step

$t-1$ indicates the previous time step

U subscript for the upper soil layer

M subscript for the middle soil layer

L subscript for the lower soil layer

P_{IN} = pollutant mass input to soil compartment (total)

P_O = pollutant mass originally in soil compartment

P_{REM} = pollutant mass remaining in soil compartment

P_{OUT} = pollutant mass output from soil compartment

P_{TRAN} = pollutant mass transformed in the soil compartment

P_{INP} = pollutant mass directly input to soil compartment

P_{INF} = pollutant mass infiltrating to a zone

P_{MOI} = pollutant mass dissolved in soil moisture

P_{SOIL} = pollutant mass associated (adsorbed, exchanged) with soil

P_{COM} = pollutant mass complexed

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

P_{VAP} = pollutant mass in vapor phase (soil air)

P_{ADS} = pollutant mass adsorbed on soil particles

P_{CEC-F} = final pollutant mass cation exchanged

P_{RS} = pollutant mass in surface runoff

P_{VOL} = pollutant mass volatilized

P_{SINK} = pollutant mass in other sinks (e.g., sediment transport)

P_{HYD-H_2O} = pollutant mass hydrolyzed from soil moisture

P_{HYD-S} = pollutant mass hydrolyzed from adsorbed pollutant

P_{HYD-C} = pollutant mass hydrolyzed from exchanged pollutant

P_{DEG} = pollutant mass degraded (other than by hydrolysis)

P_{TRANS} = pollutant mass in other transformations (e.g., fixation)

P_{RG} = pollutant mass in groundwater recharge

TABLE -5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

5. Individual Fate Process Equations

$P(t)_{INP,i} = POLIN_i/NI$

$P(t)_{INF,U} = I_M \cdot a_{SL} \cdot SL/NI$

$P(t)_{INF,M} = c_U(t) \cdot I_{M,dU}/NI$

$P(t)_{INF,L} = c_M(t) \cdot I_{M,dM}/NI$

$P(t)_{MOI,i} = c_i(t) \cdot \theta(t) \cdot d_i$

$P(t)_{SOIL,i} = s_i(t) \cdot \rho \cdot d_i$

$P(t)_{COM,i} = [ML]_i \cdot MWT \cdot 10^6 \cdot \theta(t) \cdot d_i \quad SK = [ML]_i / \left[\left(\frac{c_i(t)}{MWT \cdot 10^6} - [ML]_i \right) \left(\frac{[L]_i}{MWT_{LIG} \cdot 10^6} - b[ML]_i \right)^b \right]^*$

$P(t)_{VAP,i} = c_i(t) \cdot \left(H/\left(R \cdot (T_a + 273) \right) \right) \cdot (n - \theta(t)) \cdot d_i$.

$P(t)_{ADS,i} = c_i(t)^{1/FRN} \cdot K_i \cdot \rho \cdot d_i$

$P(t)_{CEC,i}$ = Calculated by comparing the total ion exchange capacity of the soil with the input mass

$T_{CEC,i} = (CEC_i \cdot MWT/VAL) \cdot 10 \cdot \rho \cdot d_i$

Case 1: All available pollutant is exchanged $P(t)_{CEC,i} = P(t)_{IN,i}$

Case 2: Exchange capacity of soil is exceeded $P(t)_{CEC,i} = T_{CEC,i}$

$P(t)_{RS} = c_U(t) \cdot R_{S,M} \cdot i_{RS,M}/NI$

---

*Solved numerically in subroutine COMP

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

$$P(t)_{VOL,U} = \left[c_U(t) \cdot \left(H/\left(R \cdot (T_a + 273) \cdot (d_U/2)\right)\right)\right] \left[D_a \cdot \left(\left(n-\theta(t)\right)^{10/3}/n^2\right)\right] \cdot \left(\frac{30 \cdot 86400}{NI}\right)$$

$P(t)_{VOL,M}$ = Calculated according to concentration gradient

Case 1: $C_U(t) < C_M(t)$ (Gradient is upwards.)

$$P(t)_{VOL,M} = \left[C_M(t) \cdot \left(H/\left(R \cdot (T_a + 273) \cdot \left(d_U + \frac{d_M}{2}\right)\right)\right)\right]\left[D_A \cdot \left(\left(n-\theta(t)^{10/3}\right)/n^2\right)\right]\left(\frac{30 . 86400}{NI}\right)$$

Case 2: $C_U(t) \geq C_M(t)$ (Gradient is downward or zero.)

$$P(t)_{VOL,M} = 0.0$$

$P(t)_{VOL,L}$ = Calculated according to concentration gradient

Case 1: $C_U(t)$ and $C_M(t) < C_L(t)$ (Gradient is upward.)

$$P(t)_{VOL,L} = \left[C_L(t) . \left(H/\left(R . (T_a + 273)\right)\right) . \left(d_U + d_M + \frac{d_L}{2}\right)\right]\left[D_A \cdot \left(\left(n-\theta(t)^{10/3}\right)/n^2\right)\right]\left(\frac{30 . 86400}{NI}\right)$$

Case 2: $C_U(t)$ or $C_M(t) \geq C_L(t)$ (Gradient is downward or zero.)

$$P(t)_{VOL,L} = 0.0$$

$$P(t)_{SINK,i} = P_{SINK,i}/NI$$

$$P(t)_{HYD-H_2O,i} = c_i(t) . K_{T,i} . \theta(t) . d_i . (30/NI)$$

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

$$P(t)_{HYD-S,i} = (c_i(t)^{1/FRN} \cdot K_i \cdot K_{T,i} \cdot \rho \cdot d_i \cdot (30/NI))$$

$$P(t)_{DEG,i} = c_i(t) \cdot K_{DE,i} \cdot \theta(t) \cdot d_i \cdot (30/NI)$$

$$P(t)_{TRANS,i} = P_{TRANS,i}/NI$$

$$P(t)_{RG} = c_L(t) \cdot R_{G,M}/NI$$

$$P(t)_{HYD-C,i} = P(t)_{CEC,i} \cdot K_{T,i} \cdot (30/NI)$$

6. Supporting Equations

$$I_{M,d_U} = \left(R_{G,M} + (I_M - R_{G,M}) \cdot (d_M + d_L/Z)\right) \cdot \frac{k(1)_u}{k(1)_z}$$

$$I_{M,d_L} = \left(R_{G,M} + (I_M - R_{G,M}) \cdot (d_L / Z)\right) \cdot \frac{k_2}{k_z}$$

$$k_z = \frac{Z}{\frac{d_U}{k(1)_U} + \frac{d_M}{k(1)_M} + \frac{d_L}{k(1)_L}}$$

$$MWT_{ML} = MWT + b \cdot MWT_{LIG}$$

$$K_i = K_{OC} \cdot (\%\ OC_i)/100$$
(for organics)

$$OC_M = OC_U \cdot a2_{OC}$$

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

$$OC_L = OC_U \cdot a_{OC}$$

$$CEC_M = CEC_U \cdot a2_{CEC}$$

$$CEC_L = CEC_U \cdot a_{CEC}$$

$$K_{T,i} = K_N + (K_H \cdot 10^{(-pH_i)}) + (K_{OH} \cdot 10^{-(14-pH_i)})$$

$$pH_M = pH_U \cdot a2_{pH}$$

$$pH_L = pH_U \cdot a_{pH}$$

$$K_{DE,M} = K_{DE,U} \cdot a2_{KDE}$$

$$K_{DE,L} = K_{DE,U} \cdot a_{KDE}$$

$$P(t)_{CEC-F,i} = P(t)_{CEC,i} - P(t)_{CEC,i} \cdot K_{T,i} \cdot (30/NI)$$

$$S_i(t) = \left(p(t)_{ADS,i} + P(t)_{CEC-F,i}\right) / (\rho \cdot d_i)$$

$$DEPTH(t) = (I_M + R_{G,M})/(2 \cdot \breve{\theta} \cdot n \cdot NI)$$

TABLE F (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

$$[L]_i = LIG_i / (\theta \cdot d_i)$$

$$[L]_{i,FREE} = \left([L]_i \cdot d_i \cdot \theta - B \cdot P_{COM} \cdot \left(\frac{MWTLIG}{MWT} \right) \right) / (d_i \cdot \theta)$$

$$c_{SA,i}(t) = (c_i(t) \cdot H \;/\; R \cdot (T_a + 273))$$

$$k_2 = \frac{d_U + d_M}{\left(\frac{d_U}{k(1)_U} + \frac{d_M}{k(1)_M} \right)}$$

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

Where:

			Fortran Variables
t		indicates current time step	
$t-1$		indicates previous time step	
U		subscript for upper soil layer	
M		subscript for middle soil layer	
L		subscript for lower soil layer	
i		subscript for any soil layer	
$POLIN_i$	=	monthly direct pollutant input; ($\mu g/cm^2$)	POLINU,POLINL
NI	=	number of numerical iterations per month; (-1)	NI
I_M	=	monthly rainfall infiltration; (cm)	IM
a_{SL}	=	concentration of pollutant in the infiltration as fraction of solubility; (-)	ASL
S_L	=	pollutant aqueous solubility; ($\mu g/mL$)	SL
$c_i(t)$	=	concentration of pollutant in soil moisture (layer i); ($\mu g/cm^2$)	CUM,CLM
I_{M,d_i}	=	monthly infiltration at depth d_i; (cm)	IMOU
d_i	=	depth of soil layer; (cm)	DU,DL
θ	=	average soil moisture content; (fractional)	THA
$s_i(t)$	=	concentration of pollutant on soil solids (layer i); ($\mu g/g$ [illegible])	SU[illegible] M

T/ ' PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

			Fortr· " ·iables
ρ	=	soil bulk density; (g/cm^3)	RS
MWT	=	molecular weight of pollutant; (g/mol)	MWT
MWT_{LIG}	=	molecular weight of ligand; (g/mol)	MWTLIG
MWT_{ML}	=	molecular weight of pollutant-ligand complex; (g/mol)	MWTML
k_{eq}	=	stability constant of pollutant-ligand complex; (-)	SK
$[L]_i$	=	concentration of ligand in soil moisture; (ug/mL)	LIGCU,LIGCL
b	=	number of moles of ligand per mole of pollutant complexed; (-)	B
H	=	Henry's Law constant; (m^3 . atm/mol)	H
R	=	gas constant; (8.2 x 10^{-5} m^3 · atm/mol - °K)	R
T_a	=	temperature; (°C)	T
n	=	soil effective porosity; (fractional)	N
K	=	adsorption coefficient on soil; [(μg/g)/(μg/mL)]	K
FRN	=	Freundich exponant; (-)	FRN
$T_{CEC,i}$	=	total compartment cation exchange capacity; (μg/cm^2)	TCECU,TCECL
CEC,i	=	soil cation exchange capacity; (milli equivalents/100g soil)	CECU,CECL
VAL	=	pollutant valence; (-)	VAL

TABLE PT-5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

		Fortran Variables
$R_{S,M}$	= monthly surface runoff; (cm)	RSM
$i_{RS,M}$	= index (=0,1) of surface runoff participation in pollutant distribution; (-)	IRSM
D_A	= diffusion coefficient of pollutant in air; (cm^2/S)	D
$P_{OUT,i}$	= other pollutant sinks per month; ($\mu g/cm^2$)	POUTU,POUTL
$K_{T,i}$	= total hydrolysis rate constant; (day^{-1})	KTN
K_{DE}	= total degradation rate constant; (day^{-1})	KDE
$P_{TRANS,N}$	= other pollutant transformations per month; ($\mu g/cm^2$)	PTRANU,PTRANL
R_G	= monthly groundwater recharge	RGM
Z	= depth to groundwater; (cm)	Z
K_{OC}	= adsorption coefficient on organic carbon; [(μg/g OC)/(μg/mL)]	KOC
OC	= soil organic carbon content; (o/o)	OC
a_{OC}	= ratio soil organic carbon content lower: upper; (-)	AOC
a_{CEC}	= ratio soil cation exchange capacity lower: upper; (-)	ACEC
K_N	= neutral hydrolysis rate constant; (day^{-1})	KN

TABL -5 (Continued)

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

			Fortran Variables
K_H	=	acid-catalyzed hydrolysis rate constant; $(day^{-1} . mol^{-1}/L^{-1})$	KAH
K_{OH}	=	base catalyzed hydrolysis rate constant; $(day^{-1} . mol^{-1}/L^{-1})$	KBH
pH_i	=	soil pH; (-)	PH
a_{pH}	=	ratio soil pH lower: upper; (-)	APH
a_{KDE}	=	ratio degradation rate constant lower: upper; (-)	AKDE
$P(t)_{CEC_i}$	=	pollutant mass remaining cation exchanged; $(\mu g/cm^2)$	PCECU,PCECL
$k(1)_z$	=	average intrinsic soil permeability; (cm^2)	K1
$k(1)_i$	=	intrinsic permeability of soil zone i; (cm^2)	K1U,K1L
DEPTH	=	depth rain penetration since start of simulation; (cm)	DEPTH
C	=	pore disconnectedness index; (-)	C
K(1)	=	saturated hydraulic conductivity; (cm/day)	BK1
LIG_i	=	ligand input mass; $(\mu g/cm^2)$	LIGU,LIGL
$[L]_{i,FREE}$	=	free ligand concentration; $(\mu g/mL)$	LIGCUF,LIGCLF
$c_{Sa,i}(t)$	=	pollutant concentration in soil air; $(\mu g/cm^3)$	CUSA,CLSA

MONTHLY POLLUTANT CYCLE EQUATIONS - LEVEL 3

			Fortran Variables
k_2	=	average permeability of upper and middle zone; (cm^2)	K2
$a2_{OC}$	=	ratio soil organic carbon content middle: upper; (-)	A2OC
$a2_{CEC}$	=	ratio soil cation exchange capacity middle: upper; (-)	A2CEC
$a2_{pH}$	=	ratio soil pH middle: upper; (-)	A2PH
$a2_{KDE}$	=	ratio soil degradation rate middle: upper; (-)	A2KDE
[ML]	=	concentration of ligand-pollutant complex; (mol/mL)	MLC

3.3.3.2 Constraint Criteria

Five convergence/constraint criteria have been designed to assure a solution within limits (ε). These are described below and are graphically presented in Figure PT-4.

(1) $\text{abs}(P_i[c'(t+1)]) \leq \text{abs}(P_i[c(t+1)])$ (PT-11)

This criterion assures movement of the initial P_i value towards the zero-axis.

(2) $\text{abs}(P_i) \leq \varepsilon = 0.01$ (PT-12)

This criterion implies convergence to a zero value has occurred.

(3) $(P_i[c'(t+1)]) \cdot (P_i[c(t+1)]) < 0$ (PT-13)

This criterion assures the convergence to zero, without overpassing the zero value. In the latter case the value would jump the zero-axis (from the one or the other direction) and would continue indefinitely.

(4) $\text{abs}(P_i[c(t+1)]) = 0$ (PT-14)

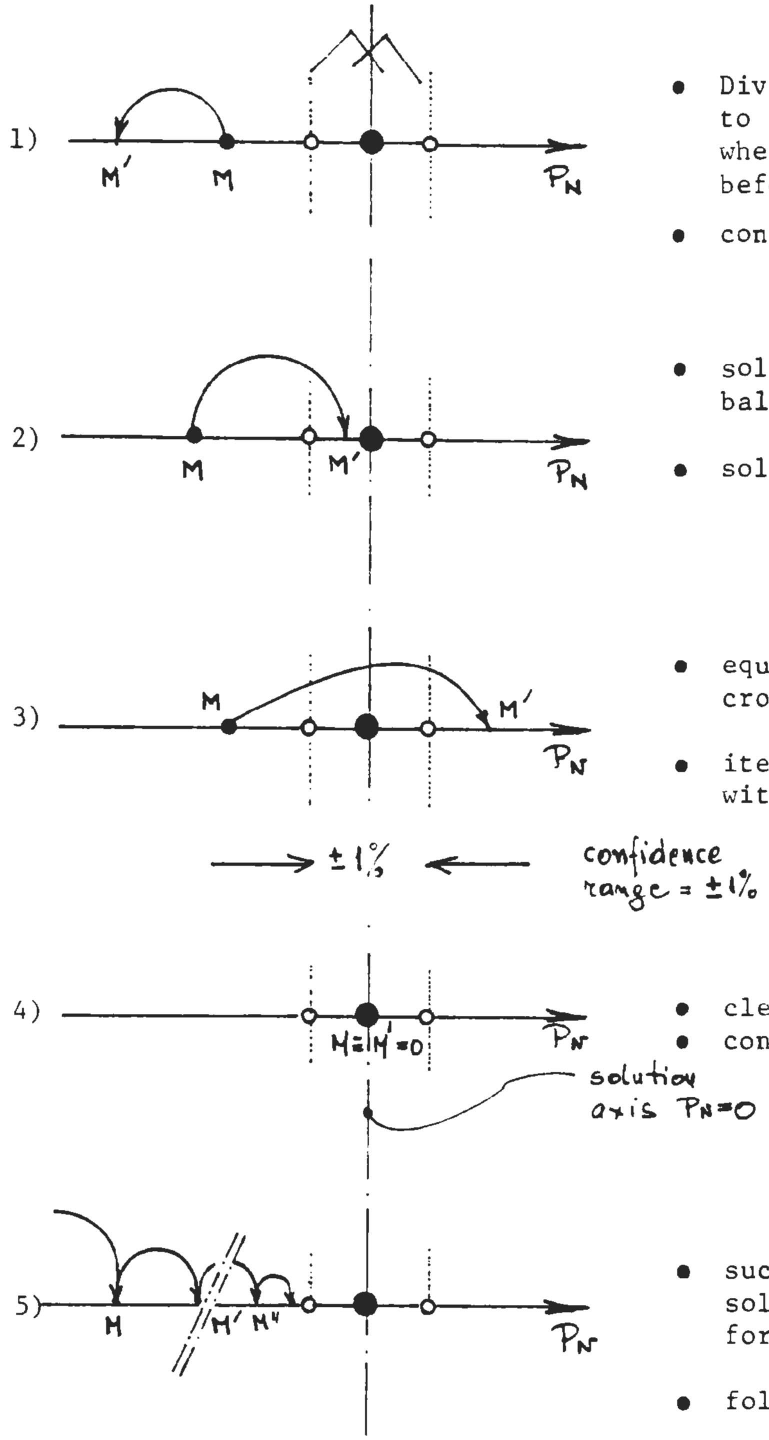
This constraint reflects the case where no pollution is in the column any more.

(5) $c(t+1)$ has been calculated to 6 significant digits. For extreme concentrations (either very small/very large pollutant load), the equations may not balance to within 1% (criterion 2) due to accumulation of round-off error. In such a case, this criteria forces convergence.

3.3.3.3 Simulation Time Step

For LEVEL2 and LEVEL3 the pollutant cycle equations are formulated on a monthly basis, and the results are reported for each month simulated. However, since all terms that are time dependent are written with an explicit time step (Δt), the model has to be run for smaller time steps (eg. week, day) in order to account for the non-linear processes (eg. volatilization). In this case the obtained monthly reports (output) represent the iterations and summations of results of many smaller iterations.

The number of iterations per month (NI) is preset in the FORTRAN code. The actual simulation time step (in days) is equal to 30 (days/month) divided by the number of iterations per month NI, or $\Delta t=30/NI$. A large



- Diverging iteration corresponding to the physico-chemical situation where the soil layer becomes "clean" before the end of the month.
- concentrations in layer = 0.0

- solution of equation system balanced within ± 1%
- solution obtained

- equation system solution has crossed origin
- iteration procedure repeated with a higher resolution

- clean soil layer criterion
- concentrations are set to 0.0

- successive approximation to solution via variable resolution for computational efficiency
- follow criterion 2 above

FIGURE PT-4: SCHEMATIC OF MATHEMATICAL CONVERGENCE CRITERIA OF EQUATION SYSTEMS number of iterations per month will increase the accuracy of the model output, and will also result in increased computational time. Presently, the model performs four iterations per month (30/4=7.5 days per simulation). It is felt that this number of iterations is a reasonable compromise between accuracy and computational cost. However, any number of iterations per month can be reprogrammed when necessary.

3.3.4 Moisture Molecule Penetration Constraint

A pollutant originating from any unsaturated soil zone layer will theoretically reach an underlying soil layer (or the groundwater) as soon as a moisture drop originating from the first layer reaches the latter layer (or the groundwater). In practice, however, a "retardation" of the pollutant front will take place with respect to the bulk mass of moisture movement. This retardation is mathematically described by Freeze and Cherry (1979 p. 404) via a retardation factor related to the adsorption capability of the pollutant on the soil particles. If no adsorption is assumed, the pollutant front <u>will</u> follow the seepage soil moisture velocity.

It is not necessary to separately account for such a pollutant in SESOIL, since the pollutant transport routine of the model will retard pollutant mass traveling vertically via the adsorption and other processes modeled. However, it is important to know whether a polluted soil moisture molecule (carrying a dissolved pollutant) originating in an upper layer has penetrated -- even at a negligible concentration -- through the entire layer to the underlying soil layer or has reached the groundwater. If so, the pollutant transport routine of the underlying layer has to be activated; otherwise, no pollutant mass input to the underlying layer will take place. The moisture molecule penetration constraint is incorporated in all levels of SESOIL operations.

Two methods of approximating estimation of the penetration depth of a soil moisture molecule into the underlying soil compartment are relevant to the SESOIL analysis: (1) via Darcy's law, (2) via soil dynamics, and these are combined below into one equation for any soil layer.

The average linear soil flow velocity in a saturated soil is given by Freeze & Cherry (1979, p.71).

$$\bar{v} = Q/n \cdot A = Q/n \qquad \text{(PT-15)}$$

where

$\bar{v}$ = average linear velocity

Q = volumetric flux (or specific discharge, or Darcy's velocity)

n = soil porosity

A = cross section of soil matrix (assumed 1)

The average linear soil moisture velocity -- known also as interstitial pore water velocity (Enfield et al 1980) -- is given by

$$\bar{v}(\Theta) = \bar{v}/\Theta = Q/n\cdot\Theta \qquad \text{(PT-16)}$$

where

$\bar{v}(\Theta)$ = average linear soil moisture velocity

Θ = soil moisture content

SESOIL employs the theoretical hydrologic routine of Eagleson (1978) as adapted for time dependent moisture storage and transfer in the course of the months. Therefore, Eagleson's principal equations have been also employed here to describe volumetric fluxes in a soil layer.

The monthly average linear volumetric flux or specific discharge in a month for a soil layer is given in SESOIL (eg. HY-28.1) by

$$Q = (I(M)+(Rg(M))/2 \qquad \text{(PT-17)}$$

Therefore, by combining above equations, we have the average moisture molecule penetration depth after t months

$$d = t\cdot(I(M)+Rg(M))/(2\Theta n) \qquad \text{(PT-18)}$$

where

d = average soil moisture penetration depth (cm)

t = 1,2,3, ... months elapsed; (integer #)

$I(M)$ = monthly infiltration (depth) to soil layer (cm)

$Rg(M)$ = monthly percolation (depth) from soil laver (cm)

Θ = soil moisture content (fraction)

n = soil porosity (fraction)

Numerical example (data from Eagleson 1977):

- Assume: $t=12$ (ie. months), $\Theta=s_o\cdot n=(0.67)\cdot(0.35)=0.235$, $I(M)=63.6/12=5.3$ cm (ie. 5.3 cm/month and for the 12 months), $Rg(M)=19.8/12=1.65$ cm, $n=0.35$
- then $d = 12(5.3+1.65)/(2*0.235*0.35) = 507$ cm (ie. cm/yr)

3.4 Storm-by-Storm Pollutant Cycle (LEVELN)

The LEVELN of SESOIL has not been developed; however, designers have conceptualized the development of this model feature. For additional information call 617/864-5770.

4.0 DISCUSSION

SESOIL is a "user friendly" model and as such the pollutant cycle subroutines are designed to be easily expandable. Processes not currently included in the simulation can be incorporated simply by adding another term to one of the mass balance terms. For example, an expression for the degradation of pollutant by soil bacteria could be added to the model by including the bacterial degradation term with the other pollutant transformation equations.

The pollutant mass added to the groundwater is estimated by all levels of operation of the model. The behavior of pollutant within the groundwater is not currently described by SESOIL, although the simulation of a groundwater "layer" can be developed and model developers have some long-term plans. However, SESOIL is also adaptable to provide information for (and/or to be interfaced with) other groundwater models of the literature.

5.0 REFERENCES

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ID - input data

SESOIL updates See notebook
July 1982

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LIST OF FIGURES

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1.0 INTRODUCTION

Four major input data categories are required by SESOIL

1. Climatological Data
2. Soil/Vegetational Data
3. Chemical Data
4. Application Specific Data

Data for these categories are handled and input to the model in different ways, depending upon the simulation level. Currently four levels of operation are available, varying from general "Exposure Assessment" simulations (annual, monthly) to "site-specific" simulations. The four levels of operation are

(1)	LEVEL0	Annual General Exposure Assessment Simulations (2 soil layers)
(2)	LEVEL1	Annual Site-Specific Exposure Assessment Simulations (2 soil layers)
(3)	LEVEL2	Monthly Site-Specific and Exposure Assessment Simulations (2 soil layers)
(4)	LEVEL3	Monthly Site-Specific and Exposure Assessment Simulations (3 soil layers)

This appendix will provide in the future a thorough background to effectively compile all input data for all above categories, in order to prove to potential users how easy it is to run SESOIL contrasted to other sophisticated models of the literature. The following sections, however, give detailed description only for the climatologic data compilation, since time and budget constraints prevented the developers (Bonazountas, Wagner 1981) to invest more time in this aspect of the model use.

Data for all data categories are stored in permanent SESOIL data files for easy retrieval at any time.

2.0 CLIMATOLOGICAL INPUT DATA

2.1 General

Site-specific simulations require monthly or annual and time and site-specific climatological input data. Non-site-specific (hypothetical) simulations require long averaged (monthly or annual) climatological input data. Data compilation for these for types of simulations can be performed

(1) Manually from the National Oceanographic and Atmospheric Administration (NOAA) climatological data records (sheets); and

(2) Computerized via a subroutine that compiles on-line data from NOAA climatological data tapes.

The LEVELO simulation does not require climatologic input data because the hydrologic cycle components are input to the model by the user (see Section 3.0, User's Manual). However, this level of operation requires soil/vegetational, chemical and application specific data, which can be compiled and stored permanently in the SESOIL data files as described in Section 3.0 through 5.0 of this appendix.

The climatological input data for levels 1, 2 and 3 can be obtained from NOAA records in the form of data sheets or data tapes. Information can be requested -- by indicating the weather station number and location (Figure ID-1) -- from the

U.S. Department of Commerce, NOAA
National Climatic Center, Federal Building
Asheville, North Carolina 28801
704/258-2850 (ext. 208, Digitized Data Dept.)

The following paragraphs describe the two methods of analyzing NOAA climatological data for input to SESOIL: (1) hand calculation based on the NOAA Monthly Data Sheets, and (2) a computer subroutine (IPDATA) which uses NOAA data tapes. The hand calculation method will be described first to provide some background on the ten parameters and how they are delivered.

2.2 Manual Estimations of Climatologic Data

NOAA reports provide daily, monthly (Figure ID-2) and annual (Figure ID-3) summaries of climatologic data for designated sites throughout the United States.

The ten SESOIL climatologic input parameters are

L	latitude; (N°)
TA	temperature; (°C)
NN	fractional cloud cover -- 24 hrs average; (-)
S	humidity (fractional)
A	albedo; (-)
REP	rate of evapotranspiration; (cm/day)
MPA	mean (annual or monthly) precipitation; (cm/yr or cm/month)

FIGURE ID-1

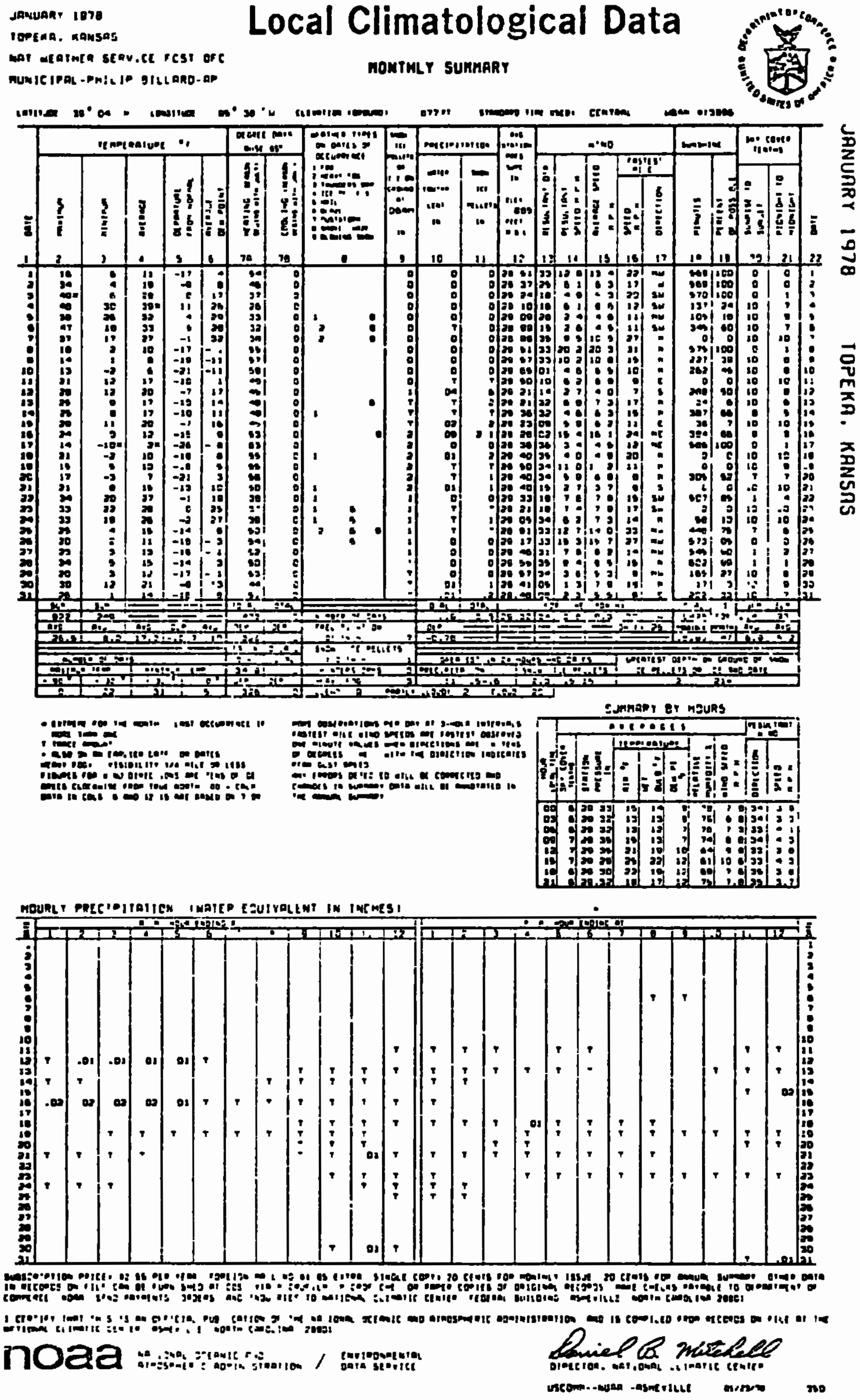
SURVEY OF TD-1440

FOR: MONTANA

STATION NO.	SERVICE	STATION		PERIOD
24033	W	Billings/Logan Fld.		01/48-
24132	F	Bozeman/Belgrade/Gallatin		01/48-12/54
24135	F	Butte/Silver Bow Fld.		01/48-12/60
24040	F	Custer		01/48-05/50
24137	F	Cut Bank/ Mun		01/48-
24138	F	Dillon/Beaverhead Cnty.		01/48-06/73
24139	F	Drummond		01/48-12/54
24034	W	Glasgow/WBO	*	01/48-10/55
94008	W	Glasgow/Int.	*	10/55-
94010	A	Glasgow		10/58-06/68
24143	W	Great Falls/Int.		01/48-
24112	A	Great Falls/Malstrom		01/49-12/70
24035	W	Havre/WBO	*	01/48-12/48;
			*	05/50-05/61
94012	W	Havre/City-Cnty.	*	02/61-
24144	W	Helena		01/48-
24146	W	Kalispell/Glacier Prk.	# *	01/48-
24036	F	Lewistown/Mun.		01/48-
24150	F	Livingston/Mission		01/48-12/54
24037	F	Miles City/Mun.		01/48-
24153	W	Missoula/Johnson-Bell Fld.		01/48-
24159	F	Superior		01/48-11/53
24161	F	Whitehall		01/48-12/54

