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AN ADVISORY SYSTEM FOR NORTH CAROLINA GROUNDWATER QUALITY MODELING AND MANAGEMENT NEEDS

By

Miguel A. Medina, Jr.
and
Jonathan B. Butcher
Department of Civil and
Environmental Engineering
School of Engineering

and

Carlos M. Marin
School of Forestry and
Environmental Studies
Duke University
Durham, North Carolina 27706

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At Duke University, Dr. Maria Moreno, a Visiting Fulbright Scholar from Spain, assisted the authors in the early stages of report preparation with model documentation and made several suggestions regarding chemical processes. Rob Runkel, a graduate student in the School of Forestry and Environmental Studies, performed several model testing and application tasks. Jo Ann Scott assisted with word-processing tasks. The first two authors must take the credit for the bulk of the word-processing, particularly the task of inserting complex equations in the manuscript with specialized software . Mr. Fred Avent accomplished the drafting of several figures and flow charts. Electronic digital computations were performed on several micro-computers within the School of Engineering, the Groundwater Section of DEM, and the authors' own personal computers. The software was tested on IBM XT's, IBM AT's and Zenith ZW 158 micro-computers.

ABSTRACT

Federal policy states that groundwater quality management is a State responsibility. Waste disposal sites that discharge or may leak to a groundwater system must undergo a permitting process. Applications are reviewed by the Division of Environmental Management, Department of Natural Resources and Community Development, State of North Carolina. This research project conditions the permitting process upon: sound mathematical modeling techniques, review of all sources of data on waste, method of disposal and hydrogeologic scenario -- all processed by a computerized advisory system capable of assessing degree of uncertainty within a sequential decision analysis framework. The advisory system is a friendly, interactive menu-driven management program which executes a large number of supporting decision algorithms and mathematical models, including 3-dimensional color graphics representation of the predicted contaminant plume.

The decision analysis framework provides the foundation for the advisory-system-based permitting process. Part of the sequential process involves a preliminary-level screening model: a computerized version of the LeGrand method. Key characteristics of a site are weighted to determine contamination potential through a numerical rating. If there is a contamination potential, the advisory system proceeds to a higher level of analysis: flow and mass transport prediction based on analytical, semi-analytical, or numerical solutions to the governing differential equations. The user is guided through the model selection process by an algorithm, CHOICE. For example, if flow in the region of the site is suspected to be strongly influenced by pumping wells, only semi-analytical or numerical models may be appropriate. Data availability is also taken into consideration, since an insufficient amount may preclude application of a numerical model. In this case, the most appropriate analytically-based model is selected which can be executed in a Monte Carlo mode to approximate site risk. A probability distribution of concentration is predicted, incorporating model error, natural uncertainty and parameter uncertainty. Permitting criteria (e.g., water quality classification and standards of groundwaters at the site) are evaluated along with probability of violation to recommend approval or denial of a permit -- with possible recommendations for reducing uncertainty by establishing a field sampling and monitoring programme.

A user's manual is presented for the advisory system in general, and for each of the component models in particular, with example applications. Technical programming considerations are reviewed, including future code development and its incorporation.

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SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

A sequential decision-analytic framework has been developed which provides the foundation for the advisory-system-based permitting process. The advisory system has been designed as a friendly, interactive menu-driven management program which executes a large number of supporting decision algorithms, screening models and predictive mathematical models. It includes 3-dimensional color graphics representation of the predicted contaminant plume: allowing selection of several color combinations, fill area designs, rotation of the graph and scaling. The management program enables the regulatory agency to process a large number of applications systematically on the basis of sound mathematical modeling techniques, review of all sources of data on waste, method of disposal and hydrogeologic scenario. An algorithm has been included to assist less experienced users in the model selection process, which can be by-passed by more experienced modelers. A user's manual has been provided with examples representative of permit applications received by the Division of Environmental Management, North Carolina Department of Natural Resources and Community Development.

All of the predictive models in the advisory system have been modified to execute in a Monte Carlo mode to approximate site risk. Thus, predictions of the probability distribution of contaminant concentration incorporate model error, natural uncertainty and parameter uncertainty. Permitting criteria (e.g., water quality standards) are evaluated along with probability of violation to recommend approval or denial of a permit. Several successful applications of the advisory system are presented. A difficult question which may only be resolved with experience deals with the level of uncertainty acceptable to the regulatory agency in making a decision. Obviously, the permit applicant can reduce the uncertainty by providing the agency with additional site data. The advisory system can indeed be used to determine minimum data requirements.

A number of recommendations follow relating directly to the advisory system. Further work is needed to:

(1) Incorporate more detailed routines for compliance monitoring, and techniques of preposterior analysis for sampling recommendations.

(2) Develop a regional data base management system to operate in conjunction with the advisory system.

(3) Develop optional methods of combining regional-data-based information with site-specific data, using techniques of Bayesian statistical analysis.

(4) Expand the advisory system to include a larger menu of the more complex geohydrochemical models for solute migration.

(5) Continue to improve the level of experience built into the model. For example, add more safeguards to reduce the possibility of entering inappropriate values for model parameters or for regionally-known aquifer characteristics (e.g., transmissivity).

(6) Incorporate work of other investigators in North Carolina aimed at specific groundwater contamination problems (e.g., leaking underground storage tanks ; chemical transport in the unsaturated zone, coupled with heat and soil moisture by Piver and Lindstrom).