FIGURE ID-2

SAMPLE NOAA MONTHLY DATA SHEET



JANUARY 1978
TOPEKA, KANSAS
NAT WEATHER SERVICE FCST OFC
MUNICIPAL-PHILIP BILLARD-AP

Local Climatological Data

MONTHLY SUMMARY

JANUARY 1978 TOPEKA, KANSAS

SUMMARY BY HOURS

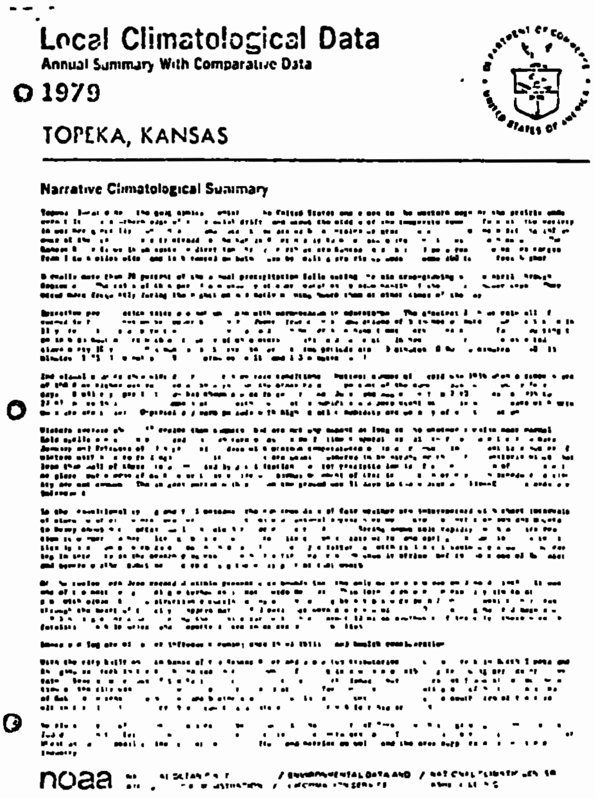
HOURLY PRECIPITATION (WATER EQUIVALENT IN INCHES)

noaa

Daniel B. Mitchell
DIRECTOR, NATIONAL CLIMATIC CENTER

FIGURE ID-3

SAMPLE NOAA ANNUAL SUMMARY DATA SHEET



Local Climatological Data

Annual Summary With Comparative Data

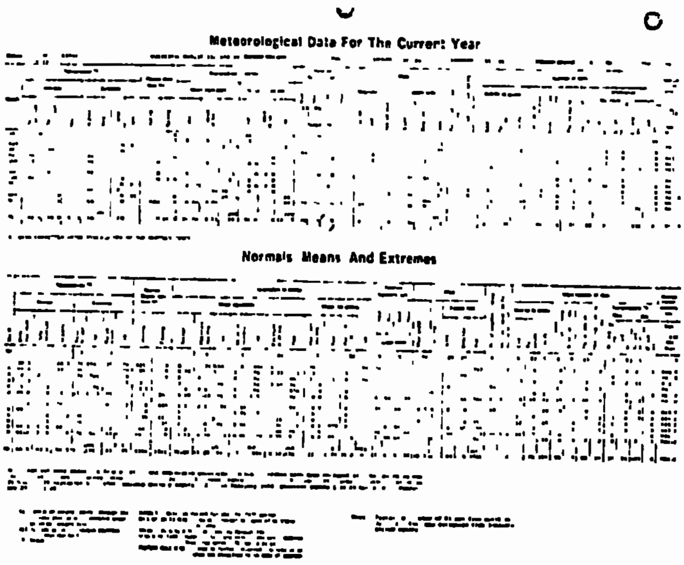
1979

TOPEKA, KANSAS

Narrative Climatological Summary

noaa

Page 1 of form

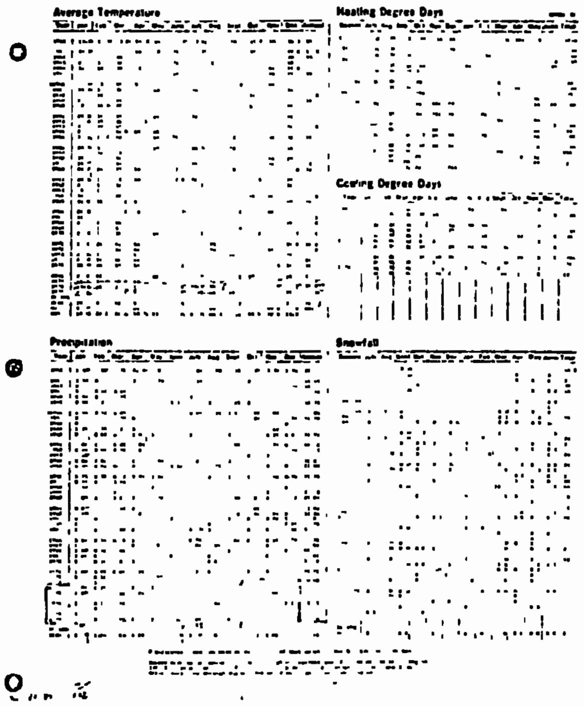


Meteorological Data For The Current Year

Normals Means And Extremes

Page 2

FIGURE ID-3 (Continued)



Page 3

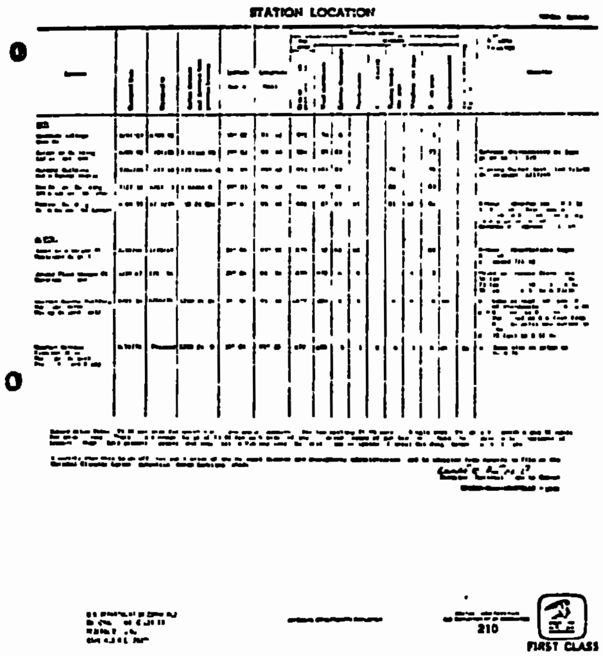
Average Temperature

Heating Degree Days

Cooling Degree Days

Precipitation

Snowfall



Page 4

STATION LOCATION

210

FIRST CLASS

MTR	mean (annual or monthly) storm duration; (days)
MN	mean number of storm events during (annual or monthly) simulation period; (-)
MT	mean length of rain period (in a year or in a month); (days)

Aside from L all other data for the above parameters are handled in four different ways when compiling SESOIL input, depending upon the simulation level; namely depending upon the time interval (months or years) and the time period (specific or general/long-term) analyzed.

2.2.1 Monthly Time-Specific Simulations

Values for all ten parameters must be provided for each month of year(s) under study in a 10 x 12 matrix, as shown in Figure ID-4. Matrix elements for each month are obtained or calculated from the NOAA climatological forms/sheets as follows

- L - The latitude is given as two digits, minutes only, and is found in the top left corner of the NOAA forms (Figure ID-5). Latitude can be also expressed (input) in decimal degrees; eg. $39^\circ\ 04' = 39+(4/60) = 39.067^\circ$.
- TA - The average temperature for the month is given in °F at the bottom of Column 4 (Figure ID-5) and must be converted to °C via $C^\circ = 5(F^\circ-32)/9$.
- NN - Cloud cover is taken as the average monthly sky cover (in tenths) from column 22 (Figure ID-5) and is divided by 10 to convert to fractional cloud cover.
- S - The average monthly humidity is estimated by averaging the relative humidity given for the 8 observations during the day in the data block shown in Figure ID-6, and is divided by 100 to convert to fractional humidity.
- A - Albedo is taken from the corresponding table of Appendix HY (Table HY-1).
- REP - Because evapotranspiration is estimated by SESOIL from the five climatic parameters previously described, this data entry can be input as 0.0. In case site-specific values are available (e.g. Table HY-1), users may input REP and disregard compilation of the previous five parameters.
- MPM - The mean monthly precipitation is given at the bottom of column 10 (Figure ID-5), in inches and must be converted to centimeters (1 inch = 2.54 cm).

FIGURE ID-4

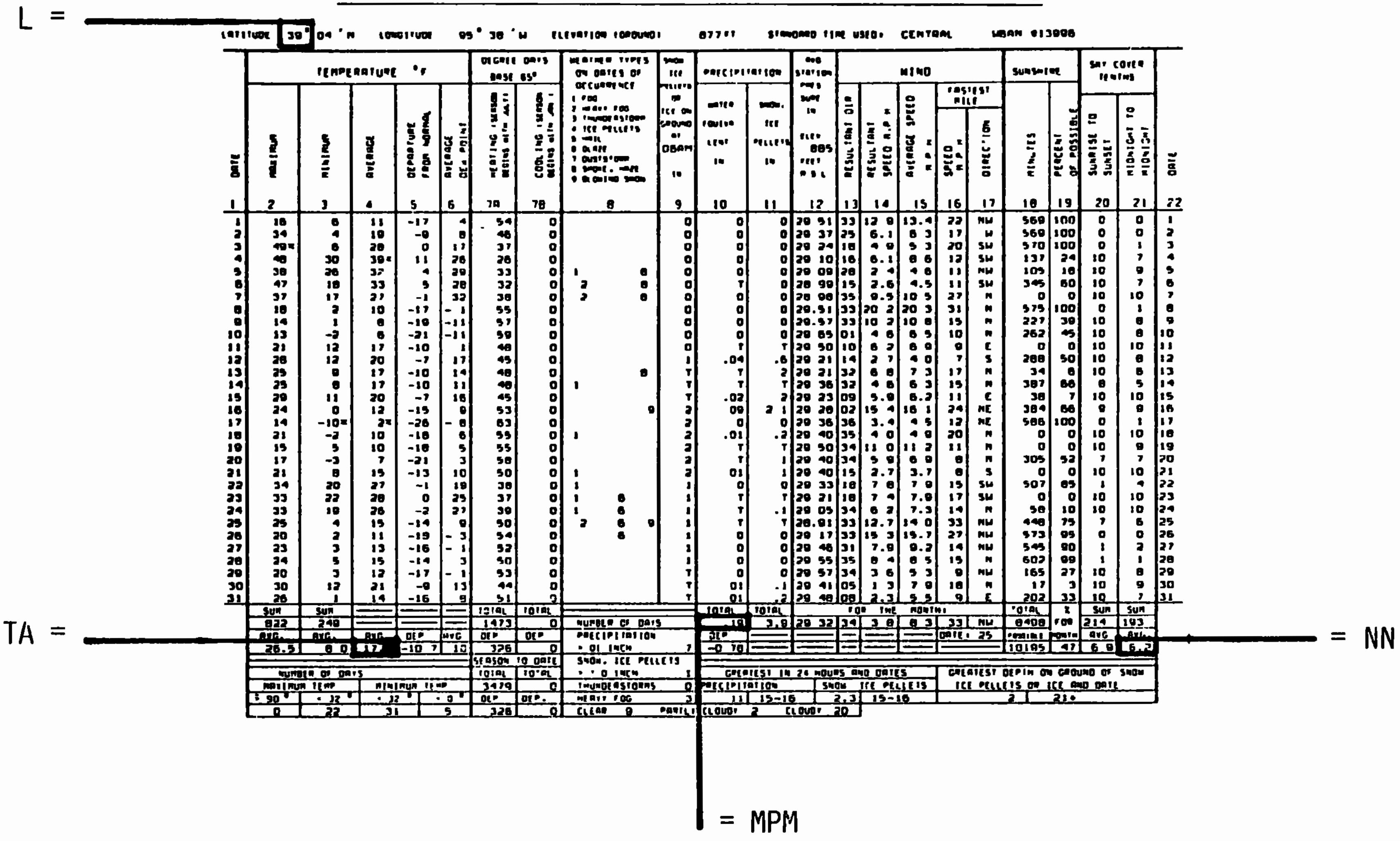
SAMPLE DATA MATRIX OF INPUT PARAMETERS FOR A TWO-YEAR MONTHLY SIMULATION

```
        TOPEKA, KANSAS:  OCTOBER 1978-SEPTEMBER 1979
        10/78  11/78  12/78  1/79   2/79   3/79   4/79   5/79   6/79   7/79   8/79   9/79
L       39.0   39.0   [illegible] [illegible] [illegible] 39.0 [illegible] 39.0 39.0 39. [illegible] [illegible]
TA      12.56  5.11   0.     0.     [illegible].7 [illegible].11 1.[illegible] 1[illegible].0[illegible] 2[illegible] [illegible].7 [illegible].11 [illegible].1
[illegible]  .32   .69   .[illegible]  .60   .6[illegible]  .67   .62   .60   .54   .[illegible]  .4[illegible]  .21
S       .6513  .7480  .[illegible] .[illegible] .75[illegible] .7500  .7375  .7150  .7513  .7[illegible] .7[illegible]7[illegible] .70[illegible]
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
FED     0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.[illegible]  0.0
[illegible]  0.91  [illegible].1[illegible]  1.[illegible]  4.[illegible]  1.[illegible]  10.0[illegible]  [illegible]  [illegible]  14.[illegible]0  1[illegible]  1[illegible]  [illegible]
[illegible]  .25   .[illegible]  .[illegible]  .[illegible]  .17   .1[illegible]  .1[illegible]  .1[illegible]  .[illegible]0  .1[illegible]  .[illegible]7  .[illegible]
[illegible]  2.0   10.0   [illegible]  [illegible]  [illegible]  1[illegible].0  1[illegible]  10.0  [illegible].0  1[illegible]  11.[illegible]  4.[illegible]
NT      30.5   [illegible] [illegible] [illegible] [illegible] 30.[illegible] [illegible] 3[illegible] 30.  30.  [illegible]  30.[illegible]

        TOPEKA, KANSAS:  OCTOBER 1979-SEPTEMBER 1980
        10/78  11/78  12/78  1/79   2/79   3/79   4/79   5/79   6/79   7/79   8/79   9/79
L       39.0   39.0   [illegible] [illegible] [illegible] 39.0 3[illegible] 39.0 39.0 39.[illegible] [illegible] [illegible].0
TA      12.89  [illegible].44  1.[illegible]  [illegible]  [illegible]  4.[illegible]  1[illegible]  17.11  2[illegible].72  [illegible]  [illegible]  [illegible]1.1
[illegible]  .46   .44   .[illegible]  .[illegible]4  .[illegible]  .64   .[illegible]7  .[illegible]1  .[illegible]  .[illegible]1  [illegible]  .47
S       .5875  .[illegible] .[illegible] .7011  .[illegible] .[illegible]7[illegible] .[illegible] .[illegible] .[illegible]1 .[illegible] .[illegible] .71[illegible]
A       0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1    0.1
[illegible]  0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   [illegible]  [illegible]
[illegible]  10.4  4.57   0.1[illegible]  3.4   2.21   10.54  2.52   12.32  12.17  2.[illegible]1  14.[illegible]  3.[illegible]2
[illegible]  .27   .24    .[illegible]4  .34   .27    .30    .14    .05    .09    .[illegible]  .1[illegible]  .0[illegible]
[illegible]  7.0   6.0    1.[illegible]  [illegible].0  7.0  10.0  [illegible]  10.0  3.0  5.[illegible]  1[illegible]  5.0
[illegible]  30.[illegible]  30.[illegible]  30.[illegible]  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  30.[illegible]  [illegible]  [illegible]  [illegible]
```

FIGURE ID-5

FIRST SAMPLE DATA BLOCK FROM MONTHLY NOAA DATA SHEETS



LATITUDE 39° 04 ' N LONGITUDE 95° 38 ' W ELEVATION (GROUND) 877 FT STANDARD TIME USED: CENTRAL WBAN #13996

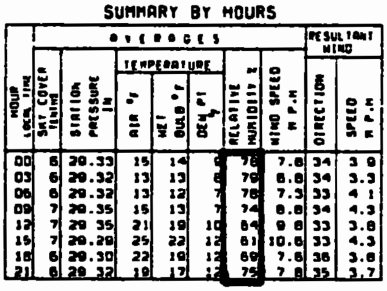
	TEMPERATURE °F					DEGREE DAYS BASE 65°		WEATHER TYPES ON DATES OF OCCURRENCE 1 FOG 2 HEAVY FOG 3 THUNDERSTORM 4 ICE PELLETS 5 HAIL 6 GLAZE 7 DUSTSTORM 8 SMOKE, HAZE 9 BLOWING SNOW	SNOW ICE PELLETS OR ICE ON GROUND AT 06AM IN	PRECIPITATION		AVG STATION PRESS IN. ELEV 885 FEET M.S.L.	WIND			FASTEST MILE		SUNSHINE		SKY COVER TENTHS		
DATE	MAXIMUM	MINIMUM	AVERAGE	DEPARTURE FROM NORMAL	AVERAGE DEW POINT	HEATING (SEASON BEGINS WITH JULY)	COOLING (SEASON BEGINS WITH JAN)			WATER EQUIVALENT IN	SNOW, ICE PELLETS IN		RESULTANT DIR	RESULTANT SPEED M.P.H.	AVERAGE SPEED M.P.H.	SPEED M.P.H.	DIRECTION	MINUTES	PERCENT OF POSSIBLE	SUNRISE TO SUNSET	MIDNIGHT TO MIDNIGHT	DATE
1	2	3	4	5	6	7A	7B	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	18	6	11	-17	4	54	0		0	0	0	29 91	33	12 8	13.4	22	NW	569	100	0	0	1
2	34	4	19	-8	8	46	0		0	0	0	29 37	25	6.1	8 3	17	W	569	100	0	0	2
3	49*	6	28	0	17	37	0		0	0	0	29 24	18	4 9	5 3	20	SW	570	100	0	1	3
4	48	30	39*	11	26	26	0		0	0	0	29 10	16	6.1	8 6	12	SW	137	24	10	7	4
5	38	26	37	4	29	33	0	1 8	0	0	0	29 09	28	2 4	4 6	11	NW	105	18	10	9	5
6	47	18	33	5	28	32	0	2 8	0	T	0	28 99	15	2.6	4.5	11	SW	345	60	10	7	6
7	37	17	27	-1	32	38	0	2 8	0	0	0	28 98	35	9.5	10 5	27	N	0	0	10	10	7
8	18	2	10	-17	- 1	55	0		0	0	0	29.51	33	20 2	20 3	31	N	575	100	0	1	8
9	14	1	8	-19	-11	57	0		0	0	0	29.57	33	10 2	10 8	15	N	227	38	10	8	9
10	13	-2	6	-21	-11	59	0		0	0	0	29 65	01	4 6	6 5	10	N	262	45	10	8	10
11	21	12	17	-10	1	48	0		0	T	T	29 50	10	6 2	6 9	9	E	0	0	10	10	11
12	28	12	20	-7	17	45	0		1	.04	.6	29 21	14	2 7	4 0	7	S	288	50	10	8	12
13	25	8	17	-10	14	48	0	8	T	T	2	29 21	32	6 8	7 3	17	N	34	8	10	8	13
14	25	8	17	-10	11	48	0	1	T	T	T	29 36	32	4 8	6 3	15	N	387	68	8	5	14
15	29	11	20	-7	16	45	0		T	.02	2	29 23	09	5.8	6.2	11	E	38	7	10	10	15
16	24	0	12	-15	9	53	0	9	2	09	2 1	29 28	02	15 4	16 1	24	NE	384	68	9	9	16
17	14	-10*	2*	-26	- 8	63	0		2	0	0	29 36	36	3.4	4 5	12	NE	586	100	0	1	17
18	21	-2	10	-18	6	55	0	1	2	.01	.2	29 40	35	4 0	4 9	20	N	0	0	10	10	18
19	15	5	10	-18	5	55	0		2	T	T	29 50	34	11 0	11 2	11	N	0	0	10	9	19
20	17	-3	7	-21	3	58	0		2	T	1	29 40	34	5 9	6 9	8	N	305	52	7	7	20
21	21	8	15	-13	10	50	0	1	2	01	1	29 40	15	2.7	3.7	8	S	0	0	10	10	21
22	34	20	27	-1	19	38	0	1	1	0	0	29 33	18	7 8	7 9	15	SW	507	85	1	4	22
23	33	22	28	0	25	37	0	1 6	1	T	T	29 21	18	7 4	7.8	17	SW	0	0	10	10	23
24	33	18	26	-2	27	39	0	1 6	1	T	.1	29 05	34	6 2	7.3	14	N	58	10	10	10	24
25	25	4	15	-14	9	50	0	2 6 9	1	T	T	28.91	33	12.7	14 0	33	NW	448	75	7	6	25
26	20	2	11	-19	- 3	54	0	6	1	0	0	29 17	33	15 3	15.7	27	NW	573	95	0	0	26
27	23	3	13	-16	- 1	52	0		1	0	0	29 46	31	7.8	8.2	14	NW	545	90	1	2	27
28	24	5	15	-14	3	50	0		1	0	0	29 55	35	8 4	8 5	15	N	602	99	1	1	28
29	20	3	12	-17	- 1	53	0		T	0	0	29 57	34	3 6	5 3	9	NW	165	27	10	8	29
30	30	12	21	-9	13	44	0		T	01	.1	29 41	05	1 3	7 8	18	N	17	3	10	9	30
31	26	1	14	-16	9	51	0		T	01	.2	29 48	08	2.3	5 5	9	E	202	33	10	7	31

SUM	SUM				TOTAL	TOTAL	
822	240				1473	0	NUMBER OF DAYS
AVG.	AVG.	AVG.	DEP	AVG	DEP	DEP	PRECIPITATION
26.5	8 0	17	-10 7	10	326	0	> .01 INCH 7
					SEASON TO DATE		SNOW, ICE PELLETS
NUMBER OF DAYS					TOTAL	TOTAL	> 1.0 INCH 1
MAXIMUM TEMP		MINIMUM TEMP			3479	0	THUNDERSTORMS 0
≥ 90°	≤ 32°	≤ 32°	≤ 0°		DEP	DEP.	HEAVY FOG 3
0	22	31	5		328	0	CLEAR 8 PARTLY CLOUDY 2 CLOUDY 20

TOTAL	TOTAL	FOR THE MONTH:						TOTAL	%	SUM	SUM
19	3.8	29 32	34	3 8	8 3	33	NW	8408	FOR	214	193
DEP						DATE: 25		POSSIBLE	MONTH	AVG	AVG.
-0 70								10195	47	6 8	6.2
GREATEST IN 24 HOURS AND DATES						GREATEST DEPTH ON GROUND OF SNOW ICE PELLETS OR ICE AND DATE					
PRECIPITATION		SNOW ICE PELLETS									
11	15-16	2.3	15-16			2	21+				

FIGURE ID-6

MIDDLE SAMPLE DATA BLOCK FROM MONTHLY NOAA DATA SHEETS



SUMMARY BY HOURS

HOUR LOCAL TIME	AVERAGES							RESULTANT WIND	
	SKY COVER TENTHS	STATION PRESSURE IN	TEMPERATURE			RELATIVE HUMIDITY %	WIND SPEED M.P.H	DIRECTION	SPEED M.P.H
			AIR °F	WET BULB °F	DEW PT °F				
00	6	29.33	15	14	9	78	7.8	34	3.9
03	6	29.32	13	13	8	79	8.8	34	3.3
06	6	29.32	13	12	7	78	7.3	33	4.1
09	7	29.35	15	13	7	74	8.8	34	4.3
12	7	29.35	21	19	10	84	9.8	33	3.8
15	7	29.29	25	22	12	81	10.6	33	4.3
18	6	29.30	22	19	12	69	7.6	36	3.8
21	6	29.32	19	17	12	75	7.8	35	3.7

$$S = \frac{\sum_{i=1}^{8}(\text{humidity}_i)}{8} / 100.$$

- MTR - Mean storm duration is obtained from the Hourly Precipitation chart shown in Figure ID-7. Three conventions are followed in demarcating storm events

(1) Hours showing the symbol "T" for "trace" precipitation are not included in storm duration if they appear at the beginning or the end of an event, or if they occur alone.

(2) "Trace" hours are counted in the middle of a rain event.

(3) Rain events that continue into the next month are included in the month which had the most hours of that event.

The mean storm duration (MTR) is obtained by: counting the number of distinct storm eve ts (MN); counting the total number of hours with quantifiable amounts of precipitation and those hours with trace amounts according to convention (2) above; and dividing the total hours by the number of events. This result must be divided by 24 (hours) to convert the units into days.

- MN - The mean number of storms is reported as counted above for determing the MTR.

- MT - Presently the model does not distinguish between months with 30 or 31 days, therefore, for a month full of rain the length of the monthly time interval MT is input as 30.5 (365 ÷ 12). In the near future, the simulation will handle the exact number of rainy days during a month (as if they were the rainy season of a year). MT in this case will be obtained by bracketing the rainy days as shown in Figure ID-7.

2.2.2 Monthly Long-Term Simulations

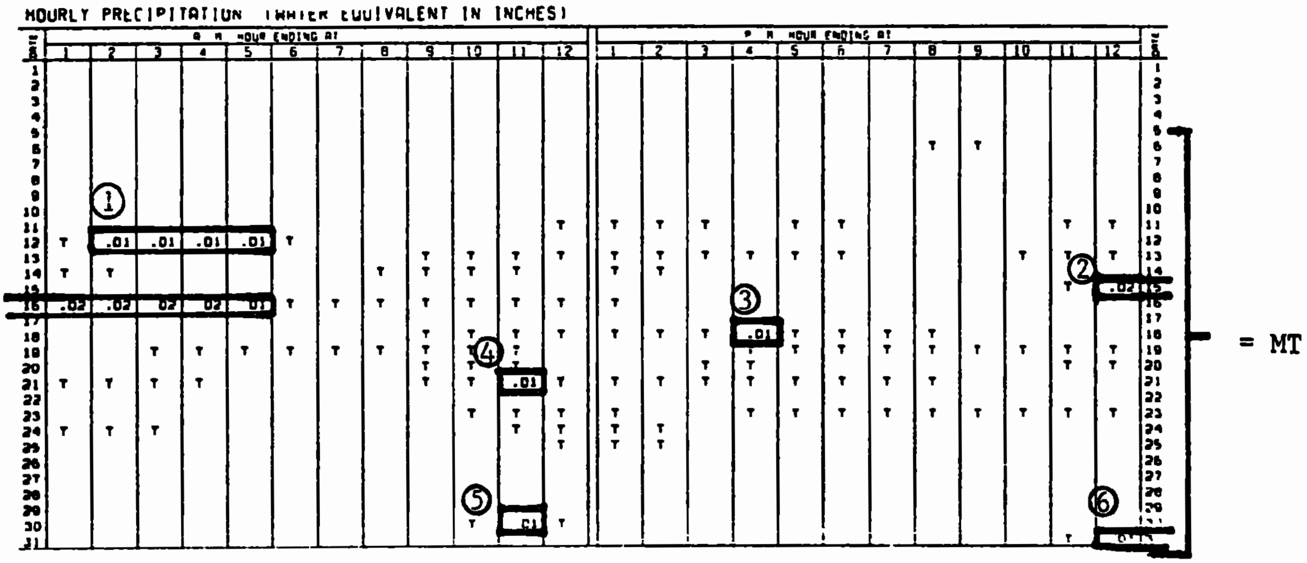
If the simulation is to provide a monthly analysis of an unspecified time period, data for at least 5 specific years can be averaged to "damp out" annual variations. The parameters which do not require averaging are: L, A, REP and MT. The remaining parameters are first handled as described above for each month of the 5 years, (with the exceptions of TA and MPM because the mean temperature (TA) and the mean rainfall (MPM) for the period of record are provided by NOAA with the annual summary, as shown in Figure ID-8) and then averaged.

2.2.3 Annual Time-Specific Simulations

To perform an analysis which covers a user specified period of time in annual time-steps (LEVEL 1), data analysis is carried out by averaging

FIGURE ID-7

SAMPLE HOURLY PRECIPITATION DATA BLOCK FROM MONTHLY NOAA DATA SHEETS



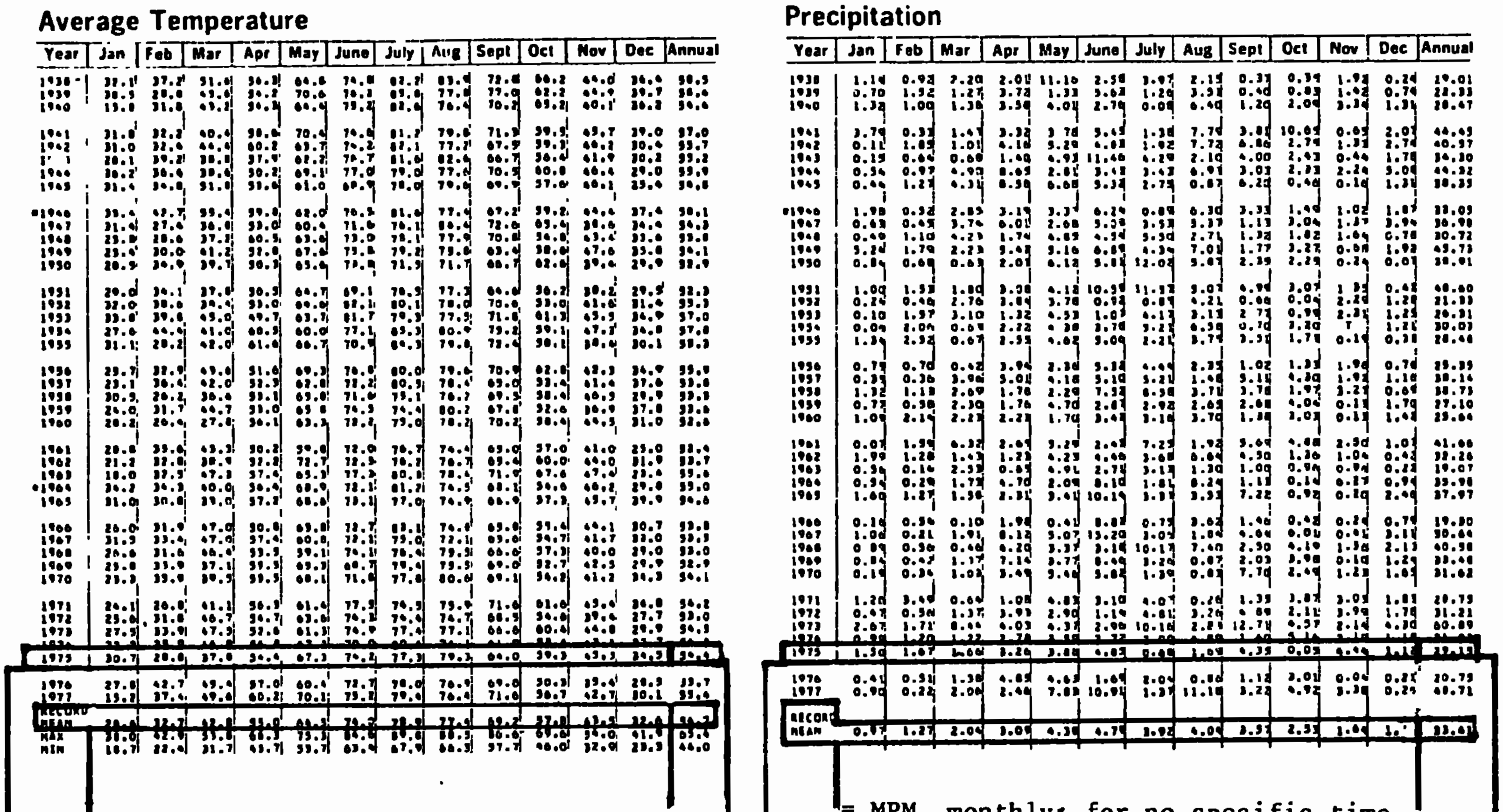
Notes: 1. This figure shows 6 rain events according to SESOIL conventions. The sixth may carry over into the next month and requires verification prior to assigning it to either. For demonstration purposes, however, it is assumed to be one complete event. Thus MN=6.

2. There are 14 hours of rainfall contained within the events bracketed above. Thus MTR=0.43.

3. The value of MT is given as 30.5 even though the rainy period covers 25 days of the month.

FIGURE ID-8

SAMPLE OF ANNUAL NOAA DATA



= TA monthly averages; for no specific time.

= TA annual general

= TA monthly, for a specific year.

= TA annual specific

= MPM, monthly; for no specific time.

= MPM, monthly; for a specific year.

= MPM annual general

= MPM annual specific

the twelve monthly averages for the year for the following five parameters: TA, NN, S, MTR and MN.

Parameters L, A, and MT do not change with time. The value for total annual mean precipitation (MPA) is found either by adding the average monthly precipitation (MPM) for all twelve months or from the totals provided in an annual summary table (Figure ID-8) and converting from centimeters to inches (if not previously converted). While MT varies seasonally, the variation is considered only for annual simulations.

2.2.4 Annual Long-Term Simulations

The data for a general annual simulation (i.e., an unspecified time period) are averaged over annual data for five or more specific consecutive years. The specific years' data are determined as described above, excepting the values for MPM and TA, which may be taken directly from NOAA data, by referring to the 40 year mean for the period of record.

2.3 Automated Estimation of Input Parameters

The ten parameters described in Section 2.2 above are determined automatically by the IPDATA subprogram, using tapes for data input. Two of the parameters (latitude and albedo) require user input to the subprogram.

The subprogram reads the data taken at a weather station from two NOAA tapes (TD-1440 and TD-9924), obtainable from the National Climatic Center by calling their Asheville offices. This Office also supplies an index of station numbers for the U.S. and the world where observations have been made called "SURVEY of TD-1440, DATA FORMAT," and user manuals for the tapes.

The data stored on TD-1440 tapes are used to calculate the monthly values for the following six parameters: TA, NN, S, MPM, MTR and MN. In addition, the IPDATA subprogram stores the total number of hours precipitation (TPPT) counted in each month. The value for REP is supplied as 0.0 by the subprogram, while MT is supplied as the number of days in the current month. The user may override the value for REP if desired by editing the input parameters (see Section 3.0, User's Manual). This would occur only in the case where certain of the input parameters were lacking or poorly supplied with data. The user might determine this either before or after scanning the data on the tapes. The second tape, TD-9924 is required to obtain values for mean monthly precipitation.

2.3.1 Monthly Time-Specific Simulations

To run the IPDATA subprograms for a simulation which will produce 10x12 matrices (10 parameters, 12 months) for all the years within a specific time period, the user first edits the FILE IP DATA. This file, along with the appropriate formats are shown in Figure ID-9. All entries but the value for REP must be changed for each site. Typical Annual Output is shown in Figure ID-10.

FIGURE ID-9

USER INPUT DATA FILE (IP DATA) SAMPLE VALUES AND FORMATS

```
STATION NAME (STANAM)                        GUANTANAMO. BAY
FIRST YEAR (IYR1),SECOND YEAR (IYR2)         45      50
OUTPUT FILE # (NFILE),DIVISION(NDIV)         99      99
ALBEDO, LATITUDE (LAT), REP                   1.0    30.0     0.0
```

Line Number	Format
1	40X, 10A4
2	40X, I2, 5X, I2
3	40X, I2, 5X, I2
4	38X, 3(F7.2)

```
*************************************************************************************************
99   GUANTANAMO, BAY                                  11706     99
*************************************************************************************************

*************************************************************************************************
        PARAMETER VALUES FOR THE WATER YEAR 1945 TO 1946
        -----------------------------------------------------------------------------------------
           OCT       NOV       DEC       JAN       FEB       MAR       APRIL     MAY       JUNE      JULY      AUG       SEPT
        -----------------------------------------------------------------------------------------
L          30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0
TA         26.5      25.0      23.0      24.2      23.9      24.4      25.0      26.1      26.9      27.5      27.7      27.1
NN          0.7    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0
S           0.8       0.8       0.8       0.8       0.7       0.7       0.7       0.8       0.8       0.7       0.7       0.8
A           1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0
REP         0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
MPM         0.0       2.5       5.1       7.5      10.2      12.7      15.2      17.8      20.3      22.9      25.4      27.9
MTR         0.2       0.1       0.1       0.0       0.1       0.0       0.3       0.1       0.0       0.1       0.1       0.1
MN         12.0      17.0      10.0       1.0       4.0      10.0      14.0      15.0       5.0       6.0       5.0       9.0
MT         31.0      30.0      31.0      31.0      28.0      31.0      30.0      31.0      30.0      31.0      31.0      30.0
TPPT       46.0      43.0      22.0       1.0       7.0      16.3      90.0      39.0       5.0       8.0       8.0      12.0
        -----------------------------------------------------------------------------------------
*************************************************************************************************
        PARAMETER VALUES FOR THE WATER YEAR 1946 TO 1947
        -----------------------------------------------------------------------------------------
           OCT       NOV       DEC       JAN       FEB       MAR       APRIL     MAY       JUNE      JULY      AUG       SEPT
        -----------------------------------------------------------------------------------------
L          30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0
TA         27.1      25.2      24.5      24.5      23.4      24.9      26.0      26.4      27.2      28.2      28.5      27.6
NN       9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0    9999.0       0.5
S           0.8       0.8       0.8       0.8       0.8       0.8       0.7       0.8       0.8       0.8       0.8       0.8
A           1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0
REP         0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
MPM         0.0       2.5       5.1       7.5      10.2      12.7      15.2      17.8      20.3      22.9      25.4      27.9
MTR         0.0       0.1       0.1       0.1       0.1       0.1       0.0       0.1       0.1       0.1       0.1       0.1
MN         13.0      11.0       6.0       6.0      14.0       4.0       5.0       7.0      20.0       8.0       9.0      21.0
MT         31.0      30.0      31.0      31.0      28.0      31.0      30.0      31.0      30.0      31.0      31.0      30.0
TPPT       20.0      24.0       7.0       3.0      35.0      10.0       6.0      16.0      41.0      13.0      17.0      50.0
        -----------------------------------------------------------------------------------------
```

FIGURE ID-10

SAMPLE PROGRAM OUTPUT

MONTHLY PARAMETER VALUES FOR THE WATER YEARS 1945-1950

```
****************************************************************************************************
          PARAMETER VALUES FOR THE WATER YEAR 1947 TO 1948
          ------------------------------------------------------------------------------------------
              OCT      NOV      DEC      JAN      FEB      MAR    APRIL     MAY     JUNE     JULY      AUG     SEPT
          ------------------------------------------------------------------------------------------
L            30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0
TA           27.4     26.8     25.0     24.7     25.1     26.0     26.3     27.5     27.9     28.7     29.1     28.0
NN            0.4   9999.0      0.2   9999.0   9999.0   9999.0   9999.0   9999.0   9999.0   9999.0   9999.0   9999.0
S             0.8      0.8      0.8      0.3      0.7      0.7      0.7      0.8      0.8      0.7      0.7      0.8
A             1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
REP           0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
MPM           0.0      2.5      5.1      7.6     10.2     12.7     15.2     17.8     20.3     22.9     25.4     27.9
MTR           0.1      0.1      0.1      0.0      0.1   9999.0      0.1      0.1      0.2      0.1      0.0      0.2
MN           13.0      4.0      5.0      3.0      8.0      0.0     11.0     24.0     12.0      6.0      7.0     14.0
MT           31.0     30.0     31.0     31.0     28.0     31.0     30.0     31.0     30.0     31.0     31.0     30.0
TPPT         12.0      6.0      9.0      3.0     12.0      9.0     19.0     73.0     47.0     12.0      7.0     76.0
          ------------------------------------------------------------------------------------------
****************************************************************************************************
          PARAMETER VALUES FOR THE WATER YEAR 1948 TO 1949
          ------------------------------------------------------------------------------------------
              OCT      NOV      DEC      JAN      FEB      MAR    APRIL     MAY     JUNE     JULY      AUG     SEPT
          ------------------------------------------------------------------------------------------
L            30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0
TA           27.2     26.5     24.9     23.4     23.7     24.2     25.7     25.9     26.7     27.5     27.6     27.3
NN         9999.0      0.3      0.2      0.2      0.1      0.2      0.3      0.6      0.6      0.5      0.5      0.5
S             0.8      0.8      0.8      0.7      0.7      0.7      0.8      0.8      0.8      0.7      0.8      0.8
A             1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
REP           0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
MPM           0.0      2.5      5.1      7.5     10.2     12.7     15.2     17.8     20.3     22.9     25.4     27.9
MTR           0.1      0.1      0.0      0.2      0.0      0.0      0.1      0.1      0.1      0.0      0.1      0.1
MN           18.0     13.0      2.0      4.0      2.0      6.0      5.0     23.0     13.0      2.0     12.0     11.0
MT           31.0     30.0     31.0     31.0     28.0     31.0     30.0     31.0     30.0     31.0     31.0     30.0
TPPT         31.0     17.0      2.0     23.0      2.0      6.0      7.0     55.0     27.0      2.0     24.0     25.0
          ------------------------------------------------------------------------------------------
****************************************************************************************************
          PARAMETER VALUES FOR THE WATER YEAR 1949 TO 1950
          ------------------------------------------------------------------------------------------
              OCT      NOV      DEC      JAN      FEB      MAR    APRIL     MAY     JUNE     JULY      AUG     SEPT
          ------------------------------------------------------------------------------------------
L            30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0     30.0
TA           26.1     25.3     24.0     23.3     23.0     24.1     24.3     25.8     27.1     27.3     27.5     26.8
NN            0.5      0.5      0.4      0.2      0.3      0.2      0.4      0.4      0.5      0.4      0.5      0.6
S             0.8      0.8      0.8      0.8      0.8      0.8      0.7      0.8      0.8      0.7      0.8      0.8
A             1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0      1.0
REP           0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
MPM           0.0      2.5      5.1      7.6     10.2     12.7     15.2     17.8     20.3     22.9     25.4     27.9
MTR           0.1      0.1      0.1      0.0      0.0      0.0      0.1      0.1      0.1      0.1      0.1      0.1
MN           20.0     13.0     12.0      3.0      8.0      2.0      5.0      9.0      3.0      9.0     20.0     20.0
MT           31.0     30.0     31.0     31.0     28.0     31.0     30.0     31.0     30.0     31.0     31.0     30.0
TPPT         49.0     19.0     15.0      3.0      9.0      2.0      9.0     14.0      8.0     14.0     35.0     45.0
          ------------------------------------------------------------------------------------------
****************************************************************************************************
```

FIGURE ID-10 (Continued)

The necessary tapes for the station under study must be loaded and labeled according to the protocols of the user's computation center. Presently the subprogram requires labels for ITAPE1 and ITAPE2, defined in the execution file for IPDATA. This latter file also determines the location to which the output is sent, i.e., disc storage, line printer, or terminal.

Output is printed as matrices (Figure ID-10), one matrix for each year in the range between the input values for IYR1 and IYR2.

2.3.2 Monthly Long-Term Simulations

The subroutine will automatically derive average values for each parameter, by month, if more than five year's data are analyzed. The results are presented as a table labeled "Average Monthly Parameter Values over the Period 19-- through 19--" where the last digits of the period are IYR1 and IYR2. Typical output shown in Figure ID-11.

2.3.3 Annual Time-Specific Simulations

Average values for each parameter over the space of a year, for each year within the specified period are also output by IPDATA. These data are output in a table titled "Annual Parameter Averages for All Months, By Year from 19-- to 19--", where the last digits of the period are IYR1 and IYR2. Typical output is displayed in Figure ID-12. Note that MT=365 and MPA is the sum of the monthly MPM values.

2.3.4 Annual Long-Term Simulations

The averages stored in the ANAV matrix described above, may again by averaged to obtain an array consisting of one average value for each parameter over, say, a 20-year period. IPDATA automatically calculates these values for any period of record specified as greater than 1 year. Typical output is shown in Figure ID-13.

2.3.5 Program Notes

The IPDATA subprogram was written to retrieve data stored by NOAA on tape. Some of the quirks used in this form of data storage necessitated the approaches used in the subprogram. This includes, checking each entry for missing, invalid or mistyped (i.e., out of range) data entries. When these circumstances are encountered, the data will be skipped. If an entire month's data were missing or invalid, as might occur in the case of monitoring equipment malfunction, the appropriate output value will be 9999. This holds true for monthly, annual and period-of-analysis averages as well. In such cases, the user will have to use best judgment as to how to proceed.

It is foreseen that averages will eventually be taken for many stations within a region and thus all IPDATA output are designed to be stored for this purpose.

The formats for all IPDATA output correspond to SESOIL-81's read format. The annual matrices must be transferred to the GE file for use as SESOIL input.

```
**************************************************************************************************************************
        AVERAGE MONTHLY PARAMETER VALUES OVER THE PERIOD 1945-1950


        --------------------------------------------------------------------------------------------------------------
            OCT       NOV       DEC       JAN       FEB       MAR       APRIL     MAY       JUNE      JULY      AUG       SEPT
        --------------------------------------------------------------------------------------------------------------
L          30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0      30.0
TA         26.9      25.8      24.4      24.0      23.5      24.7      25.5      26.3      27.2      27.9      28.1      27.4
NN          0.5       0.4       0.2       0.2       0.2       0.2       0.3       0.5       0.6       0.4       0.5       0.6
G           0.3       0.8       0.8       0.8       0.7       0.7       0.7       0.8       0.8       0.7       0.7       0.8
A           1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0       1.0
HEP         0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
MPM         0.0       2.5       5.1       7.5      10.2      12.7      15.2      17.8      20.3      22.9      25.4      27.9
MTR         0.1       0.1       0.1       0.1       0.1       0.0       0.1       0.1       0.1       0.1       0.1       0.1
MN         17.4      11.6       7.0       3.4       7.2       4.4       8.0      15.6      10.6       6.2      10.6      15.0
MT         30.5      30.5      30.5      30.5      30.5      30.5      30.5      30.5      30.5      30.5      30.5      30.5
TPPT       35.6      21.8      11.4       7.5      13.2       6.8      26.2      39.2      25.6       9.8      18.2      41.6
**************************************************************************************************************************
```

FIGURE ID-11

SAMPLE PROGRAM OUTPUT

MONTHLY PARAMETER AVERAGES FROM 1945-1950

```
*********************************************************************************
      ANNUAL PARAMETER AVERAGES FOR ALL MONTHS, BY YEAR, FROM 1945 TO 1950


      ---------------------------------------------------------------------------
YEAR  1, 1945
L   , TA  , NN  , S   , A   , REP        30.0    25.7     0.7     0.8     1.0     0.0
MPA , MTR , MN  , MT  , TPPT            167.6     0.1     9.0   365.0    24.7
---------------------------------------------------------------------------------
YEAR  2, 1946
L   , TA  , NN  , S   , A   , REP        30.0    25.1     0.5     0.8     1.0     0.0
MPA , MTR , MN  , MT  , TPPT            167.6     0.1    10.8   365.0    20.9
---------------------------------------------------------------------------------
YEAR  3, 1947
L   , TA  , NN  , S   , A   , REP        30.0    26.9     0.3     0.9     1.0     0.0
MPA , MTR , MN  , MT  , TPPT            167.6     0.1     9.3   365.0    24.7
---------------------------------------------------------------------------------
YEAR  4, 1948
L   , TA  , NN  , S   , A   , REP        30.0    25.9     0.4     0.8     1.0     0.0
MPA , MTR , MN  , MT  , TPPT            157.6     0.1     9.3   365.0    18.4
---------------------------------------------------------------------------------
YEAR  5, 1949
L   , TA  , NN  , S   , A   , REP        30.0    25.4     0.4     0.8     1.0     0.0
MPA , MTR , MN  , MT  , TPPT            167.6     0.1    10.3   365.0    18.5
---------------------------------------------------------------------------------
*********************************************************************************
```

FIGURE ID-12

SAMPLE PROGRAM OUTPUT

ANNUAL PARAMETER AVERAGES BY YEAR FROM 1945-1950

```
********************************************************************
PARAMETER AVERAGES FOR ALL OBSERVATIONS OVER THE PERIOD 1945-1950
PARAMETER                                    AVERAGE VALUE
------------------------------------------------------
L                                          30.00
TA                                         25.79
NN                                          0.47
S                                           0.76
A                                           1.00
REP                                         0.0
MPA                                       167.64
MTR                                         0.08
MN                                          9.75
MT                                        365.00
TPPT                                       21.42
********************************************************************
```

FIGURE ID-13

SAMPLE PROGRAM OUTPUT

PARAMETER AVERAGE FOR ALL OBSERVATIONS FROM 1945-1950

3.0 SOIL INPUT DATA

3.1 General

3.2 Soil Intrinsic Permeability (k)

3.3 Soil Porosity (n)

3.4 Soil Pore Disconnectedness Index (c)

The soil pore disconnectedness index c in SESOIL, is the exponent relating the "wetting" and "drying" intrinsic permeability k(s) of the soil to its saturated intrinsic permeability k(1), and is given by Eagleson (WRR p. 723 e.g. 7). This relation is given in the literature by Brook and Corey (1966) and its validity for both a cohesive and a cohesionless soil is graphically presented by Eagleson (WRR p. 724 Figure 3).

To obtain the c parameter for various soils a user has to follow the work of Talma (1974) and Moore (1939). Eagleson (1978) has presented in this work typical c parameters (Table ID-1), however, these values have to be employed with caution. The authors (Bonazountas and Wagner) of SESOIL intend to author a section for this model providing: (a) c values for the various soils of the USDA - soil classification triangle, and (b) a discussion for estimating the effective "real (of the field)" hydrologic/soil properties of soils from observations of vegetation density via the model itself. This task has not been performed yet for budget reasons only.

However, it has to be emphasized that any unsaturated soil zone of the literature (e.g. Bonazountas et al 1979) requires as a user input instead of a curve relating "permeability^{-k} vs. capillarity head ψ." This curve is obtained from experimental data. It is almost impossible to obtain this curve off-the-shelf for any type of soil, but it also is extremely difficult to obtain this curve in the laboratory. Therefore, the "one-variable" approach of Eagleson (1978) employed in SESOIL greatly simplifies data gathering. Authors of this report advise the user to employ values of Table ID-1, and to interpolate for different types of soils using also the work of Freese and Cheery (1979 p. 29).

4.0 CHEMISTRY INPUT DATA

Chemical parameters, coefficients, etc. might be compiled from the handbook "Research and Development Methods for Estimating Physicochemical Properties of Organic Compounds of Environmental Concern" (Lyman *et al.* 1981), or any other handbook.

TABLE ID-1

INDEPENDENT SOIL PROPERTIES/PARAMETERS[1)]

Properties[4)] (SESOIL Variable)	SOIL TYPE				
	Clay	Clay-Loam	Silty-Loam	Silty-Loam	Sand[2)]
k(1)	1×10^{-10}	2.8×10^{-10}	1.2×10^{-9}	2.5×10^{-9}	1×10^{-7}
n	0.45	0.35	0.35	0.25	0.25
c	12	10	5[3)]	4	3.5

1) See Table HY-3

2) Compiled from various sources

3) Personal conversation with Eagleson

4) A single relationship between k(1), n and c does not exist.

Main Source: Eagleson (1978)

5.0 REFERENCES

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Lyman, W. et al. (1981) "Research and Development Methods for Estimating Physicochemcial Properties of Organic Compounds of Environmental Concern." Prepared by Arthur D. Little, Inc., Phase II Final Report for U.S. Army Medical Bioengineering Research and Development Laboratory, Fort Detrick, Maryland; McGraw-Hill Book Company, New York.

Moore, R.E. (1939) "Water Conduction from Sahllow Water Tables," Hilgardia 12(6), 383-426.

Talsma, T. (1974) "The Effect of Initial Moisture Content and Infiltration Quantity on Redistribution of Soil Water," Aust. J. Soil Res., 12, 15-26.

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DRAFT

HB, 5.24.82

3.0 SOIL INPUT DATA

3.1 Summary of Default Values

The hydrologic routine of SESOIL employs the one-dimensional water balance model of Eagleson [1978a-g] which has been written in terms of five surface vegetation and soil parameters: the vegetation canopy M, the species-dependent plant water use coefficient k_v, the soil effective porosity n_e, the saturated intrinsic permeability k(1), and the soil pore disconnectedness index c. A state variable of the problem has been the average long-term soil moisture concentration s_o The analytic structure of this model is summarized in appendix HY, however, tailored to the needs of SESOIL, roughly for bare soils and monthly simulations. The bare soil requirement reduces the five surface parameters to the following three independent soil input parameters:

k(1) = saturated soil intrinsic permeability; (cm^2)

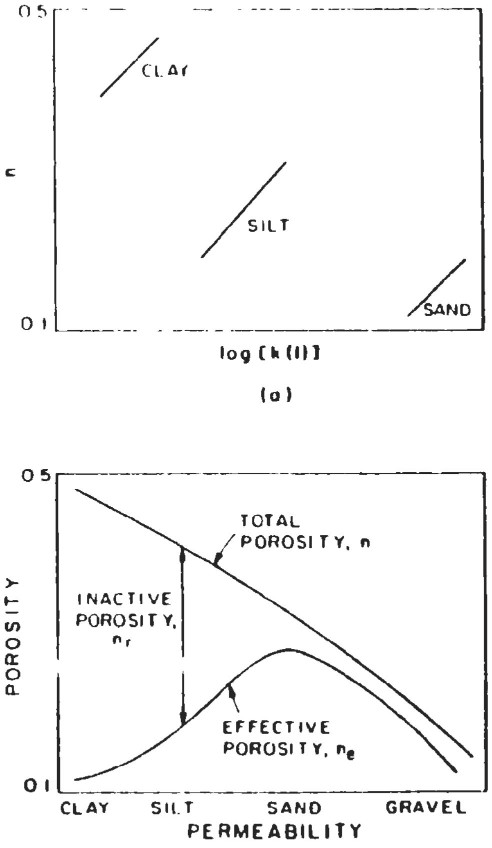
n_e = effective soil porosity; (fractional)

c = $\Delta[\ln(k)]/\Delta[\ln(s_o)]$; soil pore disconnectedness index; (-)

There is no unique association of the particular c and n regional values of a soil type with the value of a k(1). Therefore, model users should be very careful when employing the default independent soil property values presented at the end of this section. The soil properties are critical to the moisture fluxes and vary tremendously spatially. Use of point measured soil properties can yield results of only local (and hence not areally averaged) character. It would be also appropriate to use some observed water balance element such as average basin yield (surface runoff and groundwater runoff) to evaluate the effective soil properties, as discussed in section 3.5; soil parameter calibration.

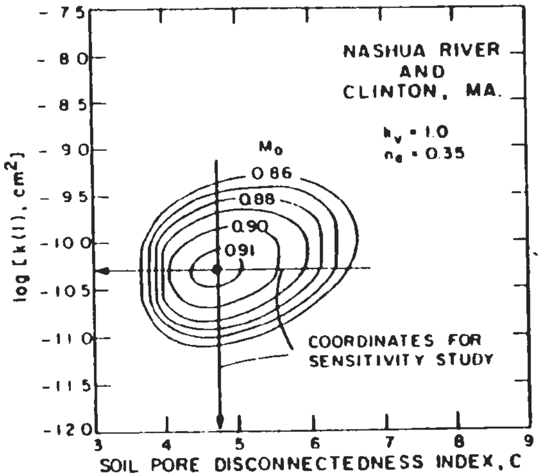
A schematic variation of soil hydraulic properties with textural class is presented in figure ID-14. Of course, soils evolve having a continuous spectrum of textures from clay through silt to sand and gravel, and the critical hydraulic properties of soils vary widely even within the same textural class, but over the variety of classes their range is enormous. Figure ID-14 is only a gross generalization of the overall soil characteristics [Eagleson 1982, p.326]. More detailed information is provided in the subsequent sections.

In a natural ecological system, Eagleson suggested [Eagleson & Tellers 1982, p.341] that there may be ecological pressures for change in natural soil-vegetation systems, which drive a synergistic development toward a water- or energy-limited equilibrium state in a given climate. Identification of the conditions for this equilibrium should allow an a priori specification of one or more of the physical parameters of the soil and vegetation, a fact that may lead to elimination of k(1) from the water balance equation in terms of the long-term average soil moisture concentration in the root zone s_o, a state variable of the



(b)

Variation of soil hydraulic properties with textural class. (a) After *Chilingar* [1964] (b) After *Bear* [1979].



Climatic climax soil-vegetation systems.

(c)

$k(l)$ = intrinsic soil permeability; (cm^2)
n = total soil porosity; (-)
n_e = effective soil porosity; (-)
c = soil pore disconnectedness indes; (-)
Mo = vegetation canopy density at maximum soil moisture
k_v = potential transpiration efficiency of plant species

Source: Eagleson [1982a-b]

Figure ID-14 - Generalized Correlation of Independent Soil Parameters; $k(l)$, n_e, c budget theory. In a bare-soil system, however, all three input variables -- k(1), n_e, and c -- have to be known and input to the model.

Ideally, one should test input values by having direct observations of k(1), n_e and c -- in addition to the various climate parameters -- from an array of spatially homogeneous natural systems covering a wide range of the dimensionless climate-soil parameter E (see appendix HY, equation HY-23). In practice, however, at least the soil parameters of natural systems are highly variable spatially [Nielsen et al 1973; Libardi et al 1982], so even if dense observations of them were available (which is rare), the problem of how to average them areally would arise [Eagleson 1982, p.342]. Because of the large spatial variability of the properties of natural soils, and because of the high degree of non linearity of the fluxes, spatial averaging over the large area elements of either climate or water resource models become a non-trivial problem [Eagleson 1982, p.325]. Therefore, given an initial set of input parameters k(1), n_e, c, it is recommended to calibrate the input data set of the model by varying the intrinsic permeability k, the pore disconnectedness index c, and the effective porosity n_e of the soil, towards obtained field records of soil moisture content or basic yield (see section 3.5; Soil Parameter Calibration).

In case of total absence of site specific input data and when non-site specific long term pollutant fate modeling efforts have to be performed for canonical climatic environments, SESOIL users may employ the information compiled in Table ID-1, namely the:

- USDA (U.S. Department of Agriculture) soil textural classification system as a guide for soil type selection; and
- Default values of k(1), n_e, c compiled for the various USDA soil-types of the soil triangle.

The figure and the table of table ID-1 are self-explanatory for easy use and for canonical environments only. The rationale behind the default values generated and the uncertainty when deriving them are outlined in the following sections for each individual soil parameter. Only fundamental concepts are discussed as they relate to the SESOIL use, therefore, model users are advised to consult original publications of this appendix.

3.2 Soil Intrinsic Permeability -- k(1)

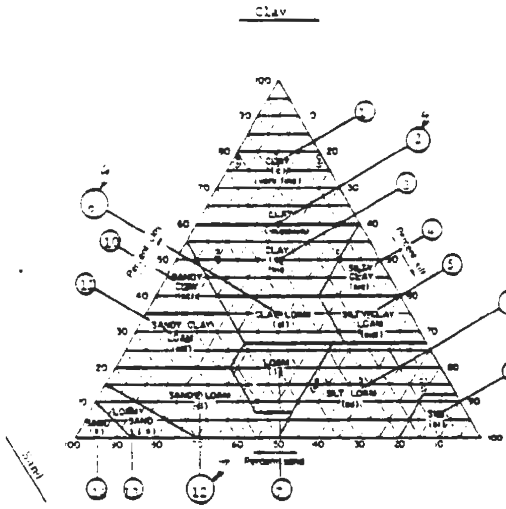
3.2.1 Definitions

When various fluids of density ρ and dynamic viscosity μ are run through a porous medium consisting of uniform glass beads of diameter d, and under a constant hydraulic gradient dh/dl, the following proportionality relationships are observed [Freeze & Cherry 1979, p.27]:

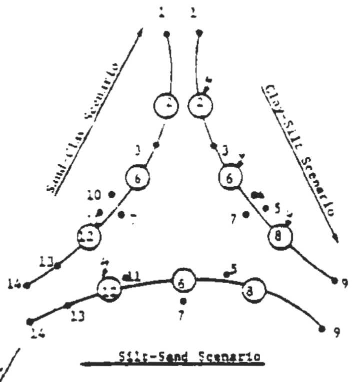
$$v = v(d^2), \qquad v = v(\rho.g), \qquad v = v(1/\mu) \qquad \text{(ID-1)}$$

Table ID-1

SESOIL Default Soil Input Parameters



Guide for USDA-SCS Soil Textural Classification



Guide for Canonical Soil Scenario Selection

Textural Soil Class		SESOIL Default Values[11)]				Supporting Information to Default Values					
#[1)]	(USDA triangle) Designation	$\rho^{9)}$ (g/cm³)	$k(1)^{3)}$ (cm²)	$n_e^{4)}$ (−)	$c^{5)}$ (−)	$n^{6)}$ (−)	$d^{7)}$ (mm)	$K^{10)}$ (cm/sec)	sand[8)] %	silt[8)] %	clay[8)] %
1[2)]	Clay (very fine)[12)]	1.35	0.75×10^{-10}	0.20	12	0.70	0.0328	7.5×10^{-4}	10	13	77
(2)	Clay (medium fine)[13)]	1.35	2.5×10^{-10}	0.20	12	0.68	0.050	2.5×10^{-3}	18	19	63
3	Clay (fine)[12)]	1.35	6.0×10^{-10}	0.22	12	0.64	0.0785	6.0×10^{-3}	25	25	50
4	Silty clay	1.35	0.5×10^{-10}	0.25	12	0.59	0.0236	5.0×10^{-4}	6	47	47
5	Silty clay loam	1.35	0.85×10^{-10}	0.27	10	0.59	0.0362	8.5×10^{-4}	10	55	35
(6)	Clay loam	1.35	6.5×10^{-10}	0.30	7.5	0.58	0.103	6.5×10^{-3}	33	33	34
7	Loam	1.35	8.0×10^{-10}	0.30	6.5	0.52	0.124	8.0×10^{-3}	40	40	20
(8)	Silt loam[12)]	1.35	3.5×10^{-10}	0.35	5.5	0.54	0.0726	3.5×10^{-3}	22	65	13
9	Silt	1.35	0.5×10^{-10}	0.27	12	0.49	0.0240	5.0×10^{-4}	5	90	5
10	Sandy clay	1.35	15×10^{-10}	0.24	6	0.44	0.157	1.5×10^{-2}	52	6	42
11	Sandy clay loam	1.35	25×10^{-10}	0.26	4	0.45	0.176	2.5×10^{-2}	58	15	27
(12)	Sandy loam	1.35	20×10^{-10}	0.25	6.33	0.44	0.167	2.0×10^{-2}	65	25	10
13	Loamy sand	1.35	500×10^{-10}	0.28	3.9	0.33	0.250	5.0×10^{-1}	83	10	7
14	Sand	1.35	100×10^{-10}	0.30	3.7	0.35	0.285	1.0×10^{-1}	95	3	2

---

[1] See USDA soil classification triangle of figure ID-15 (pictured above also)

[2] Soil class in ( ) corresponds to an overall proposed soil scenario related to the USDA soil triangle; in figure with ↗

[3] k(1) = intrinsic soil permeability; see table ID-7

[4] n_e = effective soil porosity; see table ID-9 and figure ID-18

[5] c = soil pore disconnectedness index; see table ID-10

[6] n = soil porosity; see table ID-9 and figure ID-18

[7] d = soil particle median diameter; see table ID-6

[8] see table ID-5

[9] for soil bulk density an overall constant value of 1.35 g/cm³ is assumed; see Buckman & Brady [1969], Eagleson [1970, p.257], Holton & Whelan [1967]

[10] K = soil conducting; see table ID-6

[11] only for non-site specific modeling efforts

[12] averaged value of table ID-5

[13] average values of soils #1 and #3.

Source: Bonazountas & Wagner [1981].

Together with Darcy's original observation that v=v(-dh/dl), the above three relationships lead to a new formulation of Darcy's law

$$v = -(C\ d^2 \rho . g/\mu)(dh/dl) \qquad \text{(ID-2)}$$

The parameter C is a constant of proportionality affected by the soil grain size, sphericity and other factors. Comparison of ID-2 with the Darcy equation

$$v = -K\ dh/dl \qquad \text{(ID-3)}$$

leads to

$$K = Cd^2 \rho . g/\mu \qquad \text{(ID-4)}$$

In this equation, ρ and μ are functions of the fluid alone and Cd^2 is a function of the medium. If we define

$$k = Cd^2 \quad ;\ (cm^2) \qquad \text{(ID-5)}$$

then

$$K = k \rho g/\mu \quad ;\ (cm/sec) \qquad \text{(ID-6)}$$

The parameter k is known as the specific or intrinsic permeability (or permeability) and K is known as hydraulic conductivity (or sometimes the coefficient of permeability). Table ID-2 provides values of k and K for a variety of geological materials, and values of unit conversion factors.

Beyond the above definition, Eagleson [Eagleson 1978, p.23] defined the effective intrinsic permeability (cm^2) of a soil as

$$k(s) = (\mu/\gamma_w)\ K(s) \qquad \text{(ID-7)}$$

where γ_w the specific weight of pore water in dynes per cm^3 and based on the work of Brooks and Corey [1966] he indicated for his water balance that:

$$k(s) = k(1)\ s^c \qquad \text{(ID-8)}$$

For saturated conditions --i.e. s=1 (see app. HY)-- k(1)=k and K(1)=K as indicated in expressions ID-5 and ID-6. For unsaturated soil conditions we have the definition $k(\Theta)$ and $K(\Theta)$, or k(s) and K(s) to be consistent with Eagleson.

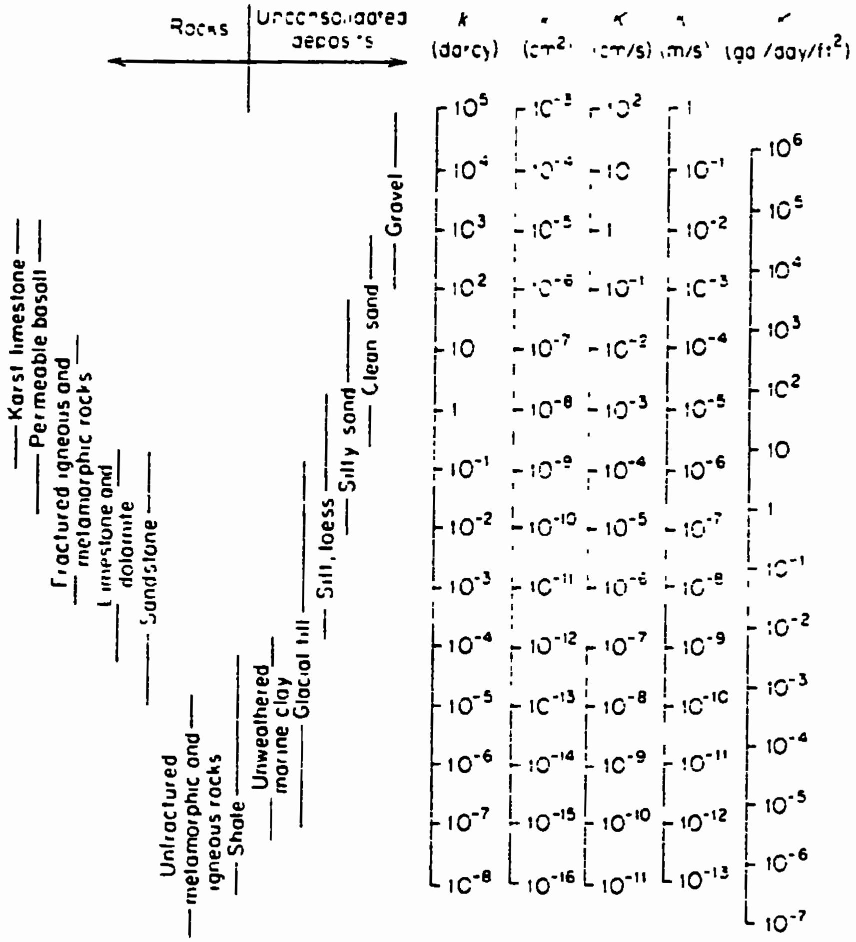
3.2.2 Hydrologic Characteristics of Soil Types

Over 4000 soils of the United States have been classified into four hydrologic groups [Chow 1964]; designated as A, B, C and D by the Soil Conservation Service (SCS). The majority of the assignments are based on the judgment of soil scientists and correlators [Chiang 1971]. A short description [Novotny 1976] of the four soil types follows:

TABLE ID-2

Range of Values of Intrinsic Permeability and Hydraulic Conductivity; Unit Conversion Factors

Range of Values of Hydraulic Conductivity and Permeability



Conversion Factors for Permeability and Hydraulic Conductivity Units

	Permeability k*			Hydraulic conductivity, K		
	cm²	ft²	darcy	m/s	ft/s	gal/day/ft²
cm²	1	1.08×10^{-3}	1.01×10^{8}	9.80×10^{2}	3.22×10^{3}	1.85×10^{9}
ft²	9.29×10^{2}	1	9.42×10^{10}	9.11×10^{5}	2.99×10^{6}	1.71×10^{12}
darcy	9.87×10^{-9}	1.06×10^{-11}	1	9.66×10^{-6}	3.17×10^{-5}	1.82×10^{1}
m/s	1.02×10^{-3}	1.10×10^{-6}	1.04×10^{5}	1	3.28	2.12×10^{6}
ft/s	3.11×10^{-4}	3.35×10^{-7}	3.15×10^{4}	3.05×10^{-1}	1	5.74×10^{5}
gal/day/ft²	5.42×10^{-10}	5.83×10^{-13}	5.49×10^{-2}	4.72×10^{-7}	1.74×10^{-6}	1

*To obtain k in ft², multiply k in cm² by 1.08×10^{-3}

Source: Freeze & Cherry [1979, p.29]

- Group A: Soils of low total runoff potential have high infiltration rates even when thoroughly wetted; these consist chiefly of deep, well to excessively-drained sand or gravel and therefore possess a high rate of water transmission.