Additional recommendations are in order for **users of the system** in the **regulatory environment** :

(7) Frequent use of the system in an operational mode, with <u>feedback</u> to the authors, will undoubtedly uncover weaknesses and/or areas for further improvement.

(8) An appreciation for the input data requirements should lead to development of better guidelines for data collection and development of a meaningful data base.

CHAPTER I

INTRODUCTION AND OVERVIEW OF METHODOLOGY

Public awareness of the potential problem of groundwater contamination has been heightened over the past decade due to highly publicized reports of toxic chemicals threatening drinking water supplies. Although Federal, State and local governments have mobilized to respond, these responses suffer from: a lack of coordination among responsible agencies, limited information about the health effects of exposure to some toxic contaminants, and a limited scientific foundation on which to base policy decisions (U.S. Environmental Protection Agency, 1984). Recognizing the high level of uncertainty associated with the problem, a framework for assessing the risk of contamination from hazardous waste sites has been adopted as the first step in a sequential methodology.

The EPA Strategy includes four major components:

(1) short-term build-up of institutions at the State level;

(2) assessing the problems that may exist from unaddressed sources of contamination (e.g., leaking storage tanks, surface impoundments, and landfills);

(3) issuing guidelines for EPA decisions affecting groundwater protection and cleanup; and

(4) strengthening the agency's coordination with other Federal and State Agencies.

The first component of the strategy is to encourage States to make use of existing grants to develop their own groundwater protection programs and strategies. Activities supported include permit systems and data management systems. Related to the EPA groundwater protection strategy, the EPA groundwater monitoring strategy will help formalize the agency's approach to groundwater protection (U.S. Environmental Protection Agency, 1985) -- once again, the States play a major role.

The State of North Carolina has developed a conceptual framework for an integrated groundwater protection strategy (Nelson and Mew, 1985). The four elements of this strategy are :

(1) an incident management program,
(2) a data integration project,
(3) an advisory groundwater modeling and decision analysis system, and
(4) a public awareness program.

The primary goals of the overall strategy are: pollution prevention of groundwater resources, response to contamination incidents and resource management. The incident management program emerged from an effort to inventory potential sources of groundwater contamination across the State (see Figure I-1). Computerization of the groundwater pollution source inventory has begun in earnest with the aid of data base management software and microcomputer hardware. The data integration project is a new initiative to bring together most groundwater quantity and quality data in a form easily accessible to all agencies or separate organizational units charged with groundwater resource responsibilities. The public awareness program will be designed to present the results of complex groundwater modeling efforts to the public and other decision makers in a format which will allow non-experts to understand alternative courses of action and reach reasoned decisions. The primary objective of the computer-based advisory system is to condition the permitting process upon sound groundwater flow and mass transport modeling strategies and all other available sources of data, within a decision analytic framework.

Through the North Carolina Administrative Code (State of North Carolina, 1985) a perimeter of compliance has been established for both new and existing facilities (which are subject to periodical review through the permit application process). For example, for new facilities, degradation of water quality beyond the first 20 feet vertically and beyond a horizontal perimeter of 250 feet from the point of discharge is not allowed. Compliance must be in accordance with State underground water classifications and water quality standards, and compliance monitoring is required. Remedial action is mandated by statutory authority if a violation of the standards occurs in adjoining underground waters or can be reasonably predicted to occur considering hydro-geologic conditions, modeling, or other available evidence (State of North Carolina, 1985).

Most sophisticated groundwater flow and mass transport analysis programs require significant experience and judgement in input data preparation (e.g., grid selection for numerical simulation, boundary conditions, etc), interpretation of model output and usage of the results to achieve meaningful management objectives. The advisory system provides guidance to the non-expert user through a CHOICE algorithm (in a friendly interactive computer mode) with all of these tasks, including selection of the appropriate model for the particular waste disposal problem and hydro-geologic scenario under review. The algorithm queries the user to determine the applicability of models based on analytical, semi-analytical or numerical solutions to the flow and mass transport governing equations. This intelligent interface incorporates the modeling experience and expertise of the developers and skilled users of the system.