- Group B: Soils of low-moderate total runoff potential have moderate infiltration rates when thoroughly wetted, and range from moderately-deep, moderately-well to well-drained soils having moderately-fine to moderately-coarse texture. Consequently, these soils have a moderate rate of water transmission.

- Group C: Soils of high-moderate total runoff potential have slow infiltration rates when thoroughly wetted and consist chiefly of soils with a layer that impedes downward movement of water, or soils with moderately-fine to fine texture. These soils have a resultant slow rate of water transmission.

- Group D: Soils of high total runoff potential have very slow infiltration rates when thoroughly wetted, and consist chiefly of clay soils with a high swelling potential, soils with a permanently high water table, soils with a clay pan or clay layer at or near the surface, and shallow soils over nearly impervious material. These have the expected very slow rate of water transmission.

Potential storage of soil moisture can be partitioned into two moisture classes: 1) gravitational water, i.e. that held between saturation and 0.33 bar tension, and 2) plant-available water, i.e. that held between 0.33 and 15 bar tension. Moisture content at 0.33 bars is assumed to represent field moisture capacity or the lower limit of gravitational water, and 15 bars the permanent wetting percentage in medium textures soils. Gravitational water, G, is derived by subtracting 0.33 bar volume percentages from total porosity. Available water capacity (AWC) is the difference between the moisture contents (volumes) at 0.33 and 15 bar tensions. [Novotny 1976.]

3.2.3 Soil Hydraulic Conductivity -- K(1)

Hydraulic conductivity of saturated soils, vary greatly and natural soils and soil materials, therefore, behave quite differently. Based on these differences in performance, soils can be classified according to their K(1) rate. For example, for earth dams the U.S. Bureau of Reclamation generally classifies soils with K-values above 10^{-4} cm/sec as pervious and soils with K-values below 10^{-6} as impervious.

In tile drainage, K-rates may be used in selecting depth and spacing of tile drains. Using relative permeabilities, guides for average depth and spacing for tile drains have been established by various agencies or investigators such as that given in table ID-3.

TABLE ID-3

Hydraulic Conductivity Classes According to the USDA-SCS

K Class	K Values		
	inch/hr	cm/sec	m/day
Very slow	Less than 0.5	Less than 0.035 x 10^{-3}	Less than 0.3
Slow	0.05 to 0.20	0.035 x 10^{-3} to 0.14 x 10^{-3}	0.3 to 0.12
Moderately slow	0.20 to 0.80	0.14 x 10^{-3} to 0.56 x 10^{-3}	0.12 to 0.48
Moderate	0.80 to 2.50	0.56 x 10^{-3} to 1.75 x 10^{-3}	0.48 to 1.52
Moderately rapid	2.50 to 5.00	1.75 x 10^{-3} to 3.5 x 10^{-3}	1.52 to 3.0
Rapid	5.00 to 10.00	3.5 x 10^{-3} to 7.0 x 10^{-3}	3.0 to 6.0
Very rapid	More than 10.00	More than 7.0 x 10^{-3}	More than 6.0

Source: Horn [1971]

3.2.4 Factors Affecting K(1)

A summary of the work of Horn [1971] is presented in this paragraph.

Particle size, gradation (particle size distribution analysis), arrangement of soil particles (fabric, structure, micromorphology), organic matter content, iron oxide content, clay mineral composition, exchangeable sodium percentage, and total concentration of salts are among the more important basic factors affecting pore size distribution and continuity, and hence, K.

Particle size and shape (it is assumed for purposes of particle size analysis that soil particles are roughly spherical in shape although many particles are platy or lath-shaped) determines the size of normal packing voids. If a soil is well graded, i.e. has a good distribution of particles throughout all size ranges, the smaller particles fit into the interstices associated with the larger particles and reduce the total porosity. Smaller clay particles may also be washed into the subsoil and deposited as films that isolate or block off larger voids that conduct water is low. Slowly permeable soils of this type are often referred to as claypan soils. Other special cases of particle arrangement occurring in natural soils are the fragipan horizons of silty soils, which also have severely restricted K.

Organic matter tends to increase the K of clayey soils by promoting aggregation. However, this is only significant when calcium ions are dominant on the soil exchange and in the soil solution. When this condition exists calcium humate compounds are formed that link clay particles into large water stable aggregates.

Iron oxides also cement finer particles together, or form coatings on aggregates that prevent their dispersion. The high K of many red, tropical soils is a result of high iron oxide contents. However, under certain conditions, iron compounds may be translocated downward in the soil and reprecipitated to eventually form dense ironpans which are very slowly permeable or sometimes impervious to water movement.

Similarly other compounds, notably those of calcium, may be precipitated in the subsoils of arid or subarid regions. Once formed, these caliche pans may drastically inhibit movement of water. Where such pans are near the soil surface waterlogging may develop under irrigation.

The kind and amount of clay in soils is extremely important in determining rate of water flow through soils. Considering the size of clay particles alone it is clear that the theoretical K rate of soil masses composed of particles with equivalent spherical diameters of less than 0.002 mm is extremely low. If it were not for the aggregation of clays into larger units (peds) most clayey soils would be virtually impervious. Some clays (those of the 2:1 layer montmorin group) swell tremendously when they are wetted and reduce permeability greatly. Others such as kaolinite do not swell. Thus, kaolinitic soils are generally quite permeable while montmorillonitic soils have very low permeability or are impervious.

Exchangeable sodium (Na) content if in excess of 10% to 15% of the soil cation exchange complex will cause dispersion of the soil particles. A highly dispersed soil is very massive and dense and lacks the high proportion of void spaces associated with strongly structured, flocculated and aggregated soils. The K may be reduced by as much as 90% due to Na-induced dispersion in some soils (Bonazountas et al 1981). Such soils include the alkali soils and have pH values of the order of 8.5 to 10.0, although NA dispersion may also be associated with soils of acid pH. Conversely, soils with a high percentage of exchangeable calcium (Ca) are usually well aggregated soils and generally have moderate to rapid permeability.

Soils containing montmorillonite, even in amounts as low as 5% to 10%, are particularly sensitive to changes in the status of the exchangeable cations and the soil solution. A well aggregated Ca-dominated soil containing montmorillonite may be affected very quickly and adversely by the addition of sodium-rich alkaline water. Therefore, the quality of irrigation water should be carefully scrutinized before applied to these soils.

Compaction of soils, by the passage of cattle, or heavy equipment (which produce traffic pans) over a field surface often causes unwanted reduction in soil infiltration and permeability rates by reducing the size and continuity of pores. Intentional compaction of canal bottoms and sideslopes causes desirable reduction in seepage losses. Frequently, however, soils will rebound significantly from initial compaction particularly where water levels fluctuate markedly.

Cultivation of soils, particularly clay soils of low organic matter content, when saturated or nearly saturated often causes destruction of natural soil structure which may then result in substantial reduction of permeability. Wet cultivation (puddling) may be done intentionally as in paddy rice cultivation to cause destruction of the large natural soil aggregates (peds) which favor rapid permeability. Puddled soils produced in this manner lose less water to deep percolation when irrigated because of the destruction of their continuous macropore system.

For most crops, however, a compacted or puddled soil is deleterious because it inhibits air, water, and root penetration. After puddling, it may take several months for the soil to fully recover its natural structure through alternate wetting and drying (thawing and freezing, or swelling and shrinking), and the influence of root activity and organisms in the soil.

Temporarily increased K-rates can be achieved by mechanical action such as subsoiling. Other features affecting permeability, but not considered inherent soil properties, include relatively short-lived macropores such as wormholes and various other animal burrows, root channels, etc. Biotic features such as these are most common to noncultivated soils and less so in cultivated soils.

3.2.5 Guides to Estimating K(1)

Most guides developed as aids in making estimates of soil K-values are based on the relationship between soil texture and various ranges in rates or K classes. The USDA has schematically presented soil textural classification with a triangle (figure ID-15). In addition the USDA-SCS rates soils into seven relative K classes as shown in table ID-3. Examples of the empirical relationships that have been established by various researchers are given in table ID-4.

The chief weaknesses of these guides are first, the inconsistency that arises in the definition and identification of various soil textural classes, and secondly, the fact that the differences in permeability due to factors other than texture (as described previously) are not accounted for [Horn 1971]. To avoid the difficulty associated with using textural class names, i.e. sandy loam, clay loam, etc., a more quantitative approach has been undertaken using mean particle size, as described subsequently.

3.2.6 Mean Soil Particle Size Estimation

This value may be calculated from particle size distribution analyses (mechanical analyses) which are often made routinely in laboratories as a part of project investigations and with much more ease than permeability determinations. This calculation is based on selecting a mean particle size (equivalent spherical diameter) of 0.3 mm for the sand fraction, 0.01 mm for the silt fraction, and 0.002 mm for the clay fraction. Values for sand and silt represent the midpoint in the size range representing each of these two fractions from a log scale (figure ID-16). For the clay fraction, its upper limit was selected. The particle size limits utilized are those of the USDA but can be equated quite readily to size limits used by other agencies by means of the scale in figure ID-16.

Using the textural triangle (figure ID-15) central points or values of sand, silt, and clay percentages representing each of the soil textural classes were selected. The clay textural class was subdivided [Horn 1971] into very fine clay (more than 60% clay) and fine clay. These values and the mean particle diameters (weighted averages) calculated from them are summarized in table ID-5 and in table ID-1 (Summary, section 3.1).

3.2.7 K(1) vs Particle Size

The mean particle diameters in millimeters as given in table ID-5 for each textural class are plotted on the ordinate axis of a log-log graph

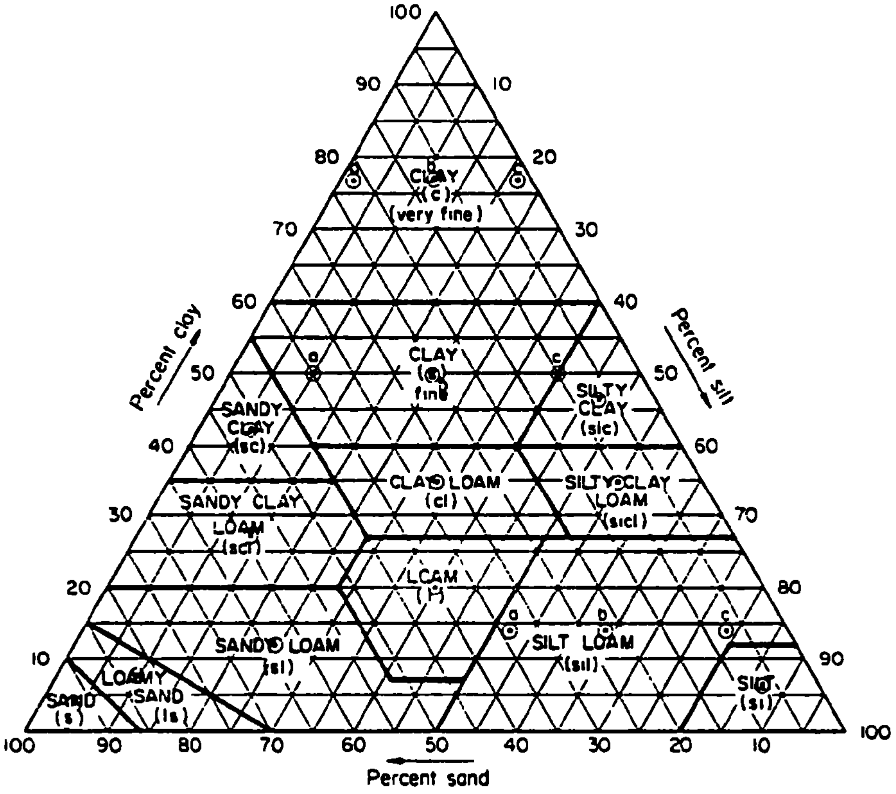


FIGURE ID-15

GUIDE FOR USDA-SCS SOIL TEXTURAL CLASSIFICATION SHOWING POINTS FOR WHICH MEAN PARTICLE DIAMETERS HAVE BEEN CALCULATED

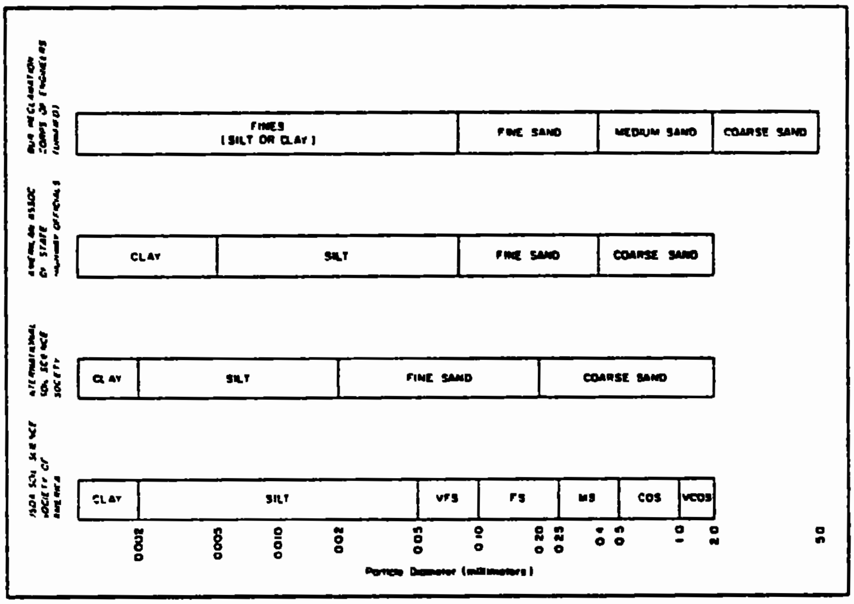


FIGURE ID-16

COMPARISON OF VARIOUS SOIL PARTICLE SIZE RANGES
USED BY VARIOUS AGENCIES

TABLE ID-4

GENERAL RELATIONSHIP BETWEEN SOIL TEXTURE AND SATURATED HYDRAULIC CONDUCTIVITY

Soil Type	Hydraulic Conductivity K (1)		
	m /day	inch/hr	cm/sec
** Jonnan et al. [1947]			
Coarse sand	120	196.8	140.0 x 10^{-3}
Sand	12	19.7	14.0 x 10^{-3}
Fine sand	4.8	7.9	5.5 x 10^{-3}
Very fine sand	2.4	3.9	2.8 x 10^{-3}
Loamy sand	1.2	2.0	1.4 x 10^{-3}
Sandy loam	0.24	0.4	0.28 x 10^{-3}
Very fine sandy loam	0.12	0.2	0.14 x 10^{-3}
Loam	0.048	0.08	0.05 x 10^{-3}
Silt loam	0.024	0.04	0.028 x 10^{-3}
Silty clay loam	0.012	0.02	0.014 x 10^{-3}
Silty clay	0.0024	0.004	0.0028 x 10^{-3}
Clay	0.0012	0.002	0.0014 x 10^{-3}
** Israelsen and Hansen [1967]			
Sandy	2 (1 - 10)	1.4 x 10^{-3}	1.2
Sandy loam	1 (0.5 - 3)	0.7 x 10^{-3}	0.6
Loam	0.5 (0.3 - 0.8)	0.35 x 10^{-3}	0.3
Clay loam	0.3 (0.1 - 0.6)	0.21 x 10^{-3}	0.18
Silty clay	0.1 (0.1 - 0.2)	0.07 x 10^{-3}	0.06
Clay	0.2 (0.05 - 0.4)	0.14 x 10^{-3}	0.12

Source: Horn [1971]

TABLE ID-5

SOIL TEXTURE, REPRESENTATIVE PARTICLE SIZE CONTENTS, AND MEAN DIAMETERS

Textural Class (USDA) (1)	Sand, as a percentage (2)	Silt, as a percentage (3)	Clay, as a percentage (4)	Mean diameter, in millimeters (5)
1. Sand	95	3	2	0.285
2. Loamy sand	83	10	7	0.250
3. Sandy clay loam	58	15	27	0.176
4. Sandy loam	55	25	10	0.167
5. Sandy clay	52	6	42	0.157
6. Loam	40	40	20	0.124
7. Clay loam	33	33	34	0.103
8. Clay (fine)	(a) 40	10	50	0.122
	(b) 25	25	50	0.0785
	(c) 10	40	50	0.035
9. Silt loam	(a) 34	53	13	0.107
	(b) 22	65	13	0.0726
	(c) 7	80	13	0.029
10. Silty clay loam	10	55	35	0.0362
Clay (very fine)	(a) 22	1	77	0.067
	(b) 10	13	77	0.0328
	(c) 1	22	77	0.007
12. Silt	5	90	5	0.0240
13. Silty clay	6	47	47	0.0236

Source : Horn [1971]

Note: (b) describes central point; (a) and (c) describe the range (see Fig. 2).

against K-rate on the abscissa (figure ID-17). It should be noted that these mean diameters represent only one of many possible values within each given textural range [Horn 1971].

The theoretical K's relative to various particle sizes, as calculated by Zunkar [1930], represent a straight line relationship (Figure ID-17). These K's are calculated for spherical particles of the same diameter with each occurring as a discrete particle. In natural soils, of course, particles are only roughly spherical or often platy, and rarely, if ever, possess uniformity of diameter. Also, cementation of particles into aggregates commonly occurs. Thus, natural soils would be expected to <u>differ</u> in K-rate from the theoretical. Nevertheless, the theoretical K serves as a good base from which K-curves for natural soils may be anticipated. With coarse, clean, well sorted sands the actual and the theoretical values approach each other but such sandy soils are quite uncommon.

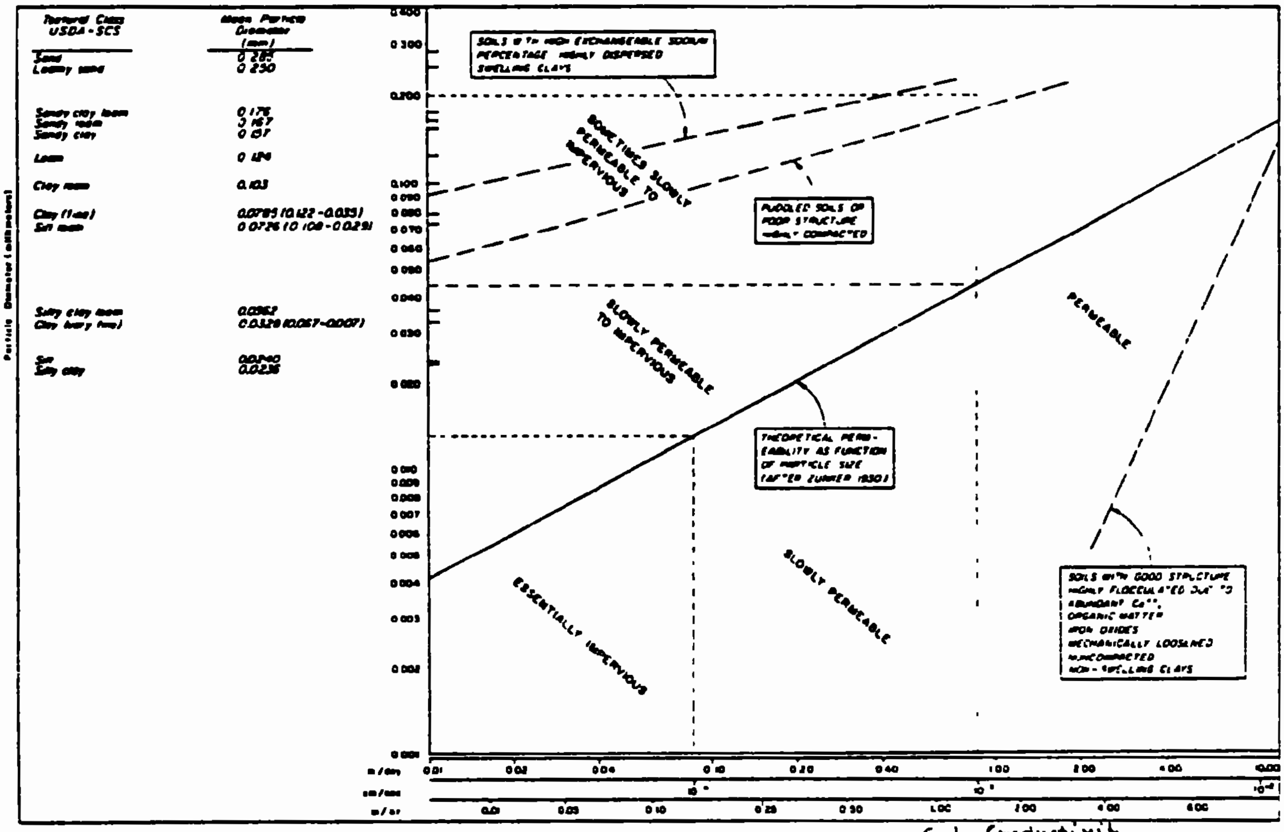
3.2.8 Selection of Working Values/Curves

For a particular application and a particular soil region, a working curve representing the soil texture-k relationship can be selected using best judgment of how existing local conditions and soil properties tend to affect soil conductivity. If some K measurements are available for known particle distributions these can be used in selecting a working curve for extrapolation to other soils. Ideally, a large number of reasonably accurate K measurements of soils along with corresponding particle size distribution data would be on hand for the locality in order to improve the accuracy of extrapolated values; however, this is rarely the case.

Without actual correlations, the working curve must be based on judgment. Best judgments are made if a thorough understanding is had of fundamental physical, mineralogical, and chemical properties of soils. Field observations, and soils data that may be available will further guide judgment. For small local areas it can often be safely assumed that nonparticle size related factors affecting soil permeability rate such as organic matter content, biotic activity, climatic conditions, clay mineralogy, and chemistry of the soil solution are more or less the same throughout. Realistic values and valid comparisons of soil K for the local area cn then be obtained from a single working curve.

Hydraulic conductivities of the very sandy soils and, at the other extreme the very clayey soils, are not affected by nonparticle size related factors as much as the in-between soils. The latter comprise the majority of natural soils and vary considerably in response to these factors.

Some very general groupings of soils according to their K are separated in figure ID-17 by the horizontal and vertical dashed lines. For example, soils with mean particle diameters greater than 0.2 mm have K rates usually in excess of about 10^{-3} cm/sec and soils with diameters



Soil Conductivity

FIGURE ID-17

SOIL TEXTURE PERMEABILITY CURVES

less than 0.015 mm have rates of 10^{-4} cm/sec and are essentially impervious. Soils between these ranges are greatly affected by the nonparticle size factors controlling K; these factors vary considerably from place to place and, in addition, are subject to in situ changes in relatively short periods of time. As a consequence the intermediate soils can range from impervious to permeable [Horn 1971].

Rigorous application of the K curves in figure ID-17 presupposes the availability of data from particle size distribution analyses for all major horizons of the soils in question. Depending on intended application, K in a vertical direction of an entire soil section may be rated according to the least permeable layer, recognizing that for some soils, the presence of very thin continuous clay laminae or other abruptly contrasting layers may exert a profound influence on the permeability behavior of the soil. Lateral K of soil sections may be rated according to the layer with greatest K. Alternatively, average K rates may be taken for the entire section.

The methods for obtaining mechanical analysis data are much easier and the results more dependable than those associated with measuring K-rates. Of course, collection of representative soil samples and laboratory facilities capable of conducting particle distribution measurements are necessary in order to quantify the soil texture variable in the estimation of K-rates.In cases where both mechanical analyses and soil K determinations are to be made, it is recommended that soil samples are taken from the same location for laboratory analyses. This not only results in reducing sampling costs and field time but also provides valuable data for correlating permeability rates with the particle size data and other measured soil properties.

When only field estimations of soil texture are available, the K estimate is less quantitative. Nevertheless, using the limits indicated in figure ID-17, a guided judgment method is provided from which tenable soil K values can be obtained for a variety of field applications.

3.2.9 K(1) vs k(1)

The hydraulic conductivity (K) is related to the intrinsic permeability (k) via equation ID-6. Since only fluid (ie. water, soil moisture) is assumed to flow in a soil system, the conversion factor from K-to-k is a constant number, to be obtained from table ID-2. By employing: the values of table ID-2; the soil classification system of table ID-15; and the soil texture graph of figure ID-17; the intrinsic permeabilities (k) for the USDA soil texture triangle of figure ID-15 have been derived (table ID-6).

3.2.10 k(1) SESOIL Default Values

As discussed in section 3.2.6, the theoretical k rates derived would be expected to differ from the field k rates of natural soils. The last column in table ID-6 (Eagleson's estimates) indicates a consistent

TABLE ID-6

SOIL TEXTURE VS. PARTICLE DIAMETER$^{(d)}$, SOIL CONDUCTIVITY$^{(K)}$ AND INTRINSIC PERMEABILITY$^{(k)}$

Textural Soil Class (USDA) #	Designation[1]	d (mm)	K (cm/sec)	k (cm^2)	Eagelson [1978,1982] (cm^2)
1	Clay (very fine)	0.0328	7.5×10^{-4}	7.5×10^{-9}	
(2)[2]	Clay (medium fine)	0.050	2.5×10^{-3}	2.5×10^{-8}	1×10^{-10}
3	Clay (fine)	0.0785	6.0×10^{-3}	6.0×10^{-8}	
4	Silty clay	0.0236	5.0×10^{-4}	5.0×10^{-9}	
5	Silty clay loam	0.0362	8.5×10^{-4}	8.5×10^{-9}	2.8×10^{-10}
(6)	Clay loam	0.103	6.5×10^{-3}	6.5×10^{-8}	6.95×10^{-11}
7	Loam	0.124	8.0×10^{-3}	8.0×10^{-8}	
(8)	Silt loam	0.0726	3.5×10^{-3}	3.5×10^{-8}	1.41×10^{-10}
9	Silt	0.0240	5.0×10^{-4}	5.0×10^{-9}	1.20×10^{-9}
10	Sandy clay	0.157	1.5×10^{-2}	1.5×10^{-7}	
11	Sandy clay loam	0.176	2.5×10^{-2}	2.5×10^{-7}	
(12)	Sandy loam	0.167	2.0×10^{-2}	2.0×10^{-7}	2.5×10^{-9}
13	Loamy sand	0.250	5.0×10^{-1}	5.0×10^{-6}	
14	Sand	0.785	1.0×10^{-1}	1.0×10^{-6}	

---

[1] See Figure ID-15.

[2] Class in ( ) corresponds to an overall proposed soil scenario related to the USDA soil triangle (Figure ID-15 and Table ID-1).

natural k-rate decrease of 10^{-1} to 10^{-2} contrasted to the theoretically derived values. Since Eagleson's theory deals with the entire seasonal water budget of the soil compartment, it is more or less expected that his field k(1) values obtained via model calibration [Eagleson & Tellers 1982, p.353] will be lower because of the number of water budget processes accounted (eg. infiltration, exfiltration). It may be appropriate, therefore, to reduce the k values derived and presented in table ID-6 to two orders of magnitude (i.e. 10^{-2}) in order to obtain some consistency with the calibrated k(1) values of Eagleson. There exist no theoretical justification for doing so (aside from engineering judgment), however, for scenarios and canonical environmental simulations or modeling efforts, the proposed action is not anticipated to drastically alter SESOIL output results. No sensitivity model analysis is performed at this stage to justify above action.

The finally derived saturated intrinsic permeabilities to be input as default values to SESOIL when dealing with fictitious or canonical environments are given in table ID-7, and in table ID-1 (summary; section 3.1).

3.3 Soil Effective Porosity -- n_e

3.3.1 Definitions

If the total unit volume V_T of a soil or rock is divided into the volume of the solid portion V_s and the volume of the voids V_v, the volumetric total porosity (or porosity) n is defined as

$$n = V_v/V_T \tag{ID-9}$$

and is usually reported as a decimal fraction or a percent. Table ID-8 [Freeze & Cherry 1979, p.37] lists representative porosity ranges for various geologic materials. In general rocks have lower porosities than soils; gravels, sands, and silts, which are made up of angular and rounded particles, have lower porosities than soils rich in platy clay minerals; and poorly sorted deposits have lower porosities than well sorted deposits [Freeze & Cherry 1979].

The porosity n is an important controlling influence on hydraulic conductivity K. In sampling programs carried out within deposits of well sorted sand or in fractured rock formations, samples with higher n have in general also higher K, but the relationship does not hold on a regional basis across the spectrum of possible rock and soil types. Clay rich soils, for example, usually have higher porosities than sandy or gravelly soils but lower hydraulic conductivities. In practice, it is difficult to saturate a soil sample and then dry it and measure its porosity. It is usual, however, to estimate the total porosity (or porosity) from the relationship [Eagleson 1970, p.286]

$$n = 1 - (\rho_b/\rho_s) \tag{ID-10}$$

Table ID-7

k(1) Default Values for SESOIL

Textural Soil Class (USDA)		k(1)		
#	Designation[1]	(cm²)		
1	Clay (very fine)	$7.5x10^{11}$	=	$0.75x10^{-10}$
(2)[2]	Clay (medium fine)	$2.5x10^{12}$	=	$2.5x10^{-10}$
3	Clay (fine)	$6.0x10^{-10}$	=	$6.0x10^{-10}$
4	Silty clay	$5.0x10^{-11}$	=	$0.5x10^{-10}$
5	Silty clay loam	$8.5x10^{-11}$	=	$0.85x10^{-10}$
(6)	Clay loam	$6.5x10^{-10}$	=	$6.5x10^{-10}$
7	Loam	$8.0x10^{-10}$	=	$8.0x10^{-10}$
(8)	Silt loam	$3.5x10^{-10}$	=	$3.5x10^{-10}$
9	Silt	$5.0x10^{-11}$	=	$0.5x10^{-10}$
10	Sandy clay	$1.5x10^{-9}$	=	$15x10^{-10}$
11	Sandy clay loam	$2.5x10^{-9}$	=	$25x10^{-10}$
(12)	Sandy loam	$2.0x10^{-9}$	=	$20x10^{-10}$
13	Loamy sand	$5.0x10^{-8}$	=	$500x10^{-10}$
14	Sand	$1.0x10^{8}$	=	$100x10^{-10}$

---

[1] See figure ID-15.

[2] Class in () corresponds to an overall proposed soil scenario related to the USDA soil triangle (figure ID-15, table ID-1).

Table ID-8

Range of Values of Porosity

Material	Porosity n %
Unconsolidated deposits	
Gravel	25-50
Sand	35-50
Clay	40-70
Rocks	
Fractured basalt	5-50
Karst limestone	5-50
Sandstone	5-30
Limestone, dolomite	0-20
Shale	0-10
Fractured crystalline rock	0-10
Dense crystalline rock	0-5

Source: Freeze & Cherry [1979, p.37].

where ρ_b is the bulk mass density of the sample, and ρ_s is the particle mass density. The bulk density is the oven-dried mass of the sample divided by its field volume. The particle density is the oven-dried mass divided by the volume of the solid particles, as determined by a water displacement test. [Freeze & Cherry 1979, p.337.] In case no great accuracy is required, it can be assumed for most mineral soils $\rho_s=2.65\ g/cm^3$.

One should be careful with the use of porosity values, when employing an unsaturated soil zone model such as SESOIL. The problem is similar to the specific yield and the porosity issue of a phreatic aquifer [Bear 1979, p.88]. As water is being drained from the interstices of the soil, the drainage is never a complete one. A certain amount of water is retained in the soil against gravity by capillary forces. After drainage has stopped, the volume of water retained is an aquifer per unit (horizontal) area and unit drop of the water table is called "specific retention" S_r, and is related to the specific aquifer yield S_y via

$$n = S_y + S_r \qquad \text{(ID-11)}$$

For this reason S_y (less than n) is also called "effective porosity" n_e. The correlation between porosity n, effective porosity n_e and median soil particle (grain) size is schematically presented in figure ID-18 [Davis & DeWiest 1966]. SESOIL requires the effective porosity n_e as an input parameters.

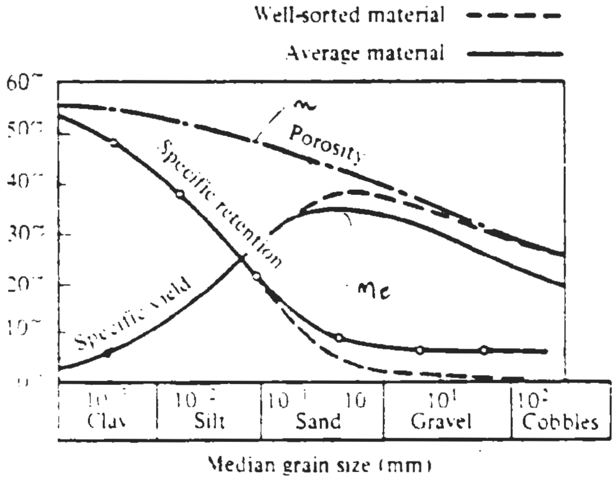
3.3.2 Soil Hydraulic Properties

An ecological and soil genesis pedologic discussion is presented by Eagleson [1982a, p.326], according to whom the overall soil properties behavior may be generalized as presented in figures ID-14 a,b (section 3.1). As discussed by Eagleson, soils evolve having a continuous spectrum of textures from clay through silt to sand and gravel, and the critical hydraulic properties of them vary widely even within the same textural class, but over the variety of classes their range is enormous. Brooks and Corey [1966] show that k(1) is related to both the shape (i.e. tortuosity) of the pores and to their total size (i.e. porosity) of a soil. Davis [1969] proposed the overall relationship [Eagleson 1982a, p.327]:

$$k(1) = Ae^{Bn} \qquad \text{(ID-12)}$$

where the coefficients A and B vary with textural class as sketched in figure ID-14 (section 3.1).

As discussed by Eagleson, for the fine-particled clayey soils the total particle surface area is enormous. The total pore volume which can be occupied by water that is bound to these surfaces through molecular forces is correspondingly large and the inactive porosity n_r dominates. With increasing sand content this volume decreases and the effective



Source: Bear [1979, p.88].

Figure ID-18 Relationships Between Porosities and Soil Grain Size porosity rises. As the sandy soil becomes gravelly, the falling total porosity takes over from the decreasing surface area and the effective porosity becomes smaller. This is sketched in figure ID-14b. We see from this diagram that over the clay to sand textural range encompassing most soil, permeability and effective porosity are directly related.

3.3.3 n_e SESOIL Default Values

The range of values of the porosity n or the effective porosity n_e is known to be quite small in field studies -- from about 0.25 to about 0.45 -- and does not have a large effect [Tellers & Eagleson 1980, Chan & Eagleson 1980] on solutions of the water balance equation HY-32 (appendix HY) as other parameters may have. The effective porosity affects directly the sigma function (equation HY-34) and consequently the gamma function of the model and the down-the-road remaining calculations, but the sensitivity of sigma vs n_e is not large.