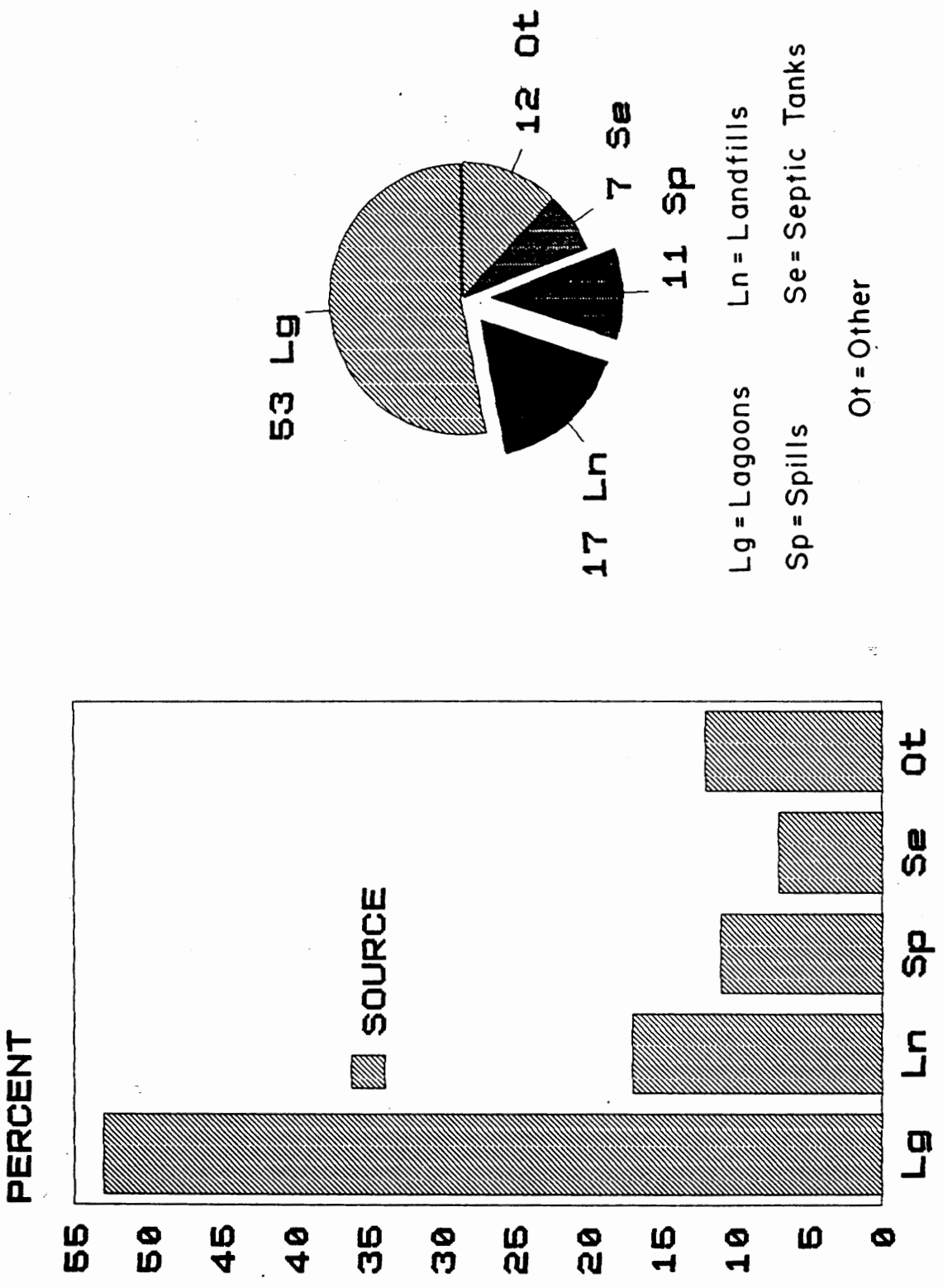

Figure I-1. Inventory of Groundwater Contamination Sources in North Carolina

A simplified representation of the logical flow of steps through the system is presented in Figure I-2. The user is guided through each step interactively. Preliminary screening procedures provide an indication of either no hazard (in which case a permit is awarded) or potential hazard (in which case the system proceeds through further refining steps).

Several hazardous waste site assessment methods were reviewed for selection as a preliminary screening procedure : (1) Hazard Ranking System (MITRE Corporation), (2) Standardized System for Evaluating Waste Disposal Sites (LeGrand), (3) Hazard Potential of Waste Disposal Facilities (JRB and Associates, Inc.), (4) Preliminary Risk Evaluation (Connecticut DEP and TRC Environmental Consultants), and (5) Prioritization of Remedial Actions (North Carolina NRCD). LeGrand's method was chosen : it begins with a numerical designation of a site's hydro-geology (LeGrand, 1980). In addition to various qualifiers, it takes into account four variables : (1) distance from the contamination source to the nearest well (ranked 0-9); (2) depth to the water table below the waste (ranked 0-9); (3) water table gradient (ranked 0-5); and (4) permeability and sorption of the earth materials (ranked 0-9). The higher numbers indicate a relatively less desirable situation : these variable ranks are summed to give a site rating.

The site rating by itself, however, does not provide a measure of the hazard potential. This is obtained by evaluating the "degree of seriousness" value -- a function of both the contaminant severity and the aquifer sensitivity. Each of these can be rated high, medium or low. Aquifer sensitivity is a measure of the likelihood and degree of groundwater contamination. It is a function of the soil permeability, water quality and thickness of the saturated aquifer. Superimposed on the contaminant severity-aquifer sensitivity matrix are the PAR values, which serve as a reference point for the site rating and permeability sorption values. Further details on the computer version of the LeGrand method are presented in later sections.

Site-specific data are evaluated along with some measure of uncertainty, or conversely, reliability. The system queries the user as to whether the facility is an existing (historical) site or a proposed (future) waste disposal site, requests information on waste characteristics, hydro-geologic setting, etc. The next step pools information from the computer-based data (e.g., built-in default values based on expert judgment), existing regional data base and the user-supplied site-specific data. The model selection step depends heavily on the previous step, since the data requirements for each model would be compared to available data. Once a model is selected, the intelligent interface acts as a preprocessor insuring that the data required by the selected model is properly coded before execution in a user-friendly interactive mode. At the next step, a probability distribution of concentration is predicted, incorporating

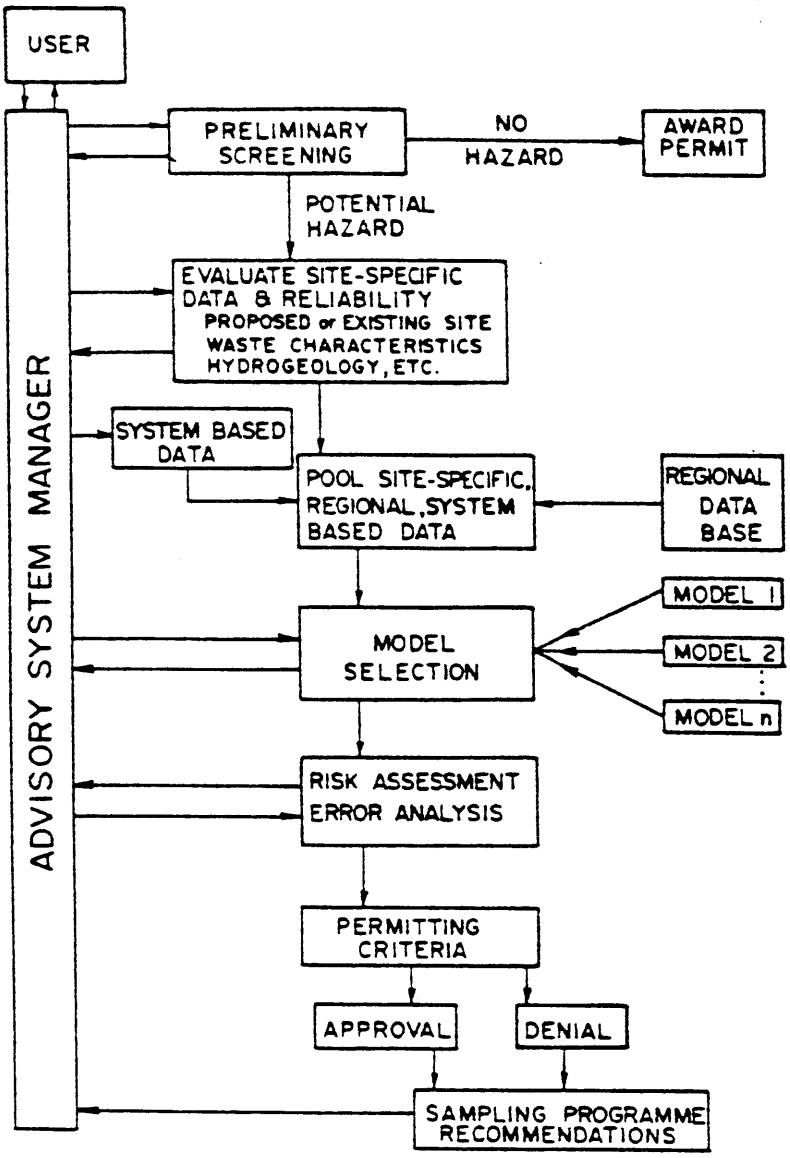

Figure I-2. General Flow Chart of Steps In Advisory System

model error, natural uncertainty, and parameter uncertainty. Permitting criteria (e.g., proximity to drinking water supplies, water quality classification of groundwaters at the site, etc.) are evaluated along with the probability of contamination to recommend approval or denial of a permit -- with possible recommendations for reducing uncertainty by establishing a field sampling and monitoring programme.

In addition to the obvious advantages of using an advisory system to evaluate the impact of these sites on groundwater quality, systematic evaluation and standardization of the method of analysis has tremendous advantages from the legal standpoint. The state agencies can claim that the very best technology available is being utilized uniformly in the decision making process: with the added advantage that the system does incorporate human experience and expertise.

Until recently, professionals involved in groundwater resources management have accepted the large-scale averaging of aquifer characteristics implicit in many of the physically-based models for flow and mass transport. However, more and more research is focusing upon the spatial variability of hydro-geologic parameters such as hydraulic conductivity, compressibility and porosity (e.g. Freeze, 1975; Smith and Schwartz, 1980; Amoozegar-Fard et al, 1982; Hoeksema and Kitanidis, 1985). Because of natural, parameter and model uncertainties, considerable uncertainty is introduced in model results even when the statistical features of the porous media are known. Thus, the need for a risk assessment framework is clearly established.

The authors have borrowed concepts from the field of expert systems and artificial intelligence in the development of the advisory system. According to Jackson (1986),

> "An expert system is a computing system capable of representing and reasoning about some knowledge-rich domain, such as internal medicine or geology, with a view to solving problems and giving advice." He further states that:
>
> -- "it deals with subject matter of realistic complexity that normally requires a considerable amount of human expertise;
>
> -- it must exhibit high performance in terms of speed and reliability in order to be a useful tool;

-- it must be capable of explaining and justifying solutions and recommendations in order to convince the user that its reasoning is, in fact, correct."

Constructing an expert system is often referred to as knowledge engineering, and is considered to be applied artificial intelligence. The advisory system presented in this report is an important first step towards achieving the goal of ultimately constructing a true expert system. As stated earlier, many well-known flow and mass transport models (most originally written in FORTRAN, some in BASIC) have been incorporated into the advisory system and its decision analytic framework. Most artificial intelligence (AI) codes have been written in languages such as LISP and PROLOG, which incorporate fast heuristic search and mechanized inference programming methods. Extensive logic has been built into the advisory system, as available with the standard PASCAL and FORTRAN 77 programming languages. Extensive use of help-screens and preprocessors for data preparation, and algorithms for model selection (e.g., CHOICE), have been included in an interactive mode. The process of incorporating human expertise into the groundwater quality advisory system is expected to be a long-term, continuing activity. The system has been designed to easily incorporate new models through batch files in the disk operating system (DOS) environment of micro-computers, the subject of further discussion in Chapter V, Technical Programming Considerations. The authors recognize and expect that new knowledge in groundwater modeling (e.g., ongoing research on the process of hydrodynamic dispersion) will require modifications to the current software. Simulation codes developed in the future by other investigators for specialized applications can be included in the menu of models available for use.