Eagleson reports in 1978 [WRR, p.769, table 2] effective porosity n (i.e. n_e) values for various soils corresponding to the "porosity" curve of figure ID-14b. In his latest publication in 1982, however, his n_e values are slightly decreased [WRR, 1982, p.329, table 1]. The newly introduced 1982 porosity vs. permeability graph [WRR 1982, p.326, figure 1] indicates potential need for employing the "effective porosity" curve of figure ID-14b (instead of the n-curve). We will follow the latter logic in the following pages when developing default values for SESOIL.

Table ID-9 lists representative porosity n values (columns (1) & (2)). They are obtained from various sources and are reported for the soil classification scheme presented on table ID-7 (derived from the USDA soil triangle). The average or the best (using best judgment) value of the various sources is designed with n. This value has been "adjusted" to an $\bar{n}_e$ value (column (5)) with the aid of figure ID-18, and the latter has been reported on table ID-1 (section 3.1) as a SESOIL default value. Adjustment has been performed by correlating the $\bar{n}$, $\bar{n}_e$ and keeping the n_e estimates for clay (#2), clay loam (#6), silt loam (#8) and sandy loam (#12) to their fixed values of 0.2, 0.30, 0.30 and 0.25 correspondingly.

3.4 Soil Disconnectedness Index -- c

3.4.1 Definition

In Eagleson's model, the soil pore disconnectedness index c is defined as [Eagleson 1982, p.328]:

$$c = \Delta[\ln(k)]/\Delta[\ln(s_o)] \qquad \text{(ID-13)}$$

where k [cm²] the intrinsic soil permeability and s_o the long-term average soil moisture concentration in the root-zone. In other words, c represents the slope of a k-s_o, or K-s curve as graphically shown in figure ID-19.

Table ID-9

Representative and SESOIL n_e-Default Values

Textural Soil Class #	Textural Soil Class USDA Designation	Porosity (n) (fractional) Perrier & Gibson[1980] (1)	 Freeze & Cherry[1979] (2)	 $\bar{n}$ 7) estimate (3)	Effective Porosity (n_e) n_e (4)	 $\bar{n}_e$ 6) estimate (5)
1	Clay (very fine)			0.70	$0.45^{1)2)}$	$0.20^{5)}$
$(2)^{8)}$	Clay (medium fine)	0.680	0.4-0.7	0.68		0.20
3	Clay (fine)			0.64		0.22
4	Silty clay	0.592		0.59		0.25
5	Silty clay loam	0.588		0.59		0.27
(6)	Clay loam	0.582		0.58	$0.35,^{1)},0.30^{2)}$	0.30
7	Loam	0.521		0.52		0.30
(8)	Silt loam	0.535		0.54	$0.35^{1)3)},0.3^{2)}-0.4^{4)}$	0.35
9	Silt		0.35-0.50	0.49		0.27
10	Sandy clay	0.442		0.44	$0.350-0.458^{4)}$	0.24
11 .	Sandy clay loam	0.453		0.45		0.26
(12)	Sandy loam	0.442		0.44	$0.25^{1)}$	0.25
13	Loamy sand	0.330		0.33		0.28
14	Sand	0.389	0.25-0.40	0.35	$0.379-0422^{4)}$	0.30

[1] Eagleson [WRR, 1978, p.769]

[2] El-Hemry & Eagleson [1980]

[3] Averaged value from clay-to-sand [Chan & Eagleson 1980]

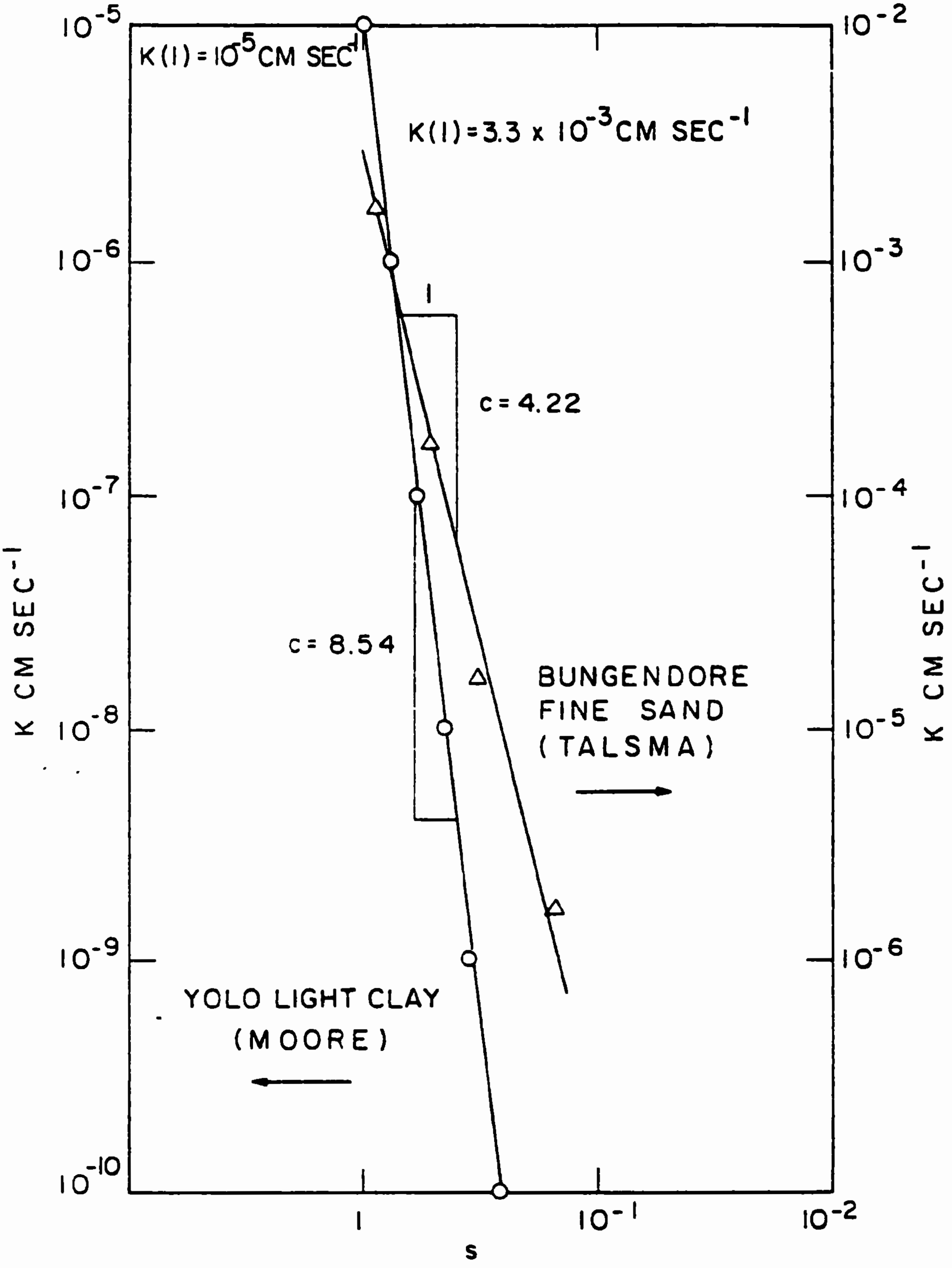
[4] Eagleson [1970, p.287]

[5] Free estimate based on Bear [1980]

[6] Interpolated values between fixed $\bar{n}_e$ values for soils # 2,6,8,12, reported on table ID-1

[7] n, $\bar{n}_e$ final estimates as SESOIL default values

[8] class in () corresponds to an overall proposed soil scenario related to the USDA soil triangle (see table ID-1)



Source: Eagleson [1979].

Figure ID-19 Hydraulic Conductivity vs Soil Moisture

Brooks and Corey [1966] show that during wetting or drying soil cycles the functional relationship

$$k(s) = k(1).s^{c} \qquad \text{(ID-14)}$$

allows integration of the simplified Burdine [1958] equations governing the relationship between effective permeability and capillary pressure in irregular pore structures to obtain the relationship

$$c = (2+3m)/m \qquad \text{(ID-15)}$$

employed in Eagleson's work [Eagleson 1978, p.723]. In that respect the pore disconnectedness index c in SESOIL can also be defined as the exponent relating the "wetting" or "drying time dependent intrinsic permeability k(s) of the soil to its saturated intrinsic permeability k(1). Relation to ID-14 has been defined by Eagleson. Theoretically k is a soil property, therefore, it should be independent from the water or moisture soil content (see equation ID-5). In practice, however, because of the effective porosity issue discussed in section 3.3.2 (figure ID-14b), k becomes moisture dependent, a fact that may have resulted to the definition of equation ID-14 via the c exponent.

At this point it is worth emphasizing that any unsaturated soil zone of the literature [eg. Bonazountas et al 1979] requires as a <u>user</u> input instead of a curve relating "conductivity k vs. capillarity head ψ." This curve is obtained from experimental data. It is almost impossible to obtain this curve off-the-shelf for any type of soil, but it is also extremely difficult to obtain this curve in the laboratory. Therefore, the "one-variable" approach of Eagleson [1978] employed in SESOIL greatly simplifies data gathering and data input to a model.

3.4.2 The c Index Sensitivity

A hydrologic balance sensitivity based on the two independent soil properties k(1) and c is presented in figure HY-38, section HY-3.5. Roughly speaking, the compartment surface runoff is insensitive to c but very sensitive to k(1).

In relation to the various soil types, and when dealing with vegetated areas, Eagleson & Tellers [1982, p.347] proves that the range of climax values of c (that is values of c at maximum vegetation canopy, given a specified soil moisture content and an ecological optimality) has been only

$$4.74 \leq c < 5.50 \quad ; \quad c > 3.0 \qquad \text{(ID-16)}$$

for six catchments studied. In addition the lower limit of c is reported [Brooks & Corey 1966] to be 3.0. Typical values of c lie around

4 to 5 and the reason for this small range has been recently analyzed by Eagleson & Tellers [1982, p.348].

The correlation of c and s_o is evaluated via the f(s) function [Eagleson & Tellers 1982, p.349].

$$(c-3).g_i(c,s_o) = f(s_o) \qquad \text{(ID-17)}$$

which by its expected value results to the very useful empirical relationship

$$(c-3).g_i(c,s_o) = 0.75 \qquad \text{(ID-18)}$$

that is presented for 6 catchments in the lower half part of figure ID-20. This relationship allows elimination of c from the water balance equation HY-32 in terms of the state variable s_o and when dealing with ecologically balanced systems. However, because variation of c is within certain limits, we may employ the equations derived by Eagleson & Tellers [1982, p.349] from ID-18, i.e.

$$s_o[k(1)]^{1/(c+5)} = f(c) \qquad \text{(ID-19)}$$

and

$$k(1) = (0.058/s_o)^{c+5} \qquad \text{(ID-20)}$$

to make some rough estimates for c values based on k(1) values as following: for a set of soils (sand, sandy loam, silty loam, loam and clay) Tellers & Eagleson [1980] report from their experience with equations ID-19, ID-20, the expression

$$k(1) = (m/512.7)^{2.75} \qquad \text{(ID-21)}$$

where m = 2/(c-3) as given by parameter set in HY-29 (app. HY) and graphically reported in figure ID-21. Therefore:

- In general (regression line; figure ID-21):

$$c = k(1)^{1/2.75} \, (512.7/2)+3 \qquad \text{(ID-22)}$$

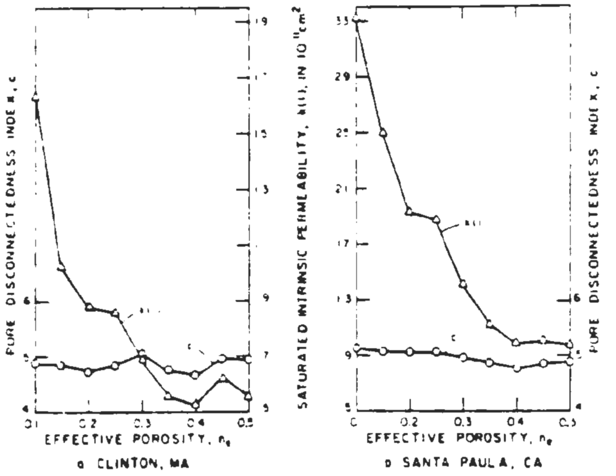
- For sandy soils (m=3, figure ID-21):

$$c = 3.7 \qquad \text{(ID-23)}$$

- For sandy loam soils (m=0.5, figure ID-21), and

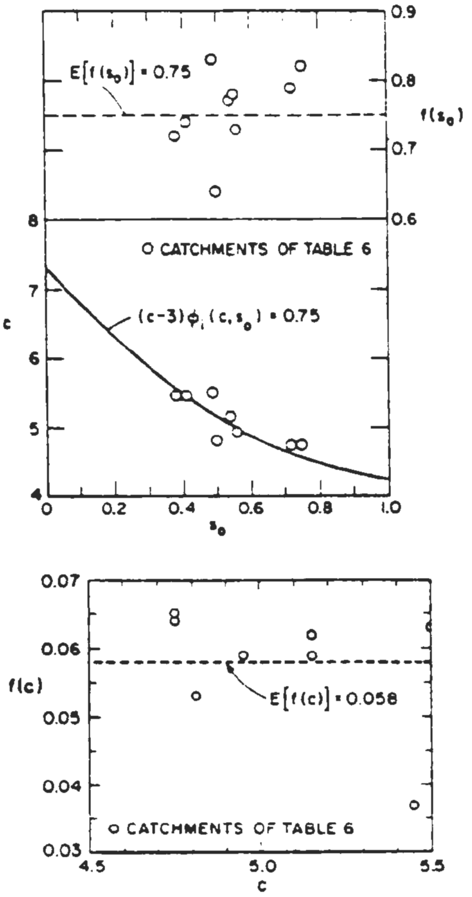
$$c = 6.33 \qquad \text{(ID-24)}$$

Table ID-10 summarizes obtained and compiled c values for the USDA soil texture classification triangle. Values of the last column are reported in table ID-1 also. Based on information obtained from the literature



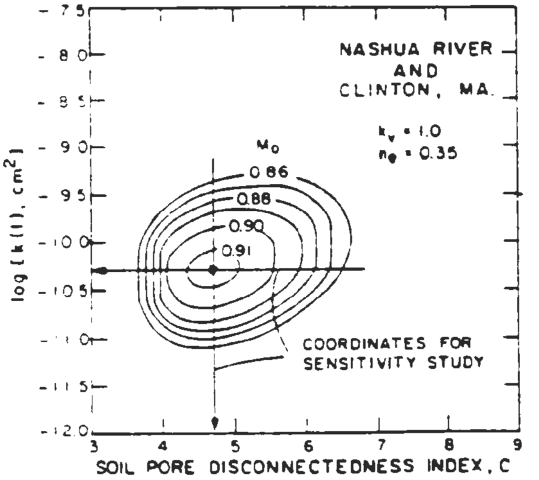
Sensitivity of flux properties of climax soils to porosity ($(k_v = 1)$).

(a)



Climatic climax soil properties. (*a*) Soil pore disconnectedness index. (*b*) Saturated intrinsic permeability.

(c)



Climatic climax soil-vegetation systems.

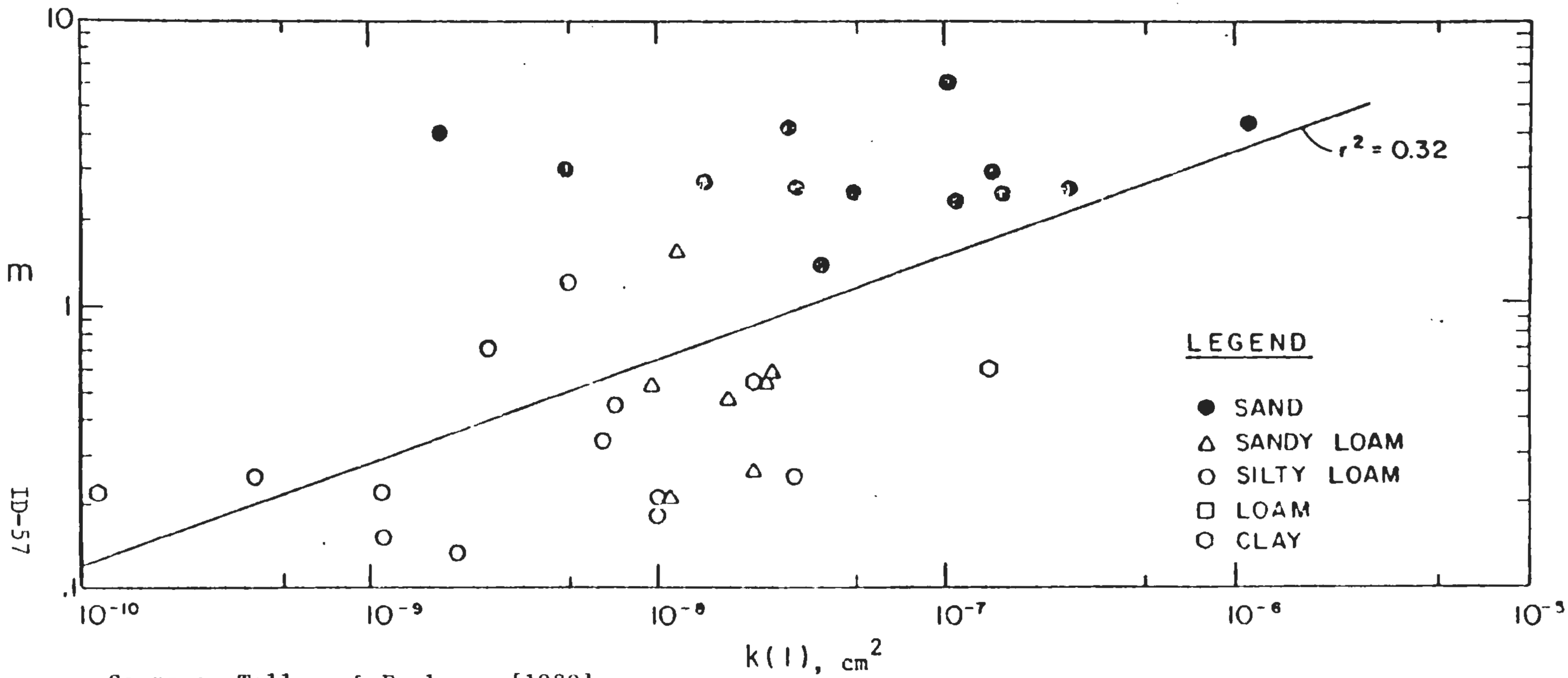
(b)

M_O = vegetation canopy density

k_V = plant coefficient

Source: Eagleson [1982], Eagleson & Tellers [1982].

Figure ID-20 Functional Relationship, $c-f(S_O)$; Saturated Intrinsic Permeability



Source: Tellers & Eagleson [1980].

Figure ID-21 Saturated Permeability vs Pore Size Distribution Index
(from Eagleson, Personal Communication)

Table ID-10

Default c Values for SESOIL

Textural Soil Class USDA		c-Soil Properties			SESOIL Default c-values 3)
#	Designation	k(1) (cm^2)	c_1 1) (-)	c_2 2) (-)	
1	Clay (very fine)	$7.5x10^{-11}$	25	12	12.0
(2) 5)	Clay (medium fine)	$2.5x10^{-10}$	16	12	12.0
3	Clay (fine)	$6.0x10^{-10}$	16	8.54 4)	12
4	Silty clay	$5.0x10^{-11}$	23		12
5	Silty clay loam	$8.5x10^{-11}$	10.6	3.8 4)	10
(6)	Clay loam	$6.5x10^{-10}$	13	10,5.05	7.5
7	loam	$8.0x10^{-10}$	11.0	8.5 4)	6.5
(8)	Silt loam	$3.5x10^{-10}$	16.0	6,4.95	5.5
9	Silt	$5.0x10^{-11}$	23.0		12
10	Sandy loam	$1.5x10^{-9}$	6.33		6
11	Sandy clay loam	$2.5x10^{-9}$	8.70		4.0
(12)	Sandy loam	$2.0x10^{-9}$	8.70	4	4.0
13	Loamy sand	$5.0x10^{-8}$	5.00		3.9
14	Sand	$1.0x10^{-8}$	3.7		3.7

---

[1] approximate values by employing equation ID-22 and the k(1) values of table ID-7

[2] Eagleson [1977, 1978, 1981, 1982]

[3] Employ primarily values of soils # 2,6,8 and 12

[4] Talsma [1974], Moore [1939], Brook & Corey [1966] from Eagleson [1978a-g].

[5] Soil class in ( ) corresponds to an overall proposed soil scenario related to the USDA soil traingle; in figure with

the c value range has been confined between c=12 [Eagleson 1978] and c=3.7 [see figure ID-21 for clay]. The c_1 theoretical estimates are kept as a guidance. The value of soil #6 (clay loam, c=7.5) equals the average of the two Eagleson studies [1982, 1978]. The same applies to soil #8 (silt loam). For the remaining soil types rough linear interpolation is performed, because the changes of c do not affect water balance estimates strongly. As information becomes available, these default values will be improved. For site specific application, model calibration to estimating the independent soil parameters c, k(1), n_e is recommended.

3.5 Soil Parameter Calibration

3.5.1 General

A single general relationship for k(1), n_e and c does not exist, because the vegetation canopy density and evapotranspiration -- both related to n_e, k(1) and c -- affect the interrelation of the three parameters in an area. Tellers & Eagleson [1980] and Eagleson & Tellers (1982] have employed the water balance theory of Eagleson [1978a-g] to estimate the effective hydrologic properties of soils from observation on vegetation density. Bonazountas et al [1981] have employed the monthly water balance of SESOIL to estimate soil moisture contents of soil, where field data were available.

Three types of input parameters are associated with Eagleson's hydro-balance routine: climatic, soil and vegetation. The climatic and vegetal properties are easily obtained from observations; this leaves the soil parameters to be determined from relationship between climate, soil and vegetation [Eagleson 1978a-g]. Four soil parameters are associated with Eagleson's theory; three independent soil properties (k(1), n_e, c) and the soil moisture state variable s_o. In calibrating the model, two methods are of major importance: (1) calibration of the soil parameters k(1), c via s_o and n, or (2) calibration of s_o via k(1), c and n. The vegetation part of Eagleson's theory has been eliminated from SESOIL, however, calibration procedures remain the same.

3.5.2 Calibration of k(1), c via s_o

The range of values of the porosity, n, is known to be quite small, from 0.25 to about 0.45 (see section 3.3), and does not have a large effect on solutions of the water balance equation. Assuming a known value for n_e, this fact leaves the soil moisture, intrinsic permeability, and pore disconnectedness index as unknowns. To solve for these variables, two equations or relationships are needed which incorporate the soil and climate as well. The first relationship is the water balance, Equation HY-32, which expresses the soil moisture, s_o, as an implicit function of the climate and soil. The second expression used is a rather weakly correlated regression between k(1) and m (figure ID-21, equation ID-21). With the information produced by Eagleson & Tellers [1982] for vegetated sites, the following calibration procedure can be designed, to estimate effective soil parameters, given a set of climatic parameters.

(1) A value of n_e is assumed, in order to estimate E (equation HY-37).

(2) The lowest possible value for c, approximately 3.5, is selected as an initial value.

(3) k(1) is calculated from equation ID-21.

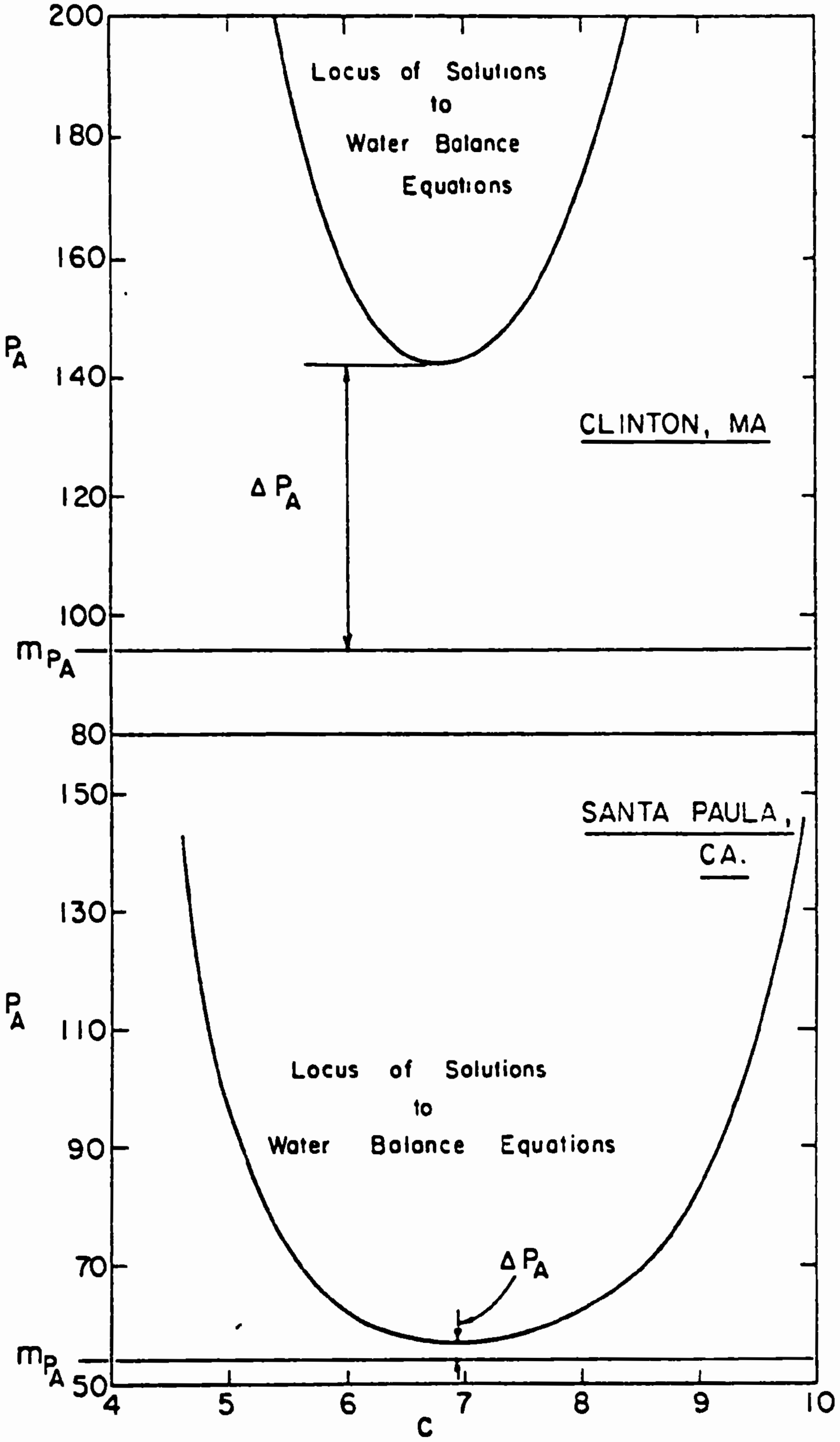
(4) With these values for the three soil parameters, n_e, k(1), and c, it can be seen from equation HY-37 that s_o remains as the only variable needed for determining E. With E known from step (1), s_o is calculated.

(5) Annual precipitation is calculated via equations HY-32 through HY-43.

(6) If the annual precipitation from the above step is not equal to the actual mean rainfall, c is incremented upward from its initially low value and steps (3)-(5) are repeated.

(7) Due to the approximation introduced by using equation ID-21, the precipitation, P_A, calculated in step (5) may never exactly equal the actual mean value, m_{PA} for any value of c. P_A will approach m_{PA} as c is increased, coming to within ΔP_A of equality at intermediate c before diverging again for large c. For low values of c, the calculated k(1) is large, representing a soil with high permeability and well connected pores. With evapotranspiration specified at the optimum (i.e. minimum) value, a large precipitation is therefore calculated in order to produce the inevitably large groundwater yield of the highly porous soil. For large c and small k(1), the soil is extremely impervious and the surface yield will be high. With minimum evapotranspiration, a large value for precipitation is again needed. Somewhere between these two extremes, a set of suitable soil parameters is obtained which gives an annual precipitation, P_A, which is closest to the actual mean, m_{PA}. This relationship is illustrated in figure ID-22. Holding c constant at the value which gives the minimum ΔP_A, k(1) is then deviated from regression equation ID-21 until another minimum in calculated precipitation is reached. If this value is above the mean precipitation, c is decreased, if it is below the mean, c is increased. Another search is done on k(1) until the minimum precipitation is found. This step is repeated until the minimum calculated precipitation is equal to the mean.

(8) If the values obtained for k(1) and c are not consistent with the assumed porosity, n is adjusted to a more appropriate



Source: Tellers & Eagleson [1980].

Figure ID-22 Water Balance Solutions Using Soil Properties from Equation ID-21 value corresponding to a more pervious or impervious soil type depending on the values of k(1) and c. Steps (1) through (7) are repeated.

The soil parameters obtained from steps (1-8) are used to construct the CDF of annual yield in the same manner as Eagleson [1978g]. The above procedure can be repeated for 3 input data categories; i.e. climate, soil and vegetation in case equation HY-32 were not simplified to the bare soil SESOIL needs (see section ID-3.1).

3.5.3 Calibration of s_o via k(1), n_e, c

The concept of procedure previously described can be repeated to calibrate SESOIL either via existing s_o field measurements, or via USGS data records for basin yields (surface runoff and groundwater runoff) [Eagleson 1978a-g]. In this particular case

(1) a n_e, c set is obtained from table ID-1.

(2) the model is run, and model yield output (equation HY-42) is compared to USGS basin yields.

(3) Depending upon the distribution of the surface vs groundwater runoff yield predictions, parameters n_e, c, and k(1) are adjusted to new values, primarily by adjusting k(1) (see section ID-3.2) and by following the sensitivity consensus of figures HY-7 and HY-8.

(4) Above steps are repeated until basin yields and averaged soil moisture s_o predictions have reached their field values.

3.5.4 Automated Calibration

It is feasible to write a program automatically calibrating SESOIL and all its input parameters given USGS data records for basin yields and some basic precompiled information such as the default data of table ID-1. However, development of such a computer code has been beyond the scope of the developers involvement.

4.0 CHEMISTRY INPUT DATA

Chemical parameters, coefficients, etc. may be compiled from the handbook "Research and Development Methods for Estimating Physicochemical Properties of Organic Compounds of Environmental Concern" [Lyman et al 1981], or any other handbook. In the future, authors of SESOIL intend to compile a data base for chemical properties relevant to the model use and a number of pollutants.

5.0 CANONICAL CLIMATIC-SOIL COMPARTMENTS

Many environmental studies, such as human exposure assessments related to hazardous waste sites, may require the design of typical or canonical soil-compartments; and SESOIL is well suited for such simulations [Bonazountas et al 1981]. The design, however, of a canonical compartment is a function of both the climate and the soil-type of the environment; therefore, only climatic or only soil canonical (default) data sets would not suffice for a model user if he has to describe a canonical soil-compartment. There may be a way to design for the entire U.S. canonical soil environments accounting for both climatologic and soil type default values, but since model developers have not yet finalized their thinking regarding this issue, and they are not confident regarding their current technical approach, they have decided not to present this information in this section. Some information may follow in the future.

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APPENDIX DF

DATA FILES (INPUT/OUTPUT)

FIGURES

1.0 INTRODUCTION

This appendix is intended to guide users through details of the data management and the computational procedures of the FORTRAN code of SESOIL. It will also help model developers (Bonazountas and Wagner) in the future, since model design and development has not been completed.

SESOIL is operational at various levels as discussed in Section 3.0, User's Manual. To organize data management and provide a quality assurance control during operations, the input, output and intermediate data are stored in data files (arrays).

SESOIL is structured around

(1) An input data file system (IDFS), and

(2) A data management array system (DMAS)

The input data file system (IDFS) contains user input or permanently stored input data (climatic, soil, chemistry; see appendix ID) required to operate the model. This input data file system consists of 5 input data files, the GE DATA, LO DATA, L1 DATA, L2 DATA and EXEC DATA. Detailed information regarding these files is given in section 3.4 (Input Data Files), of section 3.0 (User's Manual) of this documentation; therefore, it is not discussed in this appendix.

The data management array (DMAS) system contains two major types of arrays:

(2.1) Input data arrays (IDA) and

(2.2) Operational/Retrieval arrays (ORA)

The input data arrays (IDA) contain the input data relevant to a particular simulation. These data are read from the input data file system (IDFS) and are stored in the input data arrays (IDA) by subroutine RFILE (Read FILE). RFILE can access any of the 5 data files: GE DATA, EXEC DATA, LO DATA, L1 DATA, L2 DATA.

Operational/Retrieval arrays (ORA) contains data or results of intermediate calculations, and/or data for transfer to other subroutines. These arrays can be accessed (from the FORTRAN code) by a programmer or user to check on the correctness of intermediate computational steps of the model. As such, ORA-arrays serve as "control nodes" of the model code.

A schematic presentation of the SESOIL operations via its data file system is shown on the next page (Figure DF-1). Most of the DMAS arrays used in SESOIL and their contents are discussed in the following sections.