The European branch of the International Ground Water Modeling Center (Delft, The Netherlands), and the European Institute for Water (Varese, Italy), sponsored a seminar in May 1987 at Como, Italy (Jousma, 1987). Several statements were made relative to modeling as an aid to management of water resources, among which are:

a) "Modeling imposes a discipline by forcing all concerned to be explicit on goals, criteria, constraints, relevant processes, parameter values.

b) Models should be used as means for gaining insight into the physical, environmental, economic, social and other aspects of water resources problems.

c) Models can be used in their generic form to evaluate regional, national and community-wide issues. The same models can be used to investigate specific local and regional situations.

d) Models are useful in identifying existing trends and changes in trends which would result from alternative actions, even if they cannot forecast accurately the actual detailed outcomes.

e) Models are means for communication among professionals in all disciplines relevant to the water resources issues and between them and the agencies, the public and officials.

f) Models can be used to design and manage effective data collection and utilization programs.

g) Simulation models can be used to explore and evaluate the inherent uncertainties of future outcomes.

h) Model output should include an assessment of the reliability and accuracy of the results.

i) The user interface and the direct link between models and decision makers should be developed as an important part of models. Interactive techniques, symbolic representation and color graphics should be an integral part of decision-oriented models and model use."

All of the above statements apply to the advisory system presented throughout this report. It is hoped that the users (who become the modelers) will maintain frequent communication with the decision makers, since involvement of the latter contributes greatly to the acceptance of the results. The friendly, interactive user interface and color graphics are indeed intended to improve the direct use of the system and interpretation of results by those farther detached from the technical details.

For a comprehensive review of the use of numerical models in groundwater management the reader is referred to American Geophysical Union (AGU) Water Resources Monograph No. 5 (Bachmat, et al., 1980). Analytical and semi-analytical methods and codes are reviewed in AGU Water Resources Monograph No. 10 (Javandel, et al., 1984). Most of these codes are included in the advisory system, and were obtained from the International Ground Water Modeling Center, Holcomb Research Institute, Butler University, Indianapolis, Indiana. As noted earlier, pre-processors were written to assist user input of data. Other modifications were made to be able to run the models in a Monte Carlo mode. A critical review of literature reporting field-scale hydrodynamic dispersion data in saturated and unsaturated porous media was conducted by Gelhar, et al. (1985). A summary of data characterizing the parameters and variables appearing in repository siting (radioactive waste) models is provided by Mercer, et al.

(1982); however, much of the information is useful in the application of models to non-radioactive waste sites. Unquestionably, detailed long-term investigations such as those conducted since 1975 at the Borden landfill, 80 km northwest of Toronto, Canada (Cherry, 1983) are acutely needed in North Carolina and throughout the United States.

The advisory system has been designed primarily to assist the State regulatory agency with the permitting process. Therefore, a number of caveats are in order. Predictive modeling is generally performed on a site-specific basis. However, a site-specific approach is useful only for evaluation of existing land disposal units -- where compliance monitoring is in effect and/or other field data are available. Evaluations of proposed facilities must still be accomplished within a constrained decision-making time frame as specified by statute. Although screening procedures built into the advisory system range from simple to complex, even the most complex models are based on a very large number of simplifying assumptions. When coupled with lack of field data, predictions of the concentration distribution of contaminants may exhibit high levels of uncertainty. Even when the latter can be quantified, the regulatory agency must decide what level of uncertainty is acceptable in the decision-making process.

In Chapter II a sequential decision analytic framework is presented, which incorporates but is not restricted to generic scenarios of contamination developed by the U.S. Environmental Protection Agency (1986). The theoretical basis for each component model of the advisory system is presented in Chapter III. It is highly recommended that all users become familiar with the limitations imposed by the governing differential equations and their boundary conditions in representing the natural system. Safeguards and guidelines in model selection are provided within the system, but can be overridden by the user explicitly. A complete user's manual is presented in Chapter IV, supplemented by extensive use of help screens within the code. Technical programming considerations are reviewed in Chapter V for the computer-oriented users and systems programmers.

ROLE OF UNCERTAINTY IN GROUNDWATER RISK ANALYSIS

Over the past several decades many different models for contaminant transport in porous media, under varying conditions and assumptions, have been proposed and tested. These range from very simple, one-dimensional analytical solutions, which assume a completely homogeneous and isotropic medium, to complex three-dimensional numerical solutions, which allow for complete specification of the aquifer and contaminant characteristics throughout a three-dimensional grid. All contaminant transport models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes, and so can provide only an approximation of

the actual spread of contaminant from a given site and the associated risk.

This situation presents a familiar, yet difficult problem to any regulatory agency. As noted above, the North Carolina statutes specifically allow the use of mathematical modeling to assess the probability of violation of standards in groundwater. However, sufficient data on the hydrogeology are rarely, if ever, available to apply the most complex, three-dimensional contaminant transport models to a proposed or monitored site. The agency must, whether explicitly or implicitly, choose a transport model for the analysis based on a trade-off between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models. The topic of appropriate model choice is one of the important focuses of the advisory system.

Even with the choice of an appropriate transport model considerable uncertainty is likely to be present in the analysis of contamination risk. In groundwater transport models (which require estimation of parameters which are difficult to measure and spatially variable, such as hydraulic conductivity and dispersivity), there is often good reason to doubt the accuracy of the input data. For instance, if an analytical model requires the spatial average of the hydraulic conductivity throughout the local area of the aquifer, and the available data consist of only one or two slug tests, plus perhaps an expert opinion, there is good reason to doubt that the reported best estimate of the parameter accurately reflects the true mean value. Simply running the model in a deterministic mode using the best estimates of the parameters will not then provide sufficient information for a regulatory decision, because the uncertainty in the analysis has not been taken into account. For instance, if a deterministic application suggests no risk of contamination, no information is provided as to the certainty of this conclusion. If the regulatory agency determines that it should reject permits for sites with a risk of standard violation greater than some relatively small percentage (say 5%), the deterministic analysis provides only a vague and subjective answer without information on the variability of the predicted results. The recommended alternative is to explicitly consider the uncertainty that is present in the analysis, through the use of Monte Carlo analysis. The theoretical basis for the Monte Carlo analysis procedure is presented in the next section.

Uncertainty enters the modeling process in three ways: 1) through natural parameter variability; 2) through measurement error, which also introduces uncertainty in parameter estimation; and 3) through model error, representing uncertainty introduced by the degree to which the simplifying assumptions used to develop a model fail to accurately represent the actual physical processes at the site in question. The first two of these sources of uncertainty can be analyzed separately. However, the data are often insufficient : in such cases the natural and measurement uncertainty may be combined

into one source of uncertainty for the Monte Carlo analysis, through the specification of the distribution of the parameter value. For instance, the sum of the available site data (subject to measurement error), expert opinion, and available data from similar sites may enable the analyst to conclude only that : the parameter is distributed with equal probability between two bounds. It would then be appropriate to conduct the Monte Carlo risk analysis with the parameter in question specified by a uniform distribution parameterized by the two boundary values. Subsequent sampling at the site may then enable a re-specification of the parameter distribution. The conceptual framework for this process is presented in Chapter II. It should be noted that formal methods are available for incorporation of regionalized information and expert opinion through the Bayesian and Empirical Bayesian calculus. This is an area of ongoing research which has not been fully incorporated yet into the present version of the Advisory System.

The third source of uncertainty in the analysis is due to the degree to which the transport model applied may misrepresent actual processes at the site. This source of uncertainty is very difficult to quantify, and indeed may be impossible to quantify for specific sites unless extensive sampling and monitoring is carried out. Thus this source of uncertainty is not explicitly addressed in the analysis, although some of the component models do allow for the specification of a subjective amount of model error, expressed as a coefficient of variation. Lacking formal analysis of the model error, the emphasis in the system as presently constructed is on the appropriate choice of a transport model, given the current state of data availability and knowledge regarding site hydrogeology. Additional data collected may lead to different choices of models. The analyst should however always keep in mind the question of the appropriateness of a given model to a specific situation. Therefore, detailed information on the solution methods, simplifying assumptions and range of applicability of the various transport models is presented in this report.

To conduct a Monte Carlo analysis it is required that distributions be specified for the underlying parameters. The results obtained may of course be sensitive to these specifications. The criticism might therefore be raised that the Advisory System is likely to bias the analysis of contamination risk by forcing the analyst to use parameter distributions specified by the authors, which distributions may not be optimal or generally accepted. It should be clearly understood that the authors have developed the Advisory System to avoid preempting the choices of the analyst :

(1) examples of parameter distributions reported in the literature are used in the analysis of uncertainty presented in Chapter II;

(2) the analyst has the option to execute most of the

transport models in deterministic mode only; and

(3) in the two models designed for analysis under maximum parameter uncertainty (the Modified EPA Model for Monte Carlo Analysis of Impact on Groundwater, and the Modified EPA Model for Monte Carlo Analysis of Impact on Surface Water) the authors have provided maximum flexibility in the choice of distributional form -- as the user may select from among seven distributional forms.

Specification of a parameter distribution consists of two steps : choice of a distributional form, and specification of the hyperparameters of that distribution. On the first issue, the choice of distributional form, the system does of necessity provide some limitations. That is, for models which are expected to be used in cases for which the impacted aquifer is at least moderately well characterized, certain of the parameter distributions are constrained to follow specific forms, which are generally well accepted in the literature. For instance, in some of the models the mean hydraulic conductivity must be specified by a log-normal distribution. However, even in these cases a choice is present in the parameterization, as the mean hydraulic conductivity may be directly specified from the log-normal, or generated from underlying parameter distributions. In general, where the parameters are at least moderately well known the choice of a distributional form should not have a major impact on the results. In its present form, the Advisory System incorporates the framework for Monte Carlo analysis, but additional research is needed to develop the parameter distributions and values for hydrogeologic conditions in North Carolina and elsewhere.

The question of guiding specification of the hyperparameters of the distributions represents a more difficult problem, in which there is a need to balance between the provision of guidelines for input and the avoidance of improper specification by the system. The general approach taken for most of the component models incorporated into the system is that the values of the hyperparameters are <u>not</u> specified by the system, but must be specified by the user. In such cases the system merely guides input by specifying the allowable range of input parameters. The analyst will need to provide the parameterization of the distributions based on reported data <u>and</u> expert opinion, if available (the two may be formally combined by the use of Bayesian statistics). Future improvements of the system will provide a means for the automatic combination of site-specific and regional data through Empirical Bayesian methods. However, this will not be of practical significance for the State of North Carolina until an adequate data base system is designed and implemented.