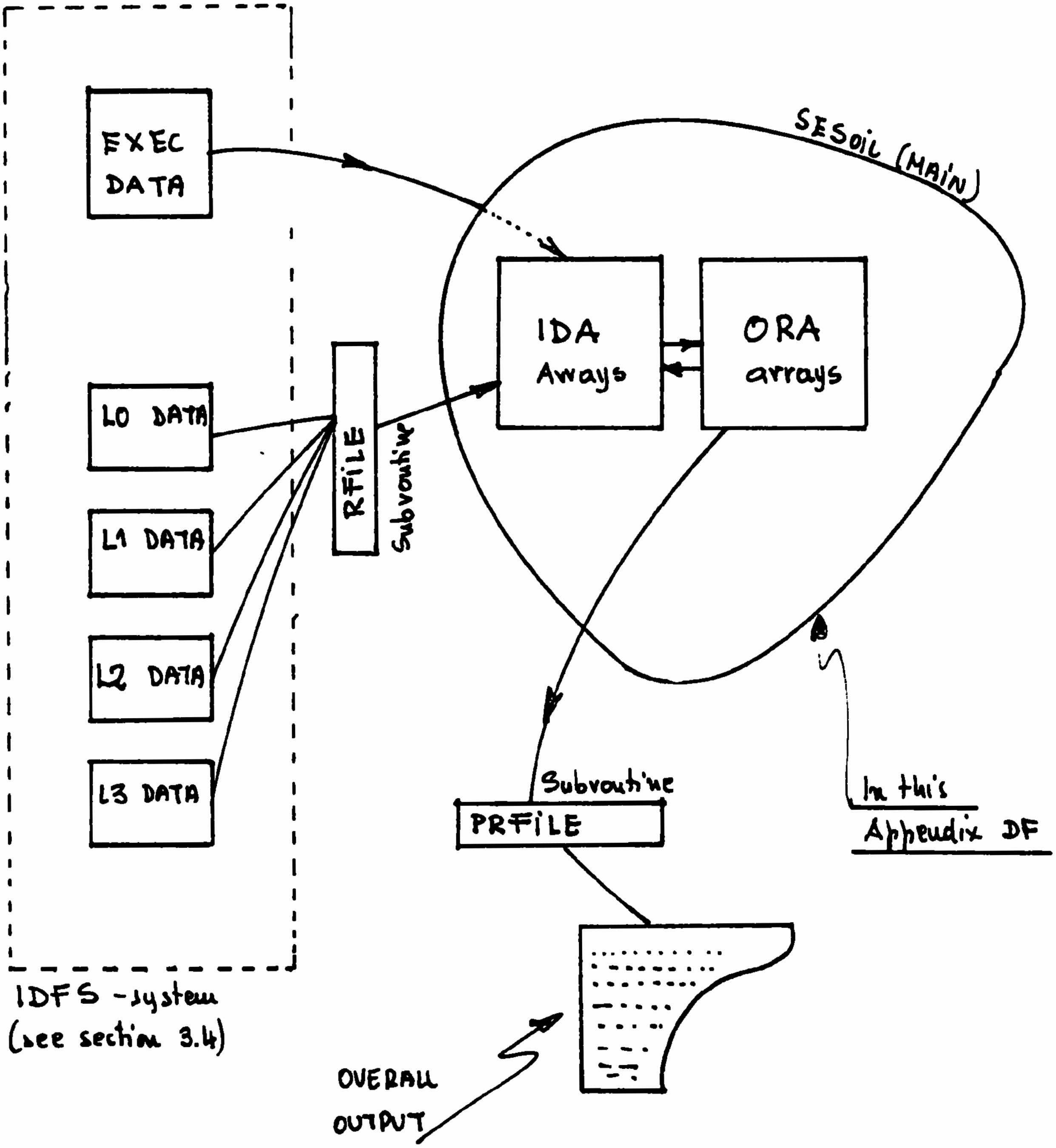

FIGURE DF-1 -- SCHEMATIC OF "SESOIL" DATA FILE/ARRAY OVERALL STRUCTURE

2.0 INPUT DATA ARRAYS (IDA)

2.1 General

The input data arrays contain the input data required for a <u>particular</u> simulation. Four major imput data arrays are available: climatologic soil, chemistry, geometric and application specific arrays. The array name, and the parameters (in FORTRAN code and their units) in each space of the arrays are given in the following sections.

2.2 Climatologic IDA Arrays

The climatological input data arrays are schematically presented in the next page (Figure DF-2) and are descirbed below:

CLIMA1(6) -- annual climatic parameters of the region

Each line of the array contains one year of data for the following 6 parameters:

1. Latitude; (L;°N)

2. Average annual soil surface temperature; (T;°C)

3. Average annual fraction of sky covered by clouds; (NN;-)

4. Average annual relative humidity (fractional); (S;-)

5. Average annual shortwave albedo of the surface; (A;-)

6. Average daily evapotranspiration; (REP;cm/day)

CLIMA2(6) -- annual storm parameters of the region

Each line contains one year's data of six storm-related parameters of the region:

1. Mean annual precipitation; (MPA;cm)

2. Mean annual storm duration; (MTR;days)

3. Mean number of storms per year; (MN;-)

4. Mean length of rainy season within a year (MT;days)

5. Empty space in array (no data)

6. Empty space in array (no data)

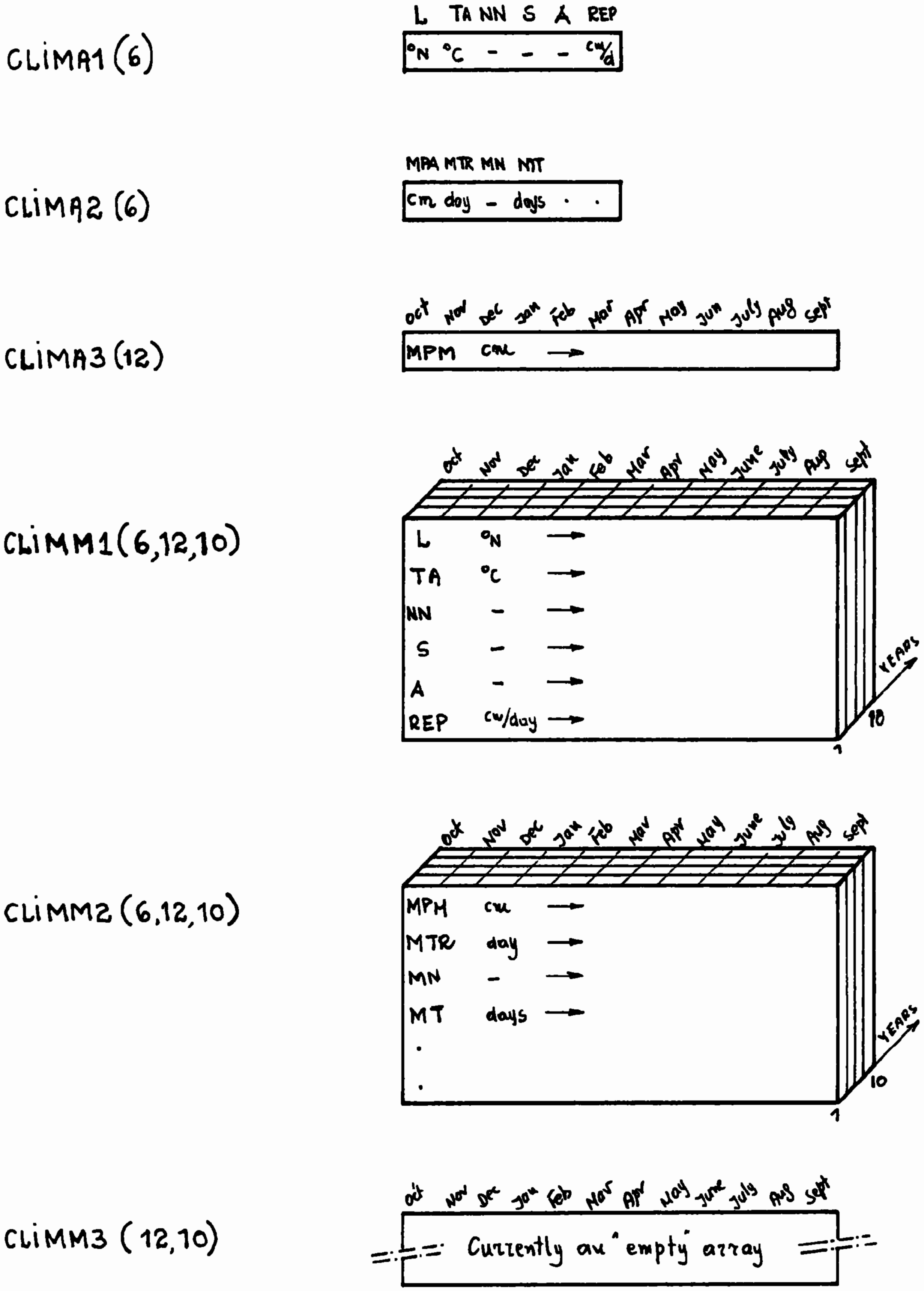

FIGURE DF-2 -- CLIMATOLOGICAL INPUT DATA ARRAYS (IDA)

CLIMA3(12) -- monthly storm depths (Oct-Sep)

This array contains one year's data of the monthly distribution of storm depths (MPM:cm) in the area, starting with the month of October (hydrologic year).

Note: Information contained in this array is not currently used by the program (see discussion of CLIMM1 and CLIMM2). The array was built into the code for a previous model version and is maintained for potential future use.

CLIMM1(6,12,10) -- monthly climatic parameters

Each block 6x12 of the 6x12x10 array contains one year of climatic parameters of a region. Ten years of data may be stored in total (IYR=1,10).

Each line of the 6x10 block contains 12 values of a particular parameter for the 12 months of the hydrologic year (Oct-Sep;IMO=1,12). These parameters are:

CLIMM1(1,1 ,IYR): (L;°N)

CLIMM1(2,IMO,IYR): surface temperature; (T;°C)

CLIMM1(3,IMO,IYR): fraction of sky covered by clouds; (NN;-)

CLIMM1(4,IMO,IYR): relative humidity (fractional); (S;-)

CLIMM1(5,IMO,IYR): shortwave albedo; (A;-)

CLIMM1(6,IMO,IYR): daily evapotranspiration rate; (REP;cm/day)

CLIMM2(6,12,10) -- monthly storm parameters of a region

Each 6x12 block of the 6x12x10 array contains one year of storm-related parameters of the region. Ten years of data may be stored in total (IYR=1,10).

Each line contains the values of a particular parameter for the twelve months of the hydrologic year (Oct-Sep;IMO=1,12). The parameters are:

CLIMM2(1,IMO,IYR): mean monthly precipitation; (MPM;cm)

CLIMM2(2,IMO,IYR): mean storm duration; (MTR;days)

CLIMM2(3,IMO,IYR): number of storms per month; (MN;-)

CLIMM2(4,IMO,IYR): mean length of rainy period within the month; (MT;days)

CLIMM2(5,IMO,IYR): empty space in array

CLIMM2(6,IMO,IYR): empty space in array

CLIMM3(12,10) -- currently an empty array

2.3 Soil IDA Arrays

The soil input data arrays are schematically presented on the next page (Figure DF-3). They are:

SOIL1(6) -- basic regional soil parameters

This array contains the following six basic soil parameters:

1. Soil density; (RS;g/cm^3)
2. Intrinsic average (depth) soil permeability; (Kl;cm^2)
3. Soil pore disconnectedness index; (c;-)
4. Effective soil porosity; (N;cm^3/cm^3)
5. Organic carbon content of the soil; (oc;%), and
6. Carbon content of the soil; (cc;%).

SOIL2(6) -- other soil related parameters

This array contains additional soil parameters of site specific simulations.

1. Soil cation exchange capacity; (CEC;m.e./100g dry w.t. soil)
2. Intrinsic soil permeability of upper soil layer; (KIU;cm^2)
3. Intrinsic soil permeability of middle soil layer; (KIM:cm^2)
4. Intrinsic soil permeability of lower soil layer; (KIL:cm^2)
5. Empty space for future use
6. Empty space for future use

SOIL1 (6)

RS	K1	C	N	OC	CC
1	2	3	4	5	6
g/cm^3	cm^2	-	cm^3/cm^3	%	%

SOIL2 (6)

CEC	K1U	K1M	K1L		
1	2	3	4	.	.
$\frac{me}{100 g s}$	cm^2	cm^2	cm^2		

CHEM1 (18)

SL	KOC	DA	KDE	H	K	MWT	VAL	KNH	KBH	KAH		SK	B	MWTLIG			
1	2	3	4	5	6	7	8	9	10	11	.	13	14	15	.	.	.
ug/mL	$\frac{ug/g\,c}{ug/mL}$	cm^2/s	day^{-1}	$\frac{m^3 \cdot atm}{°K \cdot mol}$	$\frac{ug/g\,sol}{ug/mL}$	g/mol	-	day^{-1}	L/mol·day	L/mol·day	.	-	-	g/mol	.	.	.

NUT1 (6)

empty array

GEOM (20)

AR	Z	DU	DM	DL	A2KDE	A2OC	A2CC	AKDE	AOC	ACC	ISRA	ASL	FRN	PH	A2PH	APH	A2CEC	ACEC	
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	.
cm^2	cm	cm	cm	cm	-	-	-	-	-	-	-	-	-	-	-	-	-	-	.

FIGURE DF-3 -- SOIL, CHEMISTRY, GEOMETRIC INPUT DATA ARRAYS (IDA)

2.4 Chemistry IDA Arrays

The chemistry arrays (Figure DF-3) are:

CHEM1(18) -- chemical specific parameters

This array contains 14 basic parameters of a compound, and has 4 empty spaces. These parameters are:

1. Solubility of the compound; (SL;ug/mL or mg/L)
2. Adsorption coefficient of the compound based on organic carbon; (KOC;(ug/g oc)/(ug/mL))
3. Diffusion coefficient of pollutant in air; (DA;cm^2/s)
4. Degradation rate in the upper unsaturated soil zone; (KDE;day^{-1})
5. Henry's Law Constant of the compound; (H;$m^3\cdot atm/mol$)
6. Overall adsorption coefficient of compound on soil; (K;(ug/g soil)/(ug/mL))
7. Molecular weight of compound; (MWT;g/mol)
8. Valence of compound; (VAL;-)
9. Neutral hydrolysis constant (KNH;day^{-1})
10. Base hydrolysis constant (KBH;L/(mol·day))
11. Acid hydrolysis constant (KAH;L/(mol·day))
12. Empty space
13. Stability constant of compound-ligand complex; (SK;-)
14. Number of moles of ligand per mole of compound complexed (B;-)
15. Molecular weight of ligand; (MWTLIG;g/mol)
16. Empty space
17. Empty space
18. Empty space

NUT1(6)-- nutrient cycle parameters.

The array can contain up to 6 parameters relating to the nutrient cycle. This array is presently empty, since the nutrient cycle routine is not operational

2.5 Geometric IDA Arrays

The geometric array (Figure DF-3) is:

GEOM(20) -- application related geometric parameters

The array contains 17 parameters of the application geometry and 3 empty spaces. The number of parameters input depends upon the level of operation. The 17 parameters are:

1. Area of the compartment for all levels; (AR;cm^2)
2. Depth to groundwater for all levels; (Z;m)
3. Depth of the upper soil zone for all levels; (DU;cm)
4. Depth of the middle soil zone for level 3 (DM;cm)
5. Depth of the lower soil zone for all levels; (DL;cm)
6. Ratio of biodegradation, middle/upper soil zone; (A2KDE;-) for level 3
7. Ratio of organic carbon content, middle/upper soil zone (A2OC;-) for level 3
8. Ratio of clay content, middle/upper soil zone (A2CC;-) for level 3
9. Ratio of biodegradation, lower/upper soil zone for all levels (AKDE;-)
10. Ratio of organic carbon content, lower/upper soil zone for all levels; (AOC;-)
11. Ratio of clay content, lower/upper soil zone for all levels; (ACC;-)
12. Index of pollutant participation in surface runoff for levels 0 and 1; (ISRA:-)
13. Ratio of concentration of pollutant in rainfall to maximum solubility for levels 0 and 1; (ASL;-)

14. Freundich coefficient for levels 2 and 3; (FRN;-)

15. pH in upper soil zone for all levels; (PH;-)

16. Ratio of pH middle/upper for level 3; (A2PH;-)

17. Ratio of pH, lower/upper for all levels; (APH;-)

18. Ratio of CEC, middle/upper for level 3; (A2CEC;-)

19. Ratio of CEC, lower/upper for all levels; (ACEC;m-)

20. Empty space

2.6 Application Specific IDA Arrays

The application specific arrays (Figure DF-4) are:

RUNLO(6) -- LEVELO parameters

The array contains values of 4 parameters required to run LEVELO. It also has 2 empty spaces. The 4 parameters are:

1. Soil moisture; (THA;-)

2. Infiltration; (IA ;cm)

3. Groundwater runoff; (RGA;cm)

4. Surface runoff; (RSA;cm)

5. Empty space

6. Empty space

LOAD(6) -- LEVELO and LEVEL1 pollutant loadings to compartment

The array contains 4 loading parameters and 2 empty spaces:

1. The total loading in the upper zone; (POLINU;ug/cm^2)

2. The total loading in the lower zone (POLINL;ug/cm^2)

3. The total ligand mass input to the upper zone; (LIGU;ug/cm^2)

4. The total ligand mass input to the lower zone; (LIGL;ug/cm^2)

5. Empty space

6. Empty space

LOAD (6)

POLINU	POLINL	LIGU	LI GL		
1	2	3	4	.	.
ug/cm^2	ug/cm^2	ug/cm^2	ug/cm^2		.

RUNLO (6)

THA	INF	RGA	RSA		
1	2	3	4	.	.
1	cm	cm	cm	.	.

RUNM1 (10,12)

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	June	July	Aug	Sept
1	CUM			ug/mL			→					
2	CMM			ug/mL			→					
3	CLM			ug/mL			→					
4	POLINU			ug/cm^2			→					
5	POLINM			ug/cm^2			→					
6	POLINL			ug/cm^2			→					
7	ISRM			-								
10	. .			.								

RUNM2 (10,12)

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	June	July	Aug	Sept
1	CPM			ug/mL			→					
2	TRANSU			ug/cm^2			→					
3	TRANSM			ug/cm^2			→					
4	TRANS L			ug/cm^2			→					
5	SINKU			ug/cm^2			→					
6	SINKM			ug/cm^2			→					
7	SINKL			ug/cm^2			→					
8	LIGU			g/cm^2			→					
9	LIGM			g/cm^2			→					
10	LIGL			g/cm^2			→					

TITLES (5,12)

1	REGIONAL TITLE
2	SOIL TITLE
3	COMPOUND TITLE
4	NUTRIENT TITLE
5	APPLICATION AREA TITLE

FIGURE DF-4 -- APPLICATION SPECIFIC INPUT DATA ARRAYS (IDA)

RUNM1(10,12) -- LEVEL2 and LEVEL3 loading parameters

The array contains values of 7 monthly parameters for above levels of operation. The columns represent months from October to September. The content of the lines is:

1. Concentration of pollutant in the upper zone soil moisture; (CUM;ug/mL)
2. Concentration of pollutant in the middle zone soil moisture; (CMM;ug/mL)
3. Concentration of the pollutant in the lower zone soil moisture; (CLM;ug/mL)
4. Monthly loading in the upper soil zone; (POLINU;ug/cm^2)
5. Monthly loading in the middle soil zone; (POLINM;ug/cm^2)
6. Monthly loading in the lower soil zone (POLINL;ug/cm^2)
7. Multiplier for pollutant in surface runoff by month; (ISRM;-)
8. Empty spaces
9. Empty spaces
10. Empty spaces

RUNM2(10,12) -- LEVEL2 and LEVEL3 pollutant parameters

The array contains 7 monthly pollutant parameters for above levels. The columns represent the months, from October to September. The lines contain:

1. Concentration of pollutant as fraction of solubility in the rainfall; (ASL;ug/mL)
2. Rate of pollutant transformation in the upper zone; (TRANSU;ug/cm^2)
3. Rate of pollutant transformation in the middle zone; (TRANSM;ug/cm^2)
4. Rate of pollutant transformation in the lower zone; (TRANSL;ug/cm^2)
5. Pollutant loss (by processes of source/sink) in the upper zone (SINKU;ug/cm^2)
6. Pollutant loss (by processes of source/sink) in the middle zone (SINKM;ug/cm^2)
7. Pollutant loss (by processes of source/sink) in the lower zone (SINKL;ug/cm^2)
8. Ligand mass input to the upper zone; (LIGU;ug/cm^2)

9. Ligand mass input to middle zone; (LIGM,ug/cm^2)

10. Ligand mass input to lower zone; (LIGL;ug/cm^2)

TITLES(5,12A4) -- titles of the particular simulation

This alphanumeric array contains all titles of a SESOIL.

1. Line 1 contains the regional title
2. Line 2 contains the soil title
3. Line 3 contains the compound title
4. Line 4 contains the nutrient cycle title, and
5. Line 5 contains the application area title

3.0 OPERATIONAL/RETRIEVAL ARRAYS (ORA)

The overall use of the operational/retrieval (ORA) arrays has been discussed in section 1.0 (Figure DF-1). Important operational arrays are present in the figures on the next page (Figure DF-5a,b). The parameters, the symbols in FORTRAN and the units of each array are presented below.

HYDBAL(13,10) -- hydrologic cycle array

This array is used to store and transfer results of the hydrologic cycle routine. The first 12 lines contain data for the months of the hydrologic year (Oct-Sep). The last line contains the total or the average over the year. The columns contain:

1. Moisture content; (THA; fractional)
2. Monthly precipitation; (MPM;cm)
3. Monthly infiltration; (IM;cm)
4. Monthly evapotranspiration; (REP;cm/day)
5. Monthly surface runoff; (RSM;cm)
6. Monthly groundwater recharge; (RGM;cm)
7. Convergence function; (GZ;-)
8. Empty spaces
9. Empty spaces
10. Empty spaces

PINP(13,6) -- pollutant input parameters array

This array is used to store the pollutant input masses calculated for each month of the monthly simulations (levels 2 and 3). The first 12 lines contain data for the months of the hydrologic year (Oct-Sep). The last line contains the total inputs for the year. The columns contain:

1. Pollutant input mass via rainfall; (PINFU;ug/cm^2)
2. Pollutant mass input directly to the upper zone; (POLINU;ug/cm^2)
3. Pollutant mass input directly to the lower zone; (POLINL;ug/cm^2)
4. Pollutant mass input directly to the middle zone; (POLINM;ug/cm^2)
5. Empty (spaces)
6. Total pollutant input mass for soil column; (PIN;ug/cm^2)

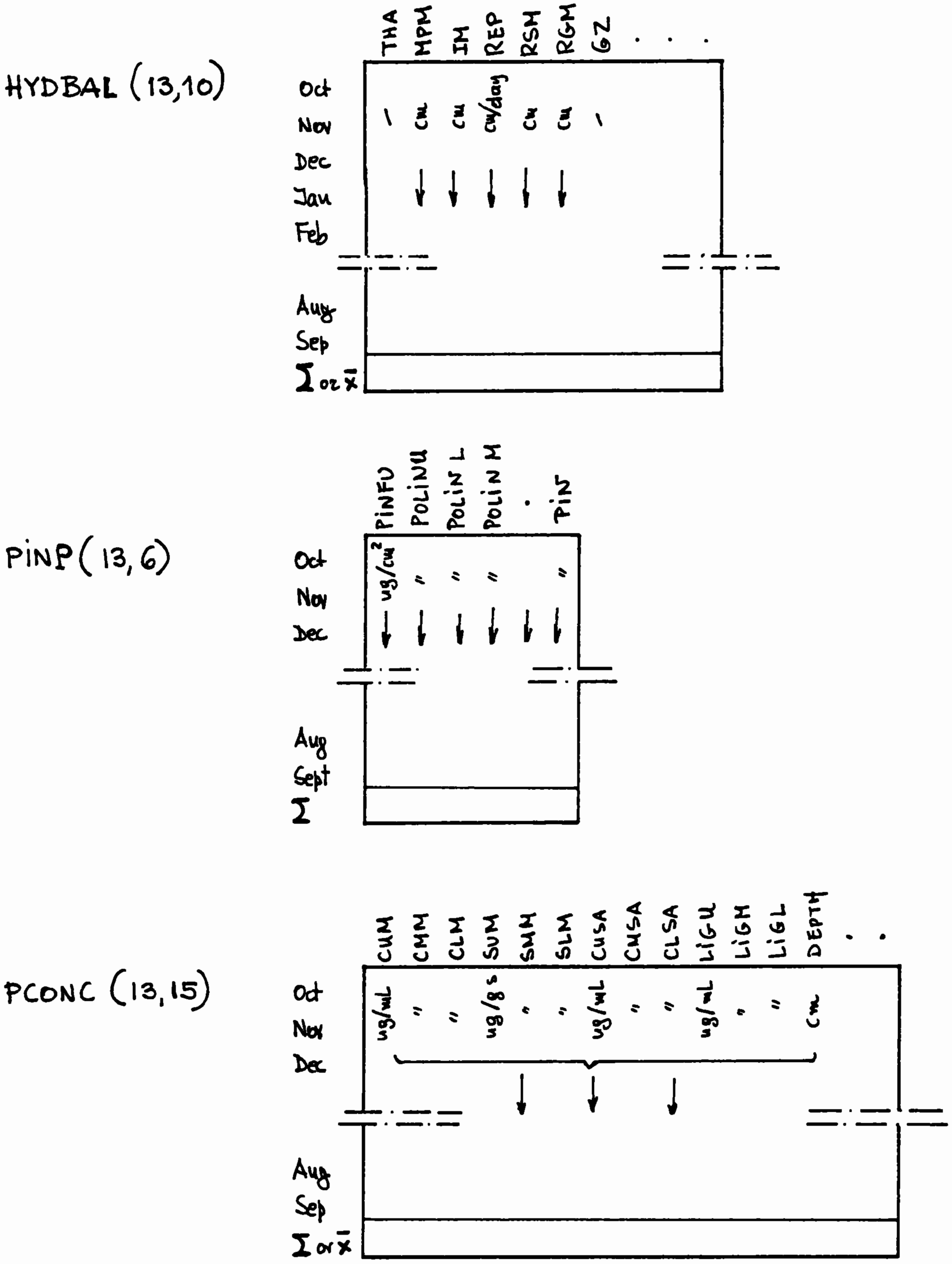

FIGURE DF-5a) -- OPERATIONAL/RETRIEVAL ARRAYS (ORA)

POLBAL (13,35)

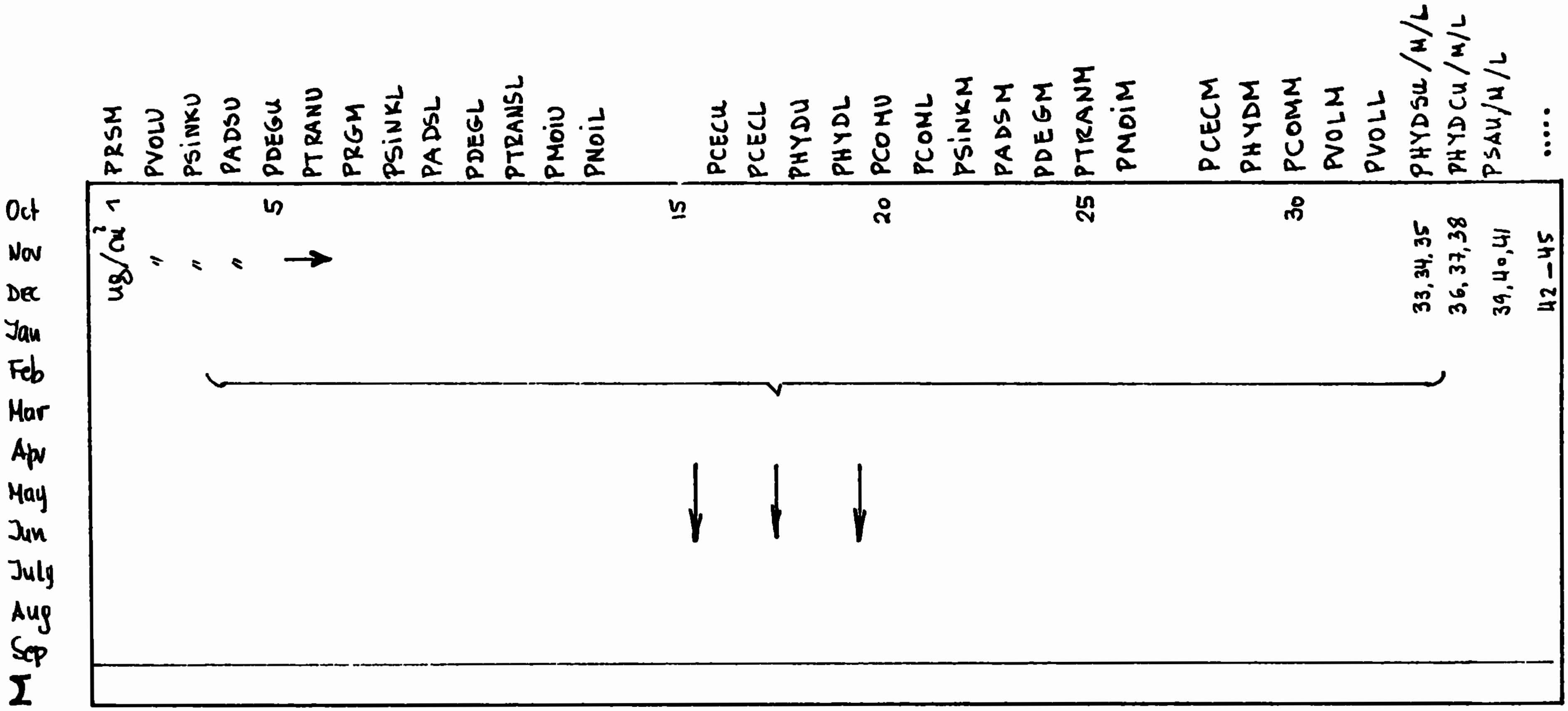

FIGURE DF-5b) -- OPERATIONAL/RETRIEVAL ARRAYS (ORA)

PCONC(13,15) -- pollutant concentrations array

This array is used to store the pollutant concentrations in the various media (air, soil, soil moisture) for each month of the monthly simulation (levels 2 and 3). The first 12 lines contain data for the months of the hydrologic year (Oct-Sep). The last line contains the total inputs for the year. The columns contain:

1. Pollutant concentration in the upper zone soil moisture; (CUM;ug/mL)
2. Pollutant concentration in the middle zone soil moisture; (CMM;ug/mL)
3. Pollutant concentration in the lower zone soil moisture; (CLM;ug/mL)
4. Pollutant concentration on the soil in the upper zone; (SUM;ug/g)
5. Pollutant concentration on the soil in the middle zone; (SMM;ug/g)
6. Pollutant concentration on the soil in the lower zone (SLM;ug/g)
7. Pollutant concentration in the soil air of the upper soil zone; (CUSA;ug/mL)
8. Pollutant concentration in the soil air of the middle soil zone; (CMSA;ug/mL)
9. Pollutant concentration in the soil air of the lower soil zone; (CLSA;ug/mL)
10. Free Ligand concentration in the soil moisture of the upper zone; (LIGCUF;ug/mL)
11. Free Ligand concentration in the soil moisture of the middle zone; (LIGCMF;ug/mL)
12. Free Ligand concentration in the soil moisture of the lower zone; (LIGCLF;ug/mL)
13. Depth of rainfall "front"; (DPTH;cm)
14. Empty column
15. Empty column

POLBAL(13,45) -- pollutant mass array

This array is used to store the pollutant masses involved in the individual fate processes for each month of the monthly simulation for levels 2 and 3. The first 12 lines contain data for the months of the hydrologic year (Oct-Sep). The last line contains the total or the remaining mass at the end of the year. The columns contain:

1. Pollutant mass in surface runoff; (PRSM;ug)
2. Pollutant mass volatilized from upper zone (PVOLU;ug)
3. Pollutant mass in other sinks from upper zone; (PSINKU;ug)
4. Pollutant mass adsorbed in upper zone (PADSU;ug)
5. Pollutant mass degraded in upper zone (PDEGU;ug)
6. Pollutant mass transformed in upper zone; (PTRANU;ug)
7. Pollutant mass released to groundwater; (PRGM;ug)
8. Pollutant mass in other sinks from lower zone; (PSINKL;ug)
9. Pollutant mass adsorbed in lower zone; (PADSL;ug)
10. Pollutant mass degraded in lower zone; (PDEGL;ug)
11. Pollutant mass transformed in lower zone; (PTRANSL;ug)
12. Pollutant mass dissolved in soil moisture in upper zone; (PMOIU;ug)
13. Pollutant mass dissolved in soil moisture in lower zone; (PMOIL;ug)
14. Empty space
15. Empty space
16. Pollutant mass cation exchanged in upper zone; (PCECU;ug)
17. Pollutant mass cation exchanged in lower zone; (PCECL;ug)
18. Pollutant mass hydrolyzed from moisture in upper zone; (PHYDMU;ug)
19. Pollutant mass hydrolyzed from moisture in lower zone; (PHYDML;ug)
20. Pollutant mass complexed in upper zone; (PCOMU;ug)

21. Pollutant mass complexed in middle zone; (PCOML;ug)

22. Pollutant mass in other sinks in middle zone; (PSINKM;ug)

23. Pollutant mass adsorbed in middle zone; (PADSM;ug)

24. Pollutant mass degraded in middle zone; (PDEGM;ug)

25. Pollutant mass transformed in middle zone; (PTRANM;ug)

26. Pollutant mass in moisture of middle zone; (PMOIM;ug)

27. Empty space

28. Pollutant mass cation exchanged in middle zone; (PCECM;ug)

29. Pollutant mass hydrolyzed from moisture in middle zone; (PHYDMM;ug)

30. Pollutant mass complexed in middle zone; (PCOMM;ug)

31. Pollutant mass volatilized from middle zone; (PVOLM;ug)

32. Pollutant mass volatilized from lower zone; (PVOLL;ug)

33. Pollutant mass hydrolyzed from upper soil layer; (PHYDSU;ug)

34. Pollutant mass hydrolyzed from middle soil layer; (PHYDSM;ug)

35. Pollutant mass hydrolyzed from lower soil layer; (PHYDSL;ug)

36. Pollutant mass hydrolyzed (upper) from cation exchanged pollutant; (PHYDCU;ug)

37. Pollutant mass hydrolyzed (middle) from cation exchanged pollutant; (PHYDCM;ug)

38. Pollutant mass hydrolyzed (lower) from cation exchanged pollutant; (PHYDCL;ug)

39. Pollutant mass in soil air of upper layer; (PSAU;ug)

40. Pollutant mass in soil air of middle layer; (PSAM;ug)

41. Pollutant mass in soil air of lower layer; (PSAL;ug)

42. Empty space

43 Empty space

44. Empty space

45. Empty space

FC - Fortran code

AP - applications

APPENDIX AP

APPLICATION SAMPLES

This section will contain abstracts and executive summaries of applications discussed in sections 2.0 and 3.0 of this documentation. Eg. see references Bonazountas et al (1981), Wagner & Bonazountas (1982) in section 3.0.