The only instances in which hyperparameter values <u>may</u> be directly specified by the system are in the two EPA models. These models are particularly designed for analysis in cases where very little site-

specific data are available. In such cases it may be necessary to perform the preliminary analysis of a site using representative regional values (and it is conceived that such an analysis would likely be followed by the submission of further data and analysis using more site-specific values, and, if appropriate, a different model). To fit the data needs of these models the authors have therefore attempted to provide hyperparameter data sets representative of reported regional parameter distributions for several of the major soil provinces of North Carolina. However, it should be stressed that the models are <u>not</u> intended to be run directly with these regional hyperparameter distributions without further thought. That is, it is intended that the analyst should examine the regional data set as a guide for input, and then alter the hyperparameter values (or distributions) based on any site specific data which are available and/or expert opinion. Indeed, one of the major advantages provided by the flexibility and data management capabilities of the system is that the analyst can readily apply a model using several different sets of parameter specifications, with the intention of examining whether the predicted results are affected by the specification.

Finally, it should be emphasized that the Advisory System is intended to be a useful tool, and not a replacement for a thorough site-specific hydrogeologic investigation. It explicitly involves interaction with the analyst in the choice of model and characterization of the parameter distributions. It is designed to aid the competent analyst while incorporating expert knowledge in a user guided format. The authors believe that adequate consideration of uncertainty is very important in the formulation of a sensible risk analysis, particularly in cases where the available site data is limited. Groundwater contaminant transport models have not been readily available in the past to regulatory agency personnel in an easily accessible format. The analyst has then been forced to either proceed with a deterministic analysis, or write a specific application program to undertake the Monte Carlo analysis. The Advisory System provides a large collection of recognized mass transport models in either Monte Carlo or deterministic format, which will hopefully serve to extend the capabilities of the analyst.

CHAPTER II

A SEQUENTIAL METHOD FOR ASSESSING WASTE DISCHARGES TO GROUNDWATER

This chapter describes a sequential decision-analytic framework within which the predictive models (presented in Chapter III) are executed as needed in the permit review process. Both general flow charts and very specific algorithms are presented. Some segments of the general flow charts refer to compliance monitoring steps which will require additional research before implementation in the advisory system, but which are included so that the reader can obtain a complete view of the operational framework.

2.1 PROXY DECISION ANALYSIS

From a decision analysis perspective, the criterion for ranking alternate levels of waste site control, say L_1 and L_2 is based on their corresponding expected net benefits, $E[NB|L_i]$. For any level of control L_i, the net benefits can be calculated, in principle, by subtracting the cost of supplying control level L_i from the benefits of the avoided hazard costs (see Figure II-1). But while supply costs present a tractable problem, the estimation of the avoided hazard costs is infinitely more problematic due to the difficulties of addressing human health damage costs. Estimates can be obtained through econometric analysis or, alternatively, through subjective valuations : for example, multiattribute utility theory (Keeney and Raiffa, 1976). But the need to explicitly value politically sensitive and imprecise health effects places practical limits on the application of a formal decision analysis to the problem of hazardous waste site management.

An alternative approach involves the specification of objectives by proxy. One such commonly used strategy is the specification of a water quality standard as an objective. Clearly, the standard represents a trade-off between health and treatment effects, but it does so implicitly. Given a legislated standard, the appropriate level of protection becomes that which meets the standard at minimum cost.

In view of the need for a practical perspective, the strategy followed in the advisory system is based on the probability distribution of the concentration of the contaminant at any point x and time t. This is consistent with a proxy objective specified by a concentration standard with a reliability constraint (e.g., the probability that the concentration at or near a drinking water supply