A typical data base and typical input/output model results are presented in the following pages for all levels 0, 1, 2 and 3.

```
************************************************************************************************************************

RUN :  1                   ****** LEVEL0 SESOIL MODEL OPERATION ******
                                  NON-SITE SPECIFIC FATE ASSESMENT



     *******************************************************************************************************************
     *****                                                                                                         *****
     ***** SESOIL-81:    SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS                   *****
     *****                                                                                                         *****
     ***** DEVELOPERS:   M. BONAZOUNTAS,ARTHUR D. LITTLE INC.   ,(617)864-5770,X5871                               *****
     *****               J. WAGNER      ,ARTHUR D. LITTLE INC.   ,(617)864-5770,X2585                               *****
     *****                                                                                                         *****
     ***** VERSION:      DECEMBER 1981                                                                             *****
     *****                                                                                                         *****
     *****                                                                                                         *****
     *******************************************************************************************************************

                       INDEX
          REGION    : (     1)     CLINTON,     MA. (SUB-HUMID):
          SOIL TYPE : (     5)     CLAY-LOAM GENERIC
          COMPOUND  : (    15)     TEST CHEM
          APPL.AREA : (     1)     CLINTON,     MA. (SUB-HUMID):


          SIMULATION INPUT PARAMETERS
          ===========================



      -- APPLICATION PARAMETERS --

  AREA(SQ.CM.): 1.0
  DEPTH TO GRW(M): .10E+03
  UPPER SOIL ZONE DEPTH(CM): 15.
  PH UPPER ZONE(-): 7.0
  PH RATIO LOWER:UPPER ZONE (-): 1.0

  TEMPERATURE(DEG. C): 8.4

  DEGRADATION RATIO LOWER:UPPER ZONE(-): .50
  ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-): .50
  CLAY CONTENT RATIO LOWER:UPPER ZONE(-): .50
  POLLUTANT RUNOFF MULTIPLIER: 1.0
  LEACHING (INPUT) RATE(FRAC. OF SOLUBILITY): .10E-02
  CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): .0

  POLLUTANT INPUT MASS-UPPER ZONE(UG/SQ.CM): .20E+03
  POLLUTANT INPUT MASS-LOWER ZONE(UG/SQ.CM): .10E+04
  LIGAND INPUT MASS-UPPER ZONE(UG/SQ.CM): .10E+04
  LIGAND INPUT MASS-LOWER ZONE(UG/SQ.CM): .20E+04
```

```
     -- HYDROLOGIC PARAMETERS --

SOIL MOISTURE(%): 26.
INFILTRATION(CM): 61.
GRW RECHARGE(CM): 26.
SURFACE RUNOFF(CM): 34.

      -- CHEMICAL PARAMETERS --

SOLUBILITY(UG/ML): .11E+04
ADSORP. COEF.(KOC): .36E+03
DIF. COEF. IN AIR(SQ.CM/SEC): .83E-05
DEGRADATION RATE(/DAY): .20
HENRYS CON.(CU.M-ATM/MOLE): .94E-02
ADSORP. COEF. ON SOIL(K): .0
MOLECULAR WT.(G/MOL): 5.0
VALENCE(-): 2.0
NEUTRAL HYDROLYSIS CONSTANT(/DAY): .70E-05
BASE HYDROLYSIS CONSTANT(L/MOL-DAY): 8.0
ACID HYDROLYSIS CONSTANT(L/MOL-DAY): 0.0
LIGAND-POLLUTANT STABILITY CONST.(-): .10E+06
NO. MOLES LIGAND/MOLE POLLUTANT(-): 2.0
LIGAND MOLECULAR WEIGHT(G/MOLE): 10.

      -- SOIL PARAMETERS --

SOIL DENSITY(G/CU.CM): 1.3
I.I. PERMEABILITY(SQ. CM): .20E-09
DISCONNECTEDNESS INDEX(-): 10.
POROSITY(-): .35
ORGANIC CARBON CONTENT(%): 1.3
CLAY CARBON CONTENT(%): .20E-01
CATION EXCHANGE COEF. (MILLI EQ./100G DRY SOIL): .0
INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM) .0
INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM) .0
INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM) .0
```

```
        SIMULATION OUTPUT
        =================


        -- POLLUTANT INPUT TO SOIL COLUMN --


     POLLUTANT INPUT W/ RAIN     66.8       UG
     DIRECT POLLUTANT INPUT:U   200.        UG
     DIRECT POLLUTANT INPUT:L   .100E+04    UG

     TOTAL POLLUTANT INPUT      .127E+04    UG


        -- POLLUTANT FATE ASSESSMENT IN SOIL COLUMN--



     UPPER SOIL ZONE DISTRIBUTION (MASS):          % OF TOTAL INPUT

     VOLATILIZED                 1.44       UG            0.11 %
     IN SOIL MOISTURE            2.33       UG            0.18 %
     ADSORBED ON SOIL            55.9       UG            4.35 %
     IMMOBILIZED-CATION EX.      .0         UG            0.0  %
     COMPLEXED                   .157E-03   UG            0.00 %
     IN SOIL AIR                 .344       UG            0.03 %
     IN SURFACE RUNOFF           20.5       UG            1.59 %
     HYDROLYZED-FROM MOI.        .733E-02   UG            0.00 %
     HYDROLYZED-FROM SOIL        .179       UG            0.01 %
     HYDROLYZED-FROM CEC         .0         UG            0.0  %
     DEGRADED                    170.       UG           13.20 %

     LOWER SOIL ZONE DISTRIBUTION (MASS):

     IN SOIL MOISTURE            20.9       UG            1.62 %
     ADSORBED ON SOIL            251.       UG           19.47 %
     IMMOBILIZED-CATION EX.      .0         UG            0.0  %
     COMPLEXED                   .127E-07   UG            0.00 %
     IN SOIL AIR                 3.09       UG            0.24 %
     HYDROLYZED-FROM MOI.        .562E-01   UG            0.01 %
     HYDROLYZED-FROM SOIL        .796       UG            0.06 %
     HYDROLYZED-FROM CEC         .0         UG            0.0  %
     DEGRADED                    761.       UG           59.13 %
     TO GROUNDWATER              .0         UG            0.0  %
```

```
UPPER SOIL ZONE DISTRIBUTION (CONCENTRATIONS):

IN SOIL MOISTURE            .6038      UG/ML
ADSORBED ON SOIL            2.826      UG/G
IN SOIL AIR                 .2468      UG/ML



LOWER SOIL ZONE DISTRIBUTION (CONCENTRATIONS):

IN SOIL MOISTURE            .8127E-02 UG/ML
ADSORBED ON SOIL            .1902E-01 UG/G
IN SOIL AIR                 .3322E-02 UG/ML


MAX. DEPTH OF POLLUTANT     483.       CM


************************************EXECUTION COMPLETED************************************
```

```
********************************************************************************

RUN :  2                 ****** LEVEL1 SESOIL MODEL OPERATION ******
                              SITE SPECIFIC ANNUAL FATE ASSESSMENT



   ******************************************************************************
   *****                                                                    *****
   *****  SESOIL-81:   SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS   *****
   *****                                                                    *****
   *****  DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.  ,(617)864-5770,X5871  *****
   *****               J. WAGNER     ,ARTHUR D. LITTLE INC.  ,(617)864-5770,X2585  *****
   *****                                                                    *****
   *****  VERSION:     DECEMBER 1981                                        *****
   *****                                                                    *****
   *****                                                                    *****
   ******************************************************************************

                 INDEX
       REGION    : (     1)     CLINTON,     MA. (SUB-HUMID):
       SOIL TYPE : (     5)     CLAY-LOAM GENERIC
       COMPOUND  : (    15)     TEST CHEM
       APPL. AREA: (     1)     CLINTON,     MA. (SUB-HUMID):


       SIMULATION INPUT PARAMETERS
       ===========================



    -- APPLICATION PARAMETERS --

AREA(SQ.CM.): 1.0
DEPTH TO GRW(M): .10E+03
UPPER SOIL ZONE DEPTH(CM): 15.
PH UPPER ZONE(-): 7.0
PH RATIO LOWER:UPPER ZONE(-): 1.0
DEGRADATION RATIO LOWER:UPPER ZONE(-): .50
ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-): .50
CLAY CONTENT RATIO LOWER:UPPER ZONE(-): .50
POLLUTANT RUNOFF MULTIPLIER: 1.0
LEACHING (INPUT) RATE(FRAC. OF SOLUBILITY): .10E-02
CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): .0

POLLUTANT INPUT MASS-UPPER ZONE(UG/SQ. CM): .20E+03
POLLUTANT INPUT MASS-LOWER ZONE(UG/SQ. CM): .10E+04
LIGAND INPUT MASS-UPPER ZONE(UG/SQ. CM): .10E+04
LIGAND INPUT MASS-LOWER ZONE(UG/SQ. CM).20E+04
```

```
UPPER SOIL ZONE DISTRIBUTION (CONCENTRATIONS):

IN SOIL MOISTURE            .6039      UG/ML
ADSORBED ON SOIL            2.626      UG/G
IN SOIL AIR                 .2459      UG/ML



LOWER SOIL ZONE DISTRIBUTION (CONCENTRATIONS):

IN SOIL MOISTURE            .8129E-02 UG/ML
ADSORBED ON SOIL            .1002E-01 UG/G
IN SOIL AIR                 .3323E-02 UG/ML


MAX. DEPTH OF POLLUTANT   463.      CM


****************************************EXECUTION COMPLETED****************************************
```

```
      -- CLIMATIC PARAMETERS --

LATITUDE(DEC. DEG): 43.
TEMPERATURE(DEG C): 8.4
CLOUD COVER(FRAC.): .35
REL. HUMIDITY(FRAC.): .70
SHORTWAVE ALBEDO(-): .30
EVAPOTRANSPIRATION(CM/DAY): .0

ANNUAL PRECIPITATION(CM): 74.
MEAN TIME OF RAIN(DAYS): .32
MEAN NUMBER OF STORM EVENTS(-): .11E+03
MEAN LENGTH OF RAINY SEASON(DAYS): .37E+03


      -- CHEMICAL PARAMETERS --

SOLUBILITY(UG/ML): .11E+0.
ADSORP. COEF.(KOC): .36E+03
DIF. COEF. IN AIR(SQ.CM./SEC): .83E-05
DEGRADATION RATE(/DAY): .20
HENRYS CON.(CU.M-ATM/MOLE): .94E-02
ADSORP. COEF. ON SOIL(K): .0
MOLECULAR WT.(G/MOL): 0.0
VALENCE(-): 2.0
NEUTRAL HYDROLYSIS CONSTANT(/DAY): .70E-05
BASE HYDROLYSIS CONSTANT(L/MOL-DAY): 8.0
ACID HYDROLYSIS CONSTANT(L/MOL-DAY): 0.0
LIGAND-POLLUTANT STABILITY CONST.(-): .10E+06
NO. MOLES LIGAND/MOLE POLLUTANT(-): 2.0
LIGAND MOLECULAR WEIGHT(G/MOLE): 10.


      -- SOIL PARAMETERS --

SOIL DENSITY(G/CU.CM): 1.5
INT. PERMEABILITY(SQ. CM.):  .28E-09
DISCONNECTEDNESS INDEX(-): 10.
POROSITY(-): .35
ORGANIC CARBON CONTENT(%): 1.3
CLAY CARBON CONTENT(%): .20E-01
CATION EXCHANGE COEF. (MILLI EQ./100G DRY SOIL): .0
INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM) .0
INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM) .0
INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM) .0
```

```
         SIMULATION OUTPUT
         =================



         -- ANNUAL HYDROLOGIC CYCLE PARAMETERS --


  SOIL MOISTURE CONTENT(THA)      25.7       %
  PRECIPITATION(PA)               94.5     CM/YR
  NET INFILTRATION(IA)            60.7     CM/YR
  EVAPOTRANSPIRATION(ETA)         34.5     CM/YR
  SURFACE RUNOFF(RSA)             33.9     CM/YR
  GROUNDWATER RUNOFF(RGA)         26.2     CM/YR
  YIELD (YA)                      60.0     CM/YR

  RATIO PA/MPA (-)                1.00



         -- POLLUTANT INPUT TO SOIL COLUMN --


     POLLUTANT INPUT W/ RAIN   66.7      UG
     DIRECT POLLUTANT INPUT:U  200.      UG
     DIRECT POLLUTANT INPUT:L  .100E+04  UG

     TOTAL POLLUTANT INPUT     .127E+04  UG
```

```
       -- POLLUTANT FATE ASSESSMENT IN SOIL COLUMN--


    UPPER SOIL ZONE DISTRIBUTION (MASS):         % OF TOTAL INPUT

    VOLATILIZED                    1.45      UG            0.11 %
    IN SOIL MOISTURE               2.33      UG            0.18 %
    ADSORBED ON SOIL               56.0      UG            4.35 %
    IMMOBILIZED-CATION EX.         .0        UG            0.0  %
    COMPLEXED                      .157E-03  UG            0.00 %
    IN SOIL AIR                    .343      UG            0.03 %
    IN SURFACE RUNOFF              20.5      UG            1.59 %
    HYDROLYZED-FROM MOI.           .739E-02  UG            0.00 %
    HYDROLYZED-FROM SOIL           .173      UG            0.01 %
    HYDROLYZED-FROM CEC            .0        UG            0.0  %
    DEGRADED                       170.      UG           13.20 %

    LOWER SOIL ZONE DISTRIBUTION (MASS):

    IN SOIL MOISTURE               20.9      UG            1.62 %
    ADSORBED ON SOIL               251.      UG           19.48 %
    IMMOBILIZED-CATION EX.         .0        UG            0.0  %
    COMPLEXED                      .127E-07  UG            0.00 %
    IN SOIL AIR                    3.09      UG            0.24 %
    HYDROLYZED-FROM MOI.           .662E-01  UG            0.01 %
    HYDROLYZED-FROM SOIL           .796      UG            0.06 %
    HYDROLYZED-FROM CEC            .0        UG            0.0  %
    DEGRADED                       761.      UG           59.13 %
    TO GROUNDWATER                 .0        UG            0.0  %
```

```
***************************************************************************************************************

RUN :   3                    ****** LEVEL2 SESOIL MODEL OPERATION ******
                                   MONTHLY SITE SPECIFIC SIMULATION


     ************************************************************************************************************
     *****                                                                                                  *****
     ***** SESOIL-81:    SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS           *****
     *****                                                                                                  *****
     ***** DEVELOPERS:   M. BONAZOUNTAS,ARTHUR D. LITTLE INC.   ,(617)864-5770,X5871                       *****
     *****               J. WAGNER      ,ARTHUR D. LITTLE INC.   ,(617)864-5770,X2585                       *****
     *****                                                                                                  *****
     ***** VERSION:      DECEMBER 1981                                                                      *****
     *****                                                                                                  *****
     *****                                                                                                  *****
     ************************************************************************************************************

                     INDEX
          REGION    : (    4)     CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)
          SOIL TYPE : (    5)     CLAY-LOAM GENERIC
          COMPOUND  : (   15)     TEST CHEM
          APPL. AREA: (    2)     TEST RUN (CLINTON, MA. 40 YEARS)



          GENERAL INPUT PARAMETERS
          ========================


       -- APPLICATION PARAMETERS --

AREA(SQ.CM.): 1.0
DEPTH TO GRW(M): .10E+03
UPPER ZONE DEPTH(CM): 15.
PH UPPER ZONE(-): 5.0
PH RATIO LOWER:UPPER ZONE(-): .88
DEGRADATION RATIO LOWER:UPPER ZONE(-): 1.1
ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-): 1.2
CLAY CONTENT RATIO LOWER:UPPER ZONE(-): 1.3
CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): .10E-02
FREUNDLICH EXPONENT(-): 1.4
```

```
      -- CHEMICAL PARAMETERS --

 SOLUBILITY(UG/ML): .11E+04
 ADSORP. COEF.(KOC): .36E+03
 DIF. COEF. IN AIR(SQ.CM./SEC): .50E-05
 DEGRADATION RATE(/DAY): .20
 HENRYS CON.(CU.M-ATM/MOLE): .94E-02
 ADSORP. COEF. ON SOIL(K): .0
 MOLECULAR  WT.(G/MOL): 0.0
 VALENCE(-): 2.0
 NEUTRAL  HYDROLYSIS CONSTANT(/DAY): .70E-05
 BASE HYDROLYSIS CONSTANT(L/MOL-DAY): 3.0
 ACID HYDROLYSIS CONSTANT(L/MOL-DAY): 9.0
 LIGAND-POLLUTANT STABILITY CONST.(-): .10E+06
 NO. MOLES LIGAND/MOLE POLLUTANT(-): 2.0
 LIGAND MOLECULAR WEIGHT(G/MOL): 10.

      -- SOIL PARAMETERS --

 SOIL DENSITY(G/CU.CM): 1.3
 INT. PERMEABILITY(SQ. CM.):  .28E-09
 DISCONNECTEDNESS INDEX(-): 10.
 POROSITY(-): .35
 ORGANIC CARBON CONTENT(%): 1.0
 CLAY CARBON CONTENT(%): .20E-01
 CATION EXCHANGE COEF. (MILLI EQ./100G DRY SOIL): .0
 INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM) .0
 INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM) .0
 INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM) .0
```

```
                              YEAR-  1     MONTHLY INPUT PARAMETERS
                              ========     ========================


                         OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP


     -- CLIMATIC PARAMETERS --

LATITUDE(DEG)           42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5
TEMP.(DEG C)            8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40
CLOUD CVR(FRAC.)        .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320
REL. HUM.(FRAC.)        .700     .700     .700     .700     .700     .700     .700     .700     .700     .700     .700     .700
ALBEDO(-)               .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300
EVAPOT.(CM/DAY):        .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0

PRECIP.(CM):            7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84
M.TIME RAIN(DAYS):      .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320
M. STORM NO.(-):        9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08
M. SEASON(DAYS):        30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4



     -- RUN DATA-SET 1 --

MOIS. CONC-UP.(UG/ML)     .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
MOIS. CONC-LO.(UG/ML)     .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
POL. INP-U(UG/SQ CM)      200.      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
POL. INP-L(UG/SQ CM)      .100E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SUR. POL. MULTIPLIER      1.00      1.00      1.00      1.00      1.00      .0        .0        .0        .0        .0        .0        .0

     -- RUN DATA-SET 2 --

POL. IN RAIN(FRAC-SL)     .100E-02  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
TRANSFORMED-U(UG/SQ CM)   .200      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
TRANSFORMED-L(UG/SQ CM)   .330      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SINKS-U(UG/SQ CM)         .400      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SINKS-L(UG/SQ CM)         .500      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

LIG. INPUT-U(UG/SQ.CM)    .100E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
LIG. INPUT-L(UG/SQ.CM)    .200E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
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                         YEAR-  1     MONTHLY RESULTS(OUTPUT)
                         ========     ======================


      -- HYDROLOGIC CYCLE COMPONENTS --

                        OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

 SOIL MOISTURE( %)     25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8
 PRECIPATION(CM)       7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86
 NET INFILTR.(CM)      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02
 EVAPOTRANSP.(CM)      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72
 SURFACE RUNOFF(CM)    2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84
 GRW RUNOFF(CM)        2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30
 YIELD (CM)            5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14

 RATIO PA/MPA(GZ)      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00


      -- POLLUTANT MASS INPUT TO COLUMN(UG) --

                        OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

 PRECIPATION           5.52      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 OTHER(UPPER)          200.      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 OTHER(LOWER)          .100E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

 TOTAL INPUT           .121E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
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      -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) --

    UPPER SOIL ZONE:

 SURFACE RUNOFF      3.58      4.70      3.14      2.18      1.50      .0        .0        .0        .0        .0        .0        .0
 VOLATILIZED         .236      .310      .207      .144      .103      .771E-01  .595E-01  .457E-01  .372E-01  .301E-01  .245E-01  .202E-01
 OTHER SINKS         .400      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 ADS. ON SOIL        161.      118.      89.7      69.7      55.4      45.7      38.2      32.3      27.5      23.7      20.6      18.0
 IMMOBILIZED-CEC     .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 DEGRADED            29.3      39.5      25.7      17.9      12.8      9.57      7.39      5.80      4.62      3.73      3.05      2.51
 HYDROLYZED-MOI      .221E-02  .291E-02  .194E-02  .135E-02  .965E-03  .722E-03  .556E-03  .438E-03  .349E-03  .282E-03  .230E-03  .189E-03
 HYDROLYZED-SOI      .479E-01  .601E-01  .451E-01  .347E-01  .273E-01  .222E-01  .185E-01  .156E-01  .132E-01  .114E-01  .982E-02  .855E-02
 HYDROLYZED-CEC      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 COMPLEXED           .748E-03  .555E-03  .355E-03  .385E-03  .387E-03  .397E-03  .194E-03  .387E-03  .355E-03  .387E-03  .387E-03  .337E-03
 OTHER TRANS.        .200      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 IN SOIL MOIST.      8.36      5.45      3.70      2.60      1.88      1.44      1.12      .884      .703      .575      .471      .387
 IN SOIL AIR         1.21      .791      .537      .378      .274      .209      .163      .128      .103      .834E-01  .683E-01  .565E-01


    LOWER SOIL ZONE:

 INTO GRWATER        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 VOLATILIZED         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 OTHER SINKS         .500      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 ADS. ON SOIL        972.      936.      901.      868.      836.      805.      776.      749.      722.      697.      673.      651.
 IMMOBILIZED-CEC     .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 DEGRADED            21.8      33.2      36.2      34.4      32.6      31.0      29.4      27.9      26.5      25.3      24.1      22.9
 HYDROLYZED-MOI      .862E-03  .151E-02  .143E-02  .136E-02  .129E-02  .122E-02  .116E-02  .110E-02  .105E-02  .100E-02  .952E-03  .907E-03
 HYDROLYZED-SOI      .159      .248      .237      .230      .221      .213      .205      .198      .191      .184      .178      .172
 HYDROLYZED-CEC      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 COMPLEXED           .181      .130      .223      .205      .202      .215      .243      .156      .211      .149      .227      .188
 OTHER TRANS.        .500      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
 IN SOIL MOIST.      5.98      5.68      5.38      5.11      4.84      4.60      4.37      4.15      3.95      3.76      3.58      3.41
 IN SOIL AIR         .868      .824      .781      .741      .703      .668      .634      .603      .573      .546      .520      .495


      -- POLLUTANT CONCENTRATIONS (UG/ML) OR (UG/G) --

 MOISTURE-UPPER      2.16      1.41      .955      .671      .486      .372      .289      .228      .183      .148      .121      .100
 SOIL-UPPER          8.11      5.97      4.53      3.52      2.80      2.31      1.93      1.63      1.39      1.20      1.04      .907
 AIR-UPPER           .883      .575      .390      .275      .199      .152      .118      .933E-01  .747E-01  .606E-01  .497E-01  .411E-01
 FREE LIGAND-UPPER   254.      258.      258.      258.      258.      258.      258.      258.      258.      258.      258.      259.

 MOISTURE-LOWER      .232E-02  .220E-02  .209E-02  .198E-02  .188E-02  .178E-02  .169E-02  .161E-02  .153E-02  .146E-02  .139E-02  .132E-02
 SOIL-LOWER          .737E-01  .710E-01  .684E-01  .658E-01  .634E-01  .611E-01  .589E-01  .568E-01  .548E-01  .529E-01  .511E-01  .494E-01
 AIR-LOWER           .948E-03  .900E-03  .853E-03  .809E-03  .768E-03  .729E-03  .693E-03  .658E-03  .626E-03  .596E-03  .568E-03  .541E-03
 FREE LIGAND-LOWER   .775      .775      .775      .775      .775      .775      .775      .775      .775      .775      .775      .775

 MAX. POL.DEPTH(CM)  45.9      75.9      108.      139.      170.      201.      232.      263.      294.      324.      355.      385.
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                                YEAR -     1  ANNUAL SUMMARY REPORT
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     -- TOTAL INPUTS (UG) --

UPPER SOIL ZONE                       205.
LOWER SOIL ZONE                       .100E+04

     -- HYDROLOGIC CYCLE COMPONENTS --

AVERAGE SOIL MOISTURE( %)             25.8
TOTAL PRECIPATION(CM)                 94.3
TOTAL INFILTRATION (CM)               60.2
TOTAL EVAPOTRANSP.(CM)                32.6
TOTAL SURFACE RUNOFF(CM)              34.1
TOTAL GRW RUNOFF(CM)                  27.6
TOTAL YIELD (CM)                      61.7

     -- POLLUTANT MASS DISTRIBUTION (UG) --

     UPPER SOIL ZONE:

TOTAL SURFACE RUNOFF                  15.2
TOTAL VOLATILIZED                     1.30
TOTAL OTHER SINKS                     .400
FINAL ADS. ON SOIL                    13.0
FINAL IMMOBILIZED-CEC                 .0
TOTAL DEGRADED                        151.
TOTAL HYDROLYZED-MOI                  .121E-01
TOTAL HYDROLYZED-SOI                  .314
TOTAL HYDROLYZED-CEC                  .0
TOTAL COMPLEXED                       .407E-02
TOTAL OTHER TRANS.                    .200
FINAL IN SOIL MOIST.                  .339
FINAL IN SOIL AIR                     .555E-01

    LOWER SOIL ZONE:

TOTAL INTO GRWATER                    .0
TOTAL VOLATALIZED                     .0
TOTAL OTHER SINKS                     .500
FINAL ADS. ON SOIL                    551.
FINAL IMMOBILIZED-CEC                 .0
TOTAL DEGRADED                        350.
TOTAL HYDROLYZED-MOI                  .133E-01
TOTAL HYDROLYZED-SOI                  2.44
TOTAL HYDROLYZED-CEC                  .0
TOTAL COMPLEXED                       2.31
TOTAL OTHER TRANS.                    .300
FINAL IN SOIL MOIST.                  3.41
FINAL IN SOIL AIR                     .435
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      -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)OR (UG/G) --



  MOISTURE-UPPER                          .593
  SOIL-UPPER                              2.94
  AIR-UPPER                               .243
  FREE LIGAND-UPPER                       253.


  MOISTURE-LOWER                          .177E-02
  SOIL-LOWER                              .635E-01
  AIR-LOWER                               .724E-03
  FREE LIGAND-LOWER                       .775

  MAX. POL. DEPTH(M)                      3.35
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                                   YEAR-  2     MONTHLY INPUT PARAMETERS
                                   ========     ========================


                         OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP


          -- CLIMATIC PARAMETERS --

     LATITUDE(DEG)       42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5
     TEMP.(DEG C)        8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40
     CLOUD CVR(FRAC.)    .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320
     REL. HUM.(FRAC.)    .700      .700      .700      .700      .700      .700      .700      .700      .700      .700      .700      .700
     ALBEDO(-)           .300      .300      .300      .300      .300      .300      .300      .300      .300      .300      .300      .300
     EVAPOT.(CM/DAY):    .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

     PRECIP.(CM):        7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84
     M.TIME RAIN(DAYS):  .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320
     M. STORM NO.(-):    9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08
     M. SEASON(DAYS):    30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4



          -- RUN DATA-SET 1 --

     MOIS. CONC-UP.(UG/ML)   .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     MOIS. CONC-LO.(UG/ML)   .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     POL. INP-U(UG/SQ CM)    .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     POL. INP-L(UG/SQ CM)    .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     SUR. POL. MULTIPLIER    .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

          -- RUN DATA-SET 2 --

     POL. IN RAIN(FRAC-SL)   .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     TRNSFORMED-U(UG/SQ CM)  .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     TRNSFORMED-L(UG/SQ CM)  .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     SINKS-U(UG/SQ CM)       .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     SINKS-L(UG/SQ CM)       .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

     LIG. INPUT-U(UG/SQ.CM)  .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
     LIG. INPUT-L(UG/SQ.CM)  .0         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
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                                   YEAR-  2      MONTHLY RESULTS(OUTPUT)
                                   ========      ======================


          -- HYDROLOGIC CYCLE COMPONENTS --

                          OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

    SOIL MOISTURE( %)    25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8      25.8
    PRECIPITATION(CM)     7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86      7.86
    NET INFILTR.(CM)      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02      5.02
    EVAPOTRANSP.(CM)      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72      2.72
    SURFACE RUNOFF(CM)    2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84      2.84
    GRW RUNOFF(CM)        2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30      2.30
    YIELD (CM)            5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14      5.14

    RATIO PA/MPA(O2)      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00


          -- POLLUTANT MASS INPUT TO COLUMN(UG) --

                          OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

    PRECIPATION           .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
    OTHER(UPPER)          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
    OTHER(LOWER)          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

    TOTAL INPUT           .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
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    -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) --

    UPPER SOIL ZONE:

 SURFACE RUNOFF      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 VOLATILIZED         .168E-01   .141E-01   .120E-01   .102E-01   .878E-02   .758E-02   .658E-02   .573E-02   .503E-02   .443E-02   .392E-02   .348E-02
 OTHER SINKS         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 ADS. ON SOIL        15.8       14.0       12.4       11.1       10.0       9.01       8.10       7.41       6.76       6.18       5.67       5.21
 IMMOBILIZD-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 DEGRADED            2.09       1.76       1.49       1.27       1.09       .941       .817       .712       .625       .550       .486       .432
 HYDROLYZED-MOI      .159E-03   .132E-03   .112E-03   .955E-04   .822E-04   .719E-04   .616E-04   .537E-04   .471E-04   .415E-04   .367E-04   .326E-04
 HYDROLYZED-SOI      .750E-02   .662E-02   .588E-02   .525E-02   .471E-02   .424E-02   .384E-02   .348E-02   .317E-02   .289E-02   .265E-02   .243E-02
 HYDROLYZED-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 COMPLEXED           .387E-03   .386E-03   .387E-03   .387E-03   .387E-03   .397E-03   .387E-03   .387E-03   .387E-03   .387E-03   .174E-03   .397E-03
 OTHER TRANS.        .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 IN SOIL MOIST.      .325       .274       .233       .199       .172       .148       .129       .113       .992E-01   .876E-01   .775E-01   .690E-01
 IN SOIL AIR         .472E-01   .398E-01   .338E-01   .289E-01   .249E-01   .215E-01   .187E-01   .164E-01   .144E-01   .127E-01   .112E-01   .100E-01


    LOWER SOIL ZONE:

 INTO GRWATER        .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 VOLATILIZED         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 OTHER SINKS         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 ADS. ON SOIL        629.       603.       583.       567.       551.       534.       517.       501.       486.       471.       457.       444.
 IMMOBILIZD-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 DEGRADED            21.9       20.6       19.8       19.0       18.2       17.4       16.6       15.9       15.2       14.6       14.0       13.4
 HYDROLYZED-MOI      .864E-03   .824E-03   .787E-03   .751E-03   .718E-03   .685E-03   .656E-03   .628E-03   .602E-03   .576E-03   .552E-03   .530E-03
 HYDROLYZED-SOI      .166       .161       .155       .150       .146       .141       .137       .132       .128       .124       .121       .117
 HYDROLYZED-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 COMPLEXED           .159       .138       .254       .250       .253       .135       .153       .176       .205       .238       .149       .173
 OTHER TRANS.        .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
 IN SOIL MOIST.      3.25       3.10       2.96       2.83       2.70       2.59       2.47       2.37       2.27       2.17       2.08       2.00
 IN SOIL AIR         .472       .451       .431       .411       .392       .375       .359       .344       .329       .315       .302       .290


    -- POLLUTANT CONCENTRATIONS (UG/ML) OR (UG/G) --

 MOISTURE-UPPER      .840E-01   .708E-01   .601E-01   .514E-01   .443E-01   .383E-01   .333E-01   .291E-01   .256E-01   .226E-01   .200E-01   .178E-01
 SOIL-UPPER          .798       .705       .628       .562       .505       .455       .412       .374       .341       .312       .286       .263
 AIR-UPPER           .343E-01   .289E-01   .245E-01   .210E-01   .181E-01   .157E-01   .136E-01   .119E-01   .105E-01   .924E-02   .818E-02   .728E-02
 FREE LIGAND-UPPER   258.       258.       258.       258.       258.       258.       258.       258.       258.       258.       258.       258.

 MOISTURE-LOWER      .126E-02   .120E-02   .115E-02   .110E-02   .105E-02   .100E-02   .959E-03   .918E-03   .879E-03   .842E-03   .808E-03   .776E-03
 SOIL-LOWER          .477E-01   .461E-01   .445E-01   .432E-01   .415E-01   .405E-01   .392E-01   .380E-01   .369E-01   .358E-01   .347E-01   .337E-01
 AIR-LOWER           .510E-03   .492E-03   .470E-03   .448E-03   .429E-03   .410E-03   .392E-03   .375E-03   .359E-03   .344E-03   .330E-03   .317E-03
 FREE LIGAND-LOWER   .775       .775       .775       .775       .775       .775       .775       .775       .775       .775       .775       .775

 MAX. POL.DEPTH(CM)  417.       448.       479.       510.       541.       572.       603.       634.       665.       696.       727.       758.
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                              YEAR -     2  ANNUAL SUMMARY REPORT
                              ================================

     -- TOTAL INPUTS (UG) --

 UPPER SOIL ZONE                     .0
 LOWER SOIL ZONE                     .0


     -- HYDROLOGIC CYCLE COMPONENTS --


 AVERAGE SOIL MOISTURE( %)           25.3
 TOTAL PRECIPITATION(CM)             94.3
 TOTAL INFILTRATION (CM)             60.2
 TOTAL EVAPOTRANSP.(CM)              32.6
 TOTAL SURFACE RUNOFF(CM)            34.1
 TOTAL GRW RUNOFF(CM)                27.5
 TOTAL YIELD (CM)                    61.7



     -- POLLUTANT MASS DISTRIBUTION (UG) --

     UPPER SOIL ZONE:


 TOTAL SURFACE RUNOFF                .0
 TOTAL VOLATILIZED                   .937E-01
 TOTAL OTHER SINKS                   .0
 FINAL ADS. ON SOIL                  5.21
 FINAL IMMOBILIZED-CEC               .0
 TOTAL DEGRADED                      12.3
 TOTAL HYDROLYZED-MOI                .724E-03
 TOTAL HYDROLYZED-SOI                .527E-01
 TOTAL HYDROLYZED-CEC                .0
 TOTAL COMPLEXED                     .445E-02
 TOTAL OTHER TRANS.                  .0
 FINAL IN SOIL MOIST.                .690E-01
 FINAL IN SOIL AIR                   .100E-01


   LOWER SOIL ZONE:

 TOTAL INTO GRWATER                  .0
 TOTAL VOLATALIZED                   .0
 TOTAL OTHER SINKS                   .0
 FINAL ADS. ON SOIL                  444.
 FINAL IMMOBILIZED-CEC               .0
 TOTAL DEGRADED                      237.
 TOTAL HYDROLYZED-MOI                .813E-02
 TOTAL HYDROLYZED-SOI                1.03
 TOTAL HYDROLYZED-CEC                .0
 TOTAL COMPLEXED                     7.30
 TOTAL OTHER TRANS.                  .0
 FINAL IN SOIL MOIST.                2.00
 FINAL IN SOIL AIR                   .200
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     -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)OR (UG/G) --



 MOISTURE-UPPER                          .939E-01
 SOIL-UPPER                              .716
 AIR-UPPER                               .372E-01
 FREE LIGAND-UPPER                       283.


 MOISTURE-LOWER                          .114E-02
 SOIL-LOWER                              .432E-01
 AIR-LOWER                               .437E-03
 FREE LIGAND-LOWER                       .843

 MAX. POL. DEPTH(M)                      7.38



 ****************************************EXECUTION COMPLETED*****************************************
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RUN :  4                    ****** LEVEL3 SESOIL MODEL OPERATION ******
                             MONTHLY SITE SPECIFIC SIMULATION(3 LAYERS)


    ******************************************************************************************
    *****                                                                               *****
    ***** SESOIL-81:   SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS   *****
    *****                                                                               *****
    ***** DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.   ,(617)864-5770,X5871         *****
    *****              J. WAGNER     ,ARTHUR D. LITTLE INC.   ,(617)864-5770,X2585         *****
    *****                                                                               *****
    ***** VERSION:     DECEMBER 1981                                                     *****
    *****                                                                               *****
    *****                                                                               *****
    ******************************************************************************************

                      INDEX
        REGION     : (    4)     CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)
        SOIL TYPE  : (    5)     CLAY-LOAM GENERIC
        COMPOUND   : (   15)     TEST CHEM
        APPL. AREA : (    1)     TEST RUN

        GENERAL INPUT PARAMETERS
        ========================


     -- APPLICATION PARAMETERS --

AREA(SQ.CM): 1.0
DEPTH TO GRW(M): .10E+03
UPPER SOIL ZONE DEPTH(CM): 15.
MIDDLE SOIL ZONE DEPTH(CM): .10E-01
FREUNDLICH EXPONENT(-): 1.4
PH UPPER ZONE(-): 5.0
PH RATIO MIDDLE:UPPER ZONE(-): 1.0
PH RATIO LOWER:UPPER ZONE(-): .83
DEGRADATION RATIO MIDDLE:UPPER ZONE(-): 1.1
DEGRADATION RATIO LOWER:UPPER ZONE(-): 1.1
ORGANIC CARBON CONTENT RATIO MIDDLE:UPPER ZONE(-): 1.2
ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-):        1.2
CLAY CONTENT RATIO MIDDLE:UPPER ZONE(-): 1.3
CLAY CONTENT RATIO LOWER:UPPER ZONE(-): 1.3
CATION EXCHANGE CAPACITY RATIO MIDDLE:LOWER ZONE(-): 1.3
CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): 1.3
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      -- CHEMICAL PARAMETERS --

SOLUBILITY(UG/ML): .11E+04
ADSORP. COEF.(KOC): .36E+03
DIF. COEF. IN AIR(SQ.CM/SEC): .83E-05
DEGRADATION RATE(/DAY): .20
HENRYS CON.(CU.M-ATM/MOLE): .94E-02
ADSORP. COEF. ON SOIL(K): .0
MOLECULAR  WT.(G/MOL): 5.0
VALENCE(-): 2.0
NEUTRAL HYDROLYSIS CONSTANT(/DAY): .70E-05
BASE HYDROLYSIS CONSTANT(L/MOL-DAY): 9.0
ACID HYDROLYSIS CONSTANT(L/MOL-DAY): 9.0
LIGAND-POLLUTANT STABILITY CONST.(-): .10E+06
NO. MOLES LIGAND/MOLE POLLUTANT(-): 2.0
LIGAND MOLECULAR WEIGHT(G/MOL): 10.


      -- SOIL PARAMETERS --

DENSITY(G/SQ.CM): 1.3
INT. PERMEABILITY(SQ.CM): .28E-09
DISCONNECTEDNESS INDEX(-): 10.
POROSITY(-): .35
ORGANIC CARBON CONTENT(%): 1.3
CLAY CARBON CONTENT(%): .20E-01
CATION EXCHANGE COEF. (MILLI EQ./100G DRY SOIL): .0
INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM): .0
INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM): .0
INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM): .0
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              YEAR- 1  MONTHLY INPUT PARAMETERS
              =======  ======================

                            OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP


     -- CLIMATIC PARAMETERS --

LATITUDE(DEG)              42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5      42.5
TEMP.(DEG C)               8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40      8.40
CLOUD CVR(FRAC.)           .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320
REL. HUMID.(FRAC.)         .700      .700      .700      .700      .700      .700      .700      .700      .700      .700      .700      .700
ALBEDO(-)                  .300      .300      .300      .300      .300      .300      .300      .300      .300      .300      .300      .300
EVAPOT.(CM/DAY)            .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0

PRECIP.(CM)                7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84      7.84
M.TIME RAIN(DAYS)          .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320      .320
M. STORM NO.(-)            9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08      9.08
M. SEASON(DAYS)            30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4      30.4



     -- RUN DATA-SET 1 --

MOIS. CONC-UP.(UG/ML)        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
MOIS. CONC-MI.(UG/ML)        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
MOIS. CONC-LO.(UG/ML)        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
POL. INP-U(UG/SQ.CM)         200.      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
POL. INP-M(UG/SQ.CM)         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
POL. INP-L(UG/SQ.CM)         .100E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SUR. RUNOFF(1=Y,0=N)         1.00      1.00      1.00      1.00      1.00      .0        .0        .0        .0        .0        .0        .0

     -- RUN DATA-SET 2 --

CONC. IN RAIN(UG/ML)         .100E-02  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
TRANSFORMED-U(UG/SQ.CM)      .200      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
TRANSFORMED-M(UG/SQ.CM)      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
TRANSFORMED-L(UG/SQ.CM)      .300      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SINKS-U(UG/SQ.CM)            .400      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SINKS-M(UG/SQ.CM)            .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
SINKS-L(UG/SQ.CM)            .500      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
LIG.INPUT-U(UG/SQ.CM)        .100E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
LIG.INPUT-M(UG/SQ.CM)        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
LIG.INPUT-L(UG/SQ.CM)        .200E+04  .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
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                         YEAR=  2     MONTHLY RESULTS(OUTPUT)
                         ========     =====================


      -- HYDROLOGIC CYCLE COMPONENTS --

                      OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP

SOIL MOISTURE( %)    25.8     25.8     25.8     25.8     25.8     25.8     25.8     25.8     25.8     25.8     25.8     25.8
PRECIPATION(CM)      7.86     7.86     7.86     7.86     7.86     7.86     7.85     7.86     7.85     7.86     7.85     7.86
NET INFILTR.(CM)     5.02     5.02     5.02     5.02     5.02     5.02     5.02     5.02     5.02     5.02     5.02     5.02
EVAPOTRANSP.(CM)     2.72     2.72     2.72     2.72     2.72     2.72     2.72     2.72     2.72     2.72     2.72     2.72
SURFACE RUNOFF(CM)   2.84     2.84     2.84     2.84     2.84     2.84     2.84     2.84     2.84     2.84     2.84     2.84
GRW RUNOFF(CM)       2.30     2.30     2.30     2.30     2.30     2.30     2.30     2.30     2.30     2.30     2.30     2.30
YIELD (CM)           5.14     5.14     5.14     5.14     5.14     5.14     5.14     5.14     5.14     5.14     5.14     5.14

RATIO PA/MPA(UZ)     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00


      -- POLLUTANT MASS INPUT TO COLUMN(UG) --

                      OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP

PRECIPATION          .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
OTHER(UPPER)         .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
OTHER(LOWER)         .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0

TOTAL INPUT          .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
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IN SOIL AIR

          MIDDLE SOIL ZONE:

VOLATILIZED          .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER SINKS          .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
ADS. ON SOIL         .122       .943E-01   .704E-01   .545E-01   .426E-01   .350E-01   .271E-01   .235E-01   .200E-01   .163E-01   .143E-01   .143E-01
IMMOBILIZED-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
DEGRADED             .172E-01   .279E-01   .185E-01   .127E-01   .899E-02   .651E-02   .507E-02   .394E-02   .311E-02   .230E-02   .183E-02   .170E-02
HYDROLYZED-MOI       .132E-05   .191E-05   .127E-05   .874E-06   .617E-06   .453E-06   .343E-06   .263E-06   .213E-06   .158E-06   .125E-06   .117E-06
HYDROLYZED-SOI       .352E-04   .477E-04   .355E-04   .272E-04   .212E-04   .170E-04   .141E-04   .116E-04   .995E-05   .802E-05   .682E-05   .645E-05
HYDROLYZED-CEC       .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
COMPLEXED            .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER TRANS.         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
IN SOIL MOIST.       .519E-02   .362E-02   .243E-02   .164E-02   .119E-02   .904E-03   .697E-03   .517E-03   .413E-03   .310E-03   .258E-03   .254E-03
IN SOIL AIR          .754E-03   .525E-03   .347E-03   .244E-03   .172E-03   .131E-03   .101E-03   .750E-04   .600E-04   .450E-04   .375E-04   .375E-04


          LOWER SOIL ZONE:

INTO GRWATER         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
VOLATILIZED          .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER SINKS          .500       .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
ADS. ON SOIL         972.       935.       901.       867.       835.       805.       776.       748.       722.       697.       673.       650.
IMMOBILIZED-CEC      .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
DEGRADED             21.8       39.2       36.2       34.4       32.6       30.9       29.4       27.9       26.6       25.3       24.1       22.9
HYDROLYZED-MOI       .861E-03   .151E-02   .143E-02   .136E-02   .129E-02   .122E-02   .116E-02   .110E-02   .105E-02   .999E-03   .951E-03   .906E-03
HYDROLYZED-SOI       .139       .249       .233       .230       .221       .213       .205       .198       .191       .184       .178       .172
HYDROLYZED-CEC       .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
COMPLEXED            .179       .257       .222       .203       .200       .213       .241       .154       .209       .147       .225       .196
OTHER TRANS.         .300       .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
IN SOIL MOIST.       5.78       5.67       5.38       5.10       4.84       4.50       4.37       4.15       3.95       3.76       3.59       3.41
IN SOIL AIR          .869       .823       .781       .741       .703       .667       .634       .603       .573       .545       .519       .495
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      -- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G)  --



 MOISTURE-UPPER      2.10      1.41      .955      .671      .486      .372      .289      .228      .183      .148      .121      .100
 SOIL-UPPER          8.11      5.97      4.53      3.52      2.80      2.31      1.93      1.63      1.39      1.20      1.04      .907
 AIR-UPPER           .833      .575      .399      .275      .199      .152      .118      .933E-01  .747E-01  .606E-01  .497E-01  .411E-01
 LIGAND-UPPER        258.      258.      258.      258.      258.      258.      258.      258.      258.      258.      258.      258.


 MOISTURE-MIDDLE     2.01      1.40      .930      .650      .460      .350      .270      .200      .160      .120      .100      .100
 SOIL-MIDDLE         9.25      7.14      5.33      4.13      3.23      2.65      2.20      1.78      1.52      1.24      1.08      1.08
 AIR-MIDDLE          .422      .372      .330      .266      .188      .143      .110      .818E-01  .654E-01  .491E-01  .409E-01  .409E-01
 LIGAND-MIDDLE       .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0


 MOISTURE-LOWER      .232E-02  .220E-02  .209E-02  .198E-02  .188E-02  .178E-02  .169E-02  .161E-02  .153E-02  .146E-02  .139E-02  .132E-02
 SOIL-LOWER          .737E-01  .710E-01  .683E-01  .658E-01  .634E-01  .611E-01  .589E-01  .568E-01  .548E-01  .529E-01  .511E-01  .493E-01
 AIR-LOWER           .948E-03  .899E-03  .853E-03  .809E-03  .768E-03  .729E-03  .692E-03  .658E-03  .625E-03  .596E-03  .567E-03  .541E-03
 LIGAND-LOWER        .775      .775      .775      .775      .775      .775      .775      .775      .775      .775      .775      .775

 MAX. POL. DEPTH(M)  45.9      75.9      108.      139.      170.      201.      232.      263.      294.      324.      355.      386.
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                              YEAR - 1  ANNUAL SUMMARY
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      -- TOTAL INPUTS --

  UPPER SOIL ZONE                        205.
  MIDDLE SOIL ZONE                       .0
  LOWER SOIL ZONE                        .100E+04


      -- HYDROLOGIC CYCLE COMPONENTS --


  AVERAGE SOIL MOISTURE( %)              25.8
  TOTAL PRECIPATION(CM)                  94.3
  TOTAL INFILTRATION (CM)                60.2
  TOTAL EVAPOTRANSP.(CM)                 32.6
  TOTAL SURFACE RUNOFF(CM)               34.1
  TOTAL GRW RUNOFF(CM)                   27.6
  TOTAL YIELD (CM)                       61.7


      -- POLLUTANT MASS DISTRIBUTION (UG) --

          UPPER ZONE:

  TOTAL SURFACE RUNOFF                   15.2
  TOTAL VOLATILIZED                      1.30
  TOTAL OTHER SINKS                      .400
  FINAL ADS. ON SOIL                     18.0
  FINAL IMMOBILIZED-CEC                  .0
  TOTAL DEGRADED                         101.
  TOTAL HYDROLYZED-MOI                   .121E-01
  TOTAL HYDROLYZED-SOI                   .314
  TOTAL HYDROLYZED-CEC                   .0
  TOTAL COMPLEXED                        .407E-02
  TOTAL OTHER TRANS.                     .200
  FINAL IN SOIL MOIST.                   .339
  FINAL IN SOIL AIR                      .555E-01


           MIDDLE SOIL ZONE:


  TOTAL VOLATILIZED                      .0
  TOTAL OTHER SINKS                      .0
  FINAL ADS. ON SOIL                     .143E-01
  FINAL IMMOBILIZED-CEC                  .0
  TOTAL DEGRADED                         .112
  TOTAL HYDROLYZED-MOI                   .757E-05
  TOTAL HYDROLYZED-SOI                   .241E-03
  TOTAL HYDROLYZED-CEC                   .0
  TOTAL COMPLEXED                        .0
  TOTAL OTHER TRANS.                     .0
  FINAL IN SOIL MOIST.                   .239E-03
  FINAL IN SOIL AIR                      .375E-04
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FINAL IN SOIL AIR                          .375E-04



            LOWER SOIL ZONE:

TOTAL INTO GRWATER                         .0
TOTAL VOLATALIZED                          .0
TOTAL OTHER SINKS                          .500
FINAL ADS. ON SOIL                         650.
FINAL IMMOBILIZED-CEC                      .0
TOTAL DEGRADED                             330.
TOTAL HYDROLYZED-MOI                       .137E-01
TOTAL HYDROLYZED-SOI                       2.44
TOTAL HYDROLYZED-CEC                       .0
TOTAL COMPLEXED                            2.44
TOTAL OTHER TRANS.                         .330
FINAL IN SOIL MOIST.                       3.41
FINAL IN SOIL AIR                          .475


    -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --



MOISTURE-UPPER                             .533
SOIL-UPPER                                 2.04
AIR-UPPER                                  .243
FREE LIGAND-UPPER                          253.


MOISTURE-MIDDLE                            .562
SOIL-MIDDLE                                3.39
AIR-MIDDLE                                 .230
FREE LIGAND-MIDDLE                         .0


MOISTURE-LOWER                             .177E-02
SOIL-LOWER                                 .605E-01
AIR-LOWER                                  .724E-03
FREE LIGAND-LOWER                          .775

MAX. POL.DEPTH(M)                          3.36
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                         YEAR- 2  MONTHLY INPUT PARAMETERS
                         =======  =======================

                     OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP


       -- CLIMATIC PARAMETERS --

LATITUDE(DEG)       42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5     42.5
TEMP.(DEG. C)       8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40     8.40
CLOUD CVR(FRAC.)    .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320
REL. HUMID.(FRAC.)  .700     .700     .700     .700     .700     .700     .700     .700     .700     .700     .700     .700
ALBEDO(-)           .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300
EVAPOT.(CM/DAY)     .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0

PRECIP.(CM)         7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84     7.84
M.TIME RAIN(DAYS)   .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320     .320
M. STORM NO.(-)     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08     9.08
M. SEASON(DAYS)     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4



       -- RUN DATA-SET 1 --

MOIS. CONC-UP.(UG/ML)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
MOIS. CONC-MI.(UG/ML)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
MOIS. CONC-LO.(UG/ML)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
POL. INP-U(UG/SQ.CM)    .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
POL. INP-M(UG/SQ.CM)    .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
POL. INP-L(UG/SQ.CM)    .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
SUR. RUNOFF(1=Y,0=N)    .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0

       -- RUN DATA-SET 2 --

CONC. IN RAIN(UG/ML)    .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
TRANSFORMED-U(UG/SQ.CM) .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
TRANSFORMED-M(UG/SQ.CM) .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
TRANSFORMED-L(UG/SQ.CM) .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
SINKS-U(UG/SQ.CM)       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
SINKS-M(UG/SQ.CM)       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
SINKS-L(UG/SQ.CM)       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
LIG.INPUT-U(UG/SQ.CM)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
LIG.INPUT-M(UG/SQ.CM)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
LIG.INPUT-L(UG/SQ.CM)   .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0
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                              YEAR - 2   MONTHLY RESULTS (OUTPUT)
                              ========   ======================



      -- HYDROLOGIC CYCLE COMPONENTS --


                          OCT        NOV        DEC        JAN        FEB        MAR        APR        MAY        JUN        JUL        AUG        SEP

SOIL MOISTURE( %)        25.8       25.8       25.8       25.8       25.8       25.8       25.8       25.8       25.8       25.8       25.8       25.8
PRECIPATION(CM)          7.86       7.86       7.86       7.86       7.86       7.86       7.86       7.86       7.86       7.86       7.86       7.86
NET INFILTR.(CM)         5.02       5.02       5.02       5.02       5.02       5.02       5.02       5.02       5.02       5.02       5.02       5.02
EVAPOTRANSP.(CM)         2.72       2.72       2.72       2.72       2.72       2.72       2.72       2.72       2.72       2.72       2.72       2.72
SURFACE RUNOFF(CM)       2.84       2.84       2.84       2.84       2.84       2.84       2.84       2.84       2.84       2.84       2.84       2.84
GRW RUNOFF(CM)           2.30       2.30       2.30       2.30       2.30       2.30       2.30       2.30       2.30       2.30       2.30       2.30
YIELD (CM)               5.14       5.14       5.14       5.14       5.14       5.14       5.14       5.14       5.14       5.14       5.14       5.14
RATIO PA/MPA(GZ)         1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00


      -- POLLUTANT MASS INPUT TO COLUMN (UG) --


PRECIPATION               .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER(UPPER)              .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER(MIDDLE)             .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
OTHER(LOWER)              .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0


TOTAL INPUT               .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0


      -- POLLUTANT MASS DISTRIBUTION IN COLUMN(UG) --

          UPPER SOIL ZONE:


SURFACE RUNOFF            .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
VOLATILIZED              .168E-01   .141E-01   .120E-01   .102E-01   .878E-02   .758E-02   .658E-02   .573E-02   .503E-02   .443E-02   .392E-02   .348E-02
OTHER SINKS               .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
ADS. ON SOIL             15.8       14.0       12.4       11.1       10.0       9.01       8.16       7.41       6.76       6.18       5.67       5.21
IMMOBILIZED-CEC           .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
DEGRADED                 2.09       1.76       1.49       1.27       1.09       .941       .817       .712       .625       .550       .486       .432
HYDROLYZED-MOI           .158E-03   .132E-03   .112E-03   .956E-04   .822E-04   .710E-04   .616E-04   .537E-04   .471E-04   .415E-04   .367E-04   .326E-04
HYDROLYZED-SOI           .750E-02   .662E-02   .593E-02   .525E-02   .471E-02   .424E-02   .384E-02   .348E-02   .317E-02   .289E-02   .265E-02   .243E-02
HYDROLYZED-CEC            .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
COMPLEXED                .387E-03   .386E-03   .387E-03   .387E-03   .387E-03   .387E-03   .387E-03   .387E-03   .387E-03   .387E-03   .194E-03   .387E-03
OTHER TRANS.              .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0         .0
IN SOIL MOIST.           .325       .274       .233       .199       .172       .148       .129       .113       .992E-01   .876E-01   .775E-01   .690E-01
IN [illegible]           [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] .137E-01 .104E-01 .144E-01 .127E-01 .112E-01 .100E-01
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IN SOIL AIR

         MIDDLE SOIL ZONE:

VOLATILIZED          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
OTHER SINKS          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
ADS. ON SOIL         .994E-02  .872E-02  .744E-02  .606E-02  .453E-02  .453E-02  .276E-02  .276E-02  .276E-02  .0        .0        .0
IMMOBILIZED-CEC      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
DEGRADED             .115E-02  .395E-03  .582E-03  .511E-03  .426E-03  .341E-03  .213E-03  .170E-03  .170E-03  .128E-03  .0        .0
HYDROLYZED-MOI       .789E-07  .614E-07  .455E-07  .351E-07  .292E-07  .234E-07  .145E-07  .117E-07  .117E-07  .877E-08  .0        .0
HYDROLYZED-SOI       .499E-05  .409E-05  .337E-05  .274E-05  .240E-05  .205E-05  .145E-05  .125E-05  .125E-05  .938E-06  .0        .0
HYDROLYZED-CEC       .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
COMPLEXED            .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
OTHER TRANS.         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
IN SOIL MOIST.       .155E-03  .129E-03  .103E-03  .775E-04  .517E-04  .517E-04  .258E-04  .258E-04  .258E-04  .0        .0        .0
IN SOIL AIR          .225E-04  .187E-04  .150E-04  .112E-04  .750E-05  .750E-05  .375E-05  .375E-05  .375E-05  .0        .0        .0


         LOWER SOIL ZONE:

INTO GRWATER         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
VOLATILIZED          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
OTHER SINKS          .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
ADS. ON SOIL         629.      608.      588.      569.      551.      533.      517.      501.      486.      471.      457.      443.
IMMOBILIZED-CEC      .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
DEGRADED             21.8      20.8      19.9      19.0      18.1      17.3      16.6      15.9      15.2      14.6      14.0      13.4
HYDROLYZED-MOI       .864E-03  .824E-03  .786E-03  .751E-03  .717E-03  .686E-03  .656E-03  .628E-03  .601E-03  .576E-03  .552E-03  .529E-03
HYDROLYZED-SOI       .166      .161      .155      .150      .145      .141      .136      .132      .128      .124      .121      .117
HYDROLYZED-CEC       .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
COMPLEXED            .137      .136      .252      .243      .251      .133      .159      .173      .202      .236      .146      .190
OTHER TRANS.         .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0        .0
IN SOIL MOIST.       3.25      3.10      2.96      2.83      2.70      2.58      2.47      2.37      2.27      2.17      2.08      2.00
IN SOIL AIR          .472      .450      .430      .410      .392      .375      .359      .343      .329      .315      .302      .290
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-- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --



MOISTURE-UPPER      .840E-01 .708E-01 .601E-01 .514E-01 .443E-01 .383E-01 .333E-01 .291E-01 .256E-01 .226E-01 .200E-01 .178E-01
SOIL-UPPER          .798     .706     .628     .562     .505     .455     .412     .374     .341     .312     .286     .253
AIR-UPPER           .343E-01 .289E-01 .246E-01 .210E-01 .181E-01 .157E-01 .136E-01 .119E-01 .105E-01 .924E-02 .819E-02 .728E-02
LIGAND-UPPER        258.     258.     258.     258.     258.     258.     258.     258.     258.     258.     258.     258.


MOISTURE-MIDDLE     .600E-01 .500E-01 .400E-01 .300E-01 .200E-01 .200E-01 .100E-01 .100E-01 .100E-01 .0       .0       .0
SOIL-MIDDLE         .753     .661     .564     .457     .343     .343     .209     .209     .209     .0       .0       .0
AIR-MIDDLE          .245E-01 .204E-01 .164E-01 .123E-01 .818E-02 .818E-02 .409E-02 .409E-02 .409E-02 .0       .0       .0
LIGAND-MIDDLE       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0       .0


MOISTURE-LOWER      .126E-02 .120E-02 .115E-02 .110E-02 .105E-02 .100E-02 .958E-03 .917E-03 .873E-03 .841E-03 .807E-03 .774E-03
SOIL-LOWER          .477E-01 .461E-01 .446E-01 .432E-01 .418E-01 .405E-01 .392E-01 .380E-01 .368E-01 .357E-01 .347E-01 .336E-01
AIR-LOWER           .515E-03 .492E-03 .469E-03 .448E-03 .428E-03 .410E-03 .392E-03 .375E-03 .359E-03 .344E-03 .330E-03 .316E-03
LIGAND-LOWER        .775     .775     .775     .775     .775     .775     .775     .775     .775     .775     .775     .775

MAX. POL. DEPTH(M)  417.     448.     479.     510.     541.     572.     603.     634.     665.     696.     727.     758.
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                                    YEAR - 2   ANNUAL SUMMARY
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      -- TOTAL INPUTS --

 UPPER SOIL ZONE                             .0
 MIDDLE SOIL ZONE                            .0
 LOWER SOIL ZONE                             .0



      -- HYDROLOGIC CYCLE COMPONENTS --

 AVERAGE SOIL MOISTURE( %)                   25.8
 TOTAL PRECIPATION(CM)                       94.3
 TOTAL INFILTRATION (CM)                     60.2
 TOTAL EVAPOTRANSP.(CM)                      32.6
 TOTAL SURFACE RUNOFF(CM)                    34.1
 TOTAL GRW RUNOFF(CM)                        27.6
 TOTAL YIELD (CM)                            61.7



      -- POLLUTANT MASS DISTRIBUTION (UG) --

          UPPER ZONE:


 TOTAL SURFACE RUNOFF                        .0
 TOTAL VOLATILIZED                           .937E-01
 TOTAL OTHER SINKS                           .0
 FINAL ADS. ON SOIL                          5.21
 FINAL IMMOBILIZED-CEC                       .0
 TOTAL DEGRADED                              12.3
 TOTAL HYDROLYZED-MOI                        .924E-03
 TOTAL HYDROLYZED-SOI                        .327E-01
 TOTAL HYDROLYZED-CEC                        .0
 TOTAL COMPLEXED                             .443E-02
 TOTAL OTHER TRANS.                          .0
 FINAL IN SOIL MOIST.                        .600E-01
 FINAL IN SOIL AIR                           .100E-01



           MIDDLE SOIL ZONE:


 TOTAL VOLATILIZED                           .0
 TOTAL OTHER SINKS                           .0
 FINAL ADS. ON SOIL                          .0
 FINAL IMMOBILIZED-CEC                       .0
 TOTAL DEGRADED                              .459E-02
 TOTAL HYDROLYZED-MOI                        .322E-06
 TOTAL HYDROLYZED-SOI                        .244E-04
 TOTAL HYDROLYZED-CEC                        .0
 TOTAL COMPLEXED                             .0
 TOTAL OTHER TRANS.                          .0
 FINAL IN SOIL MOIST.                        .0
 FINAL IN SOIL AIR                           .0
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 FINAL IN SOIL AIR-- ----



          LOWER SOIL ZONE:

 TOTAL INTO GRWATER                 .0
 TOTAL VOLATALIZED                  .0
 TOTAL OTHER SINKS                  .0
 FINAL ADS. ON SOIL                 443.
 FINAL IMMOBILIZED-CEC              .0
 TOTAL DEGRADED                     207.
 TOTAL HYDROLYZED-MOI               .317E-02
 TOTAL HYDROLYZED-SOI               1.04
 TOTAL HYDROLYZED-CEC               .0
 TOTAL COMPLEXED                    2.27
 TOTAL OTHER TRANS.                 .0
 FINAL IN SOIL MOIST.               2.00
 FINAL IN SOIL AIR                  .200


     -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --



 MOISTURE-UPPER                     .909E-01
 SOIL-UPPER                         .716
 AIR-UPPER                          .372E-01
 FREE LIGAND-UPPER                  280.


 MOISTURE-MIDDLE                    .677E-01
 SOIL-MIDDLE                        .505
 AIR-MIDDLE                         .277E-01
 FREE LIGAND-MIDDLE                 .0


 MOISTURE-LOWER                     .114E-02
 SOIL-LOWER                         .432E-01
 AIR-LOWER                          .407E-03
 FREE LIGAND-LOWER                  .840

 MAX. POL.DEPTH(M)                  7.50


 ****************************************EXECUTION COMPLETED****************************************
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MI - miscellaneous

APPENDIX MI

SYMBOLS & MISCELLANEOUS

The appendix will contain sections such as

1.0 INDEX

2.0 DEFINITIONS

  2.1 Soil Moisture Content (see next page)

3.0 NOTATIONS (also presented in each scientific appendix separately)

4.0 FORTRAN/NONFORTRAN VARIABLE CORRESPONDENCE

5.0 LIST OF FIGURES (also presented in each appendix)

6.0 LIST OF TABLES (also presented in each appendix)

7.0 TABLE FOR NUMERICAL CALCULATIONS

8.0 TYPICAL INPUT/OUTPUT (attached)

2.1 SOIL MOISTURE CONTENT

The soil moisture content (θ) is defined as:

$$\theta = V_w/V_t \qquad \text{in mL/mL} = \text{cm}^3/\text{cm}^3$$

where:

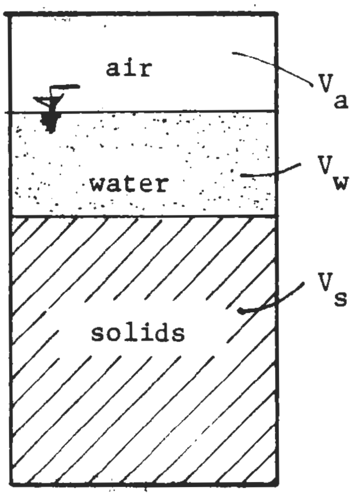
$$V_t = V_s + V_w + V_a$$

V_t = total volume of soil matrix (mL)

V_s = volume of solid portion (mL)

V_w = volume of water (mL)

V_a = volume of air (mL)



Like the porosity (n), volumetric moisture content is usually reported as a decimal fraction or a percent. For saturation flow, $\theta = n$; for unsaturated flow, $\theta < n$.

Above definition is employed by most of hydrology engineers and SESOIL. Soil scientists, however, frequently use as a moisture content definition the effective "degree of medium saturation" (s), that is equivalent to the volume of active soil moisture (water) divided by the effective volume of voids . In this case

$$s = \theta/n \quad (0 \leq s \leq 1)$$

or $$\theta = s \cdot n \quad (0 \leq \theta \leq n)$$

where n is the effective medium porosity, or the effective volume of voids divided by the total volume.

MARCOS BONAZOUNTAS

Dr. Bonazountas, a civil and environmental engineer, is a senior member of the Bio/Enviro Systems Section of Arthur D. Little, Inc. who specializes in mathematical environmental modeling.

Since joining Arthur D. Little, Inc., in 1977, Dr. Bonazountas has coordinated modeling teams and has developed, applied and validated models for: soils, groundwater, biology, water resources and air; multi-media models for pollutant fate in the environment; estuarine and hydrodynamic models with a continuous emphasis on both the physics and the chemistry of the environmental systems; and water resources economic and optimization models. Recent models developed include: an unsaturated soil/biotic zone model, which can be interfaced with any numerical finite difference or finite element groundwater model; a time series water resource model; a civil engineering construction containment model for hazardous waste sites; an oceanic oil slick model; a river quality and sedimentation model; an economic model for waste underground injection; an environmental exposure/ risk model for toxic substances; and a river basin model for the Maqarin Dam and the Jordan River in Jordan. He recently headed a multi-media (air, water, soil, biota) mathematical effort whose objective was to describe fate, pathways, and exposure of toxics in the environment. The SESOIL model encompasses his lengthy experience in soil, groundwater and general environmental modeling.

Dr. Bonazountas received his engineering degree in civil engineering (1969) from the National Technical University of Athens, Greece; his doctoral degree in river hydromechanics and sediment transportation (1973) from the Technical University of Munich, Germany; and his diploma in computer sciences (1969) from the Data Processing Institute in Athens, Greece. He undertook further studies at the Massachusetts Institute of Technology and at Harvard University. He is a member of the ASCE, AGU, AWRA, IAHR, and has authored several publications concerning his research.

JANET M. WAGNER

Ms. Wagner, a chemist and computer scientist, is a member of the Analytical and Environmental Chemistry Section. Her interests focus on the use of computers for solving environmental and chemical problems.

Since joining Arthur D. Little, Inc. in 1978, Ms. Wagner has been involved in the application of numerical and mathematical techniques to the modeling of environmental processes, in the development of software packages for data management, and in the analysis of several toxic substances in the environment. Recent projects, other than SESOIL, include: design and implementation of a data management system for a project involving utility disposal wastes, which is designed to facilitate data entry and storage and to perform further statistical and numerical analyses on subsets of the data; analysis of chemical properties, laboratory studies, and environmental models to assess the environmental fate of some of the priority pollutants for EPA risk assessment reports; and a multi-media environmental computer modeling effort, encompassing air, soil and water-body modeling issues, such as air quality, river flow and quality, and exposure to humans and biota. Ms. Wagner was a member on the ADLPIPE/DIS project, where she contributed to the development, implementation, and quality control of large FORTRAN based software packages used for piping system design and pipe stress analysis. Prior to joining Arthur D. Little, Inc., Ms. Wagner participated in the design and implementation of computer models in the areas of quantum chemistry and chemical kinetics.

In her computer applications, Ms. Wagner has employed the computer languages of FORTRAN, APL, BASIC, ALGOL and COBOL; has worked on IBM, VAX, CDC, UNIVAC, and Data General systems; and has developed and worked with computer graphics packages.

Ms. Wagner received her B.A. in Chemistry and Computer Sciences (1980) from Williams College, Massachusetts.