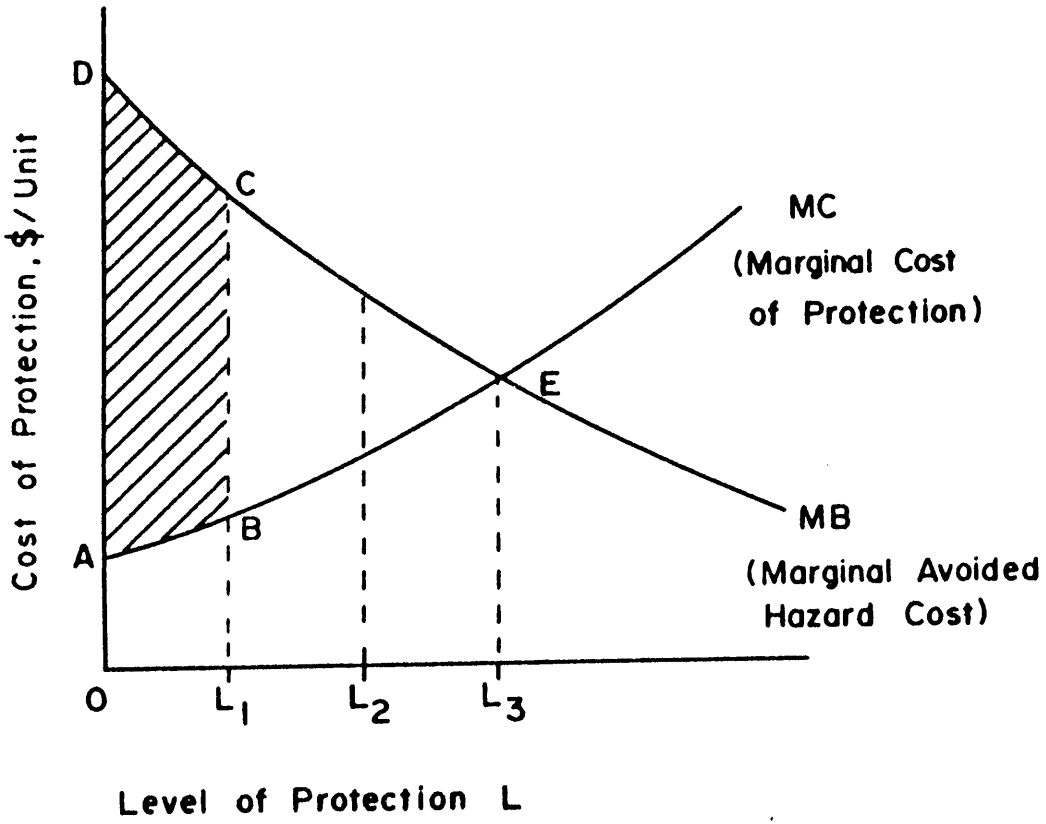

Figure II-1. Net Benefits of Avoided Hazard Costs

exceeds c_s must be less than p %). The reliability factor is introduced to acknowledge the uncertainty inherent in the prediction/occurrence of field concentrations. Even beyond economically feasible levels of protection, there will be a finite, though small, probability of exceeding a concentration standard.

2.2 GENERAL ALGORITHM

The calculation of the fate of contaminant releases from a hazardous waste site involves the simultaneous consideration of a number of factors: the reliability of the waste site, the type and quantity of stored materials, and the direction and rate of transport. Each of these, however, is characterized by various uncertainties (natural, parameter, model) which make their prediction inherently imprecise and force a risk assessment. In an operational mode, such as that of a permit reviewing agency, such a detailed computation is not practical for every site. The results of such an approach are presented later to illustrate the effect of the various types of uncertainties on the prediction.

The general algorithm for the sequential method is outlined in Figure II-2. Note that the steps listed below do not necessarily imply a sequence. Steps 2 through 7 apply to existing sites only. The current version of the advisory system focuses primarily on proposed sites.

STEP 1 The first step in the algorithm determines whether the site is existing or proposed. In the case where it is an existing site, the algorithm continues at step two, where it is assumed that routine compliance monitoring data is being intermittently collected in the area surrounding the site. If it is a proposed site, the algorithm proceeds to step eight from step one.

STEP 2 Since the intent of compliance monitoring is to determine whether a change in the leachate release pattern has occurred, previous data is useful only for defining a reference point or background. The second step is concerned with calculating the posterior probability, p, that the measured concentration exceeds the standard. The algorithm now proceeds to the third step.

STEP 3 In the third step, a site decision is made on the basis of the probability criteria adopted by the agency. If p is less than the criteria I level, C_I, the site passes its routine compliance test and is scheduled for its next sampling cycle. If p exceeds the criteria II level, C_{II}, the site is recommended for remedial action. On the other hand, if $C_I \leq p \leq C_{II}$, the site evaluation proceeds to step four, the preposterior analysis, for consideration of additional sampling.

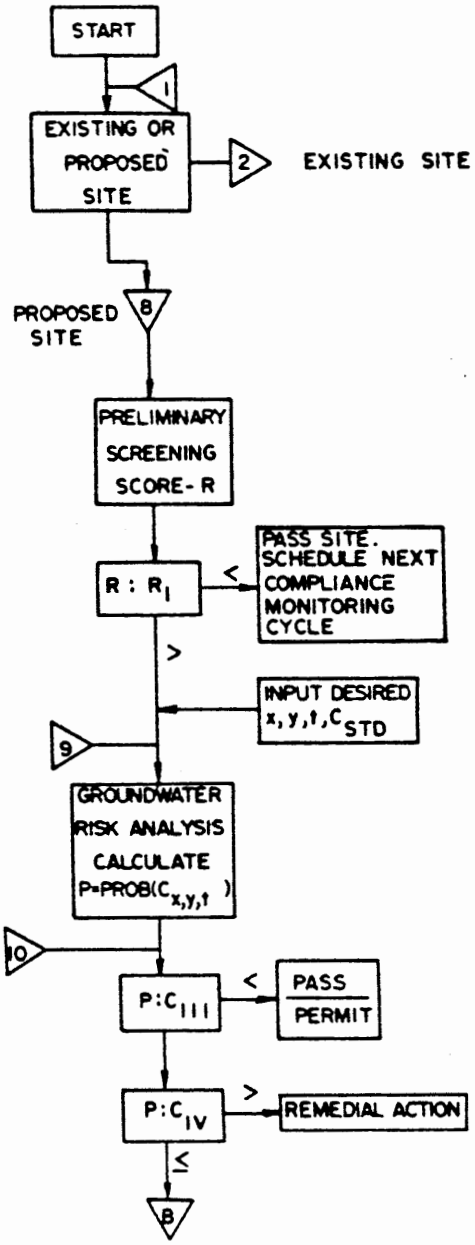

Figure II-2. Algorithm for the Sequential Decision-Analytic Framework (Proposed Sites)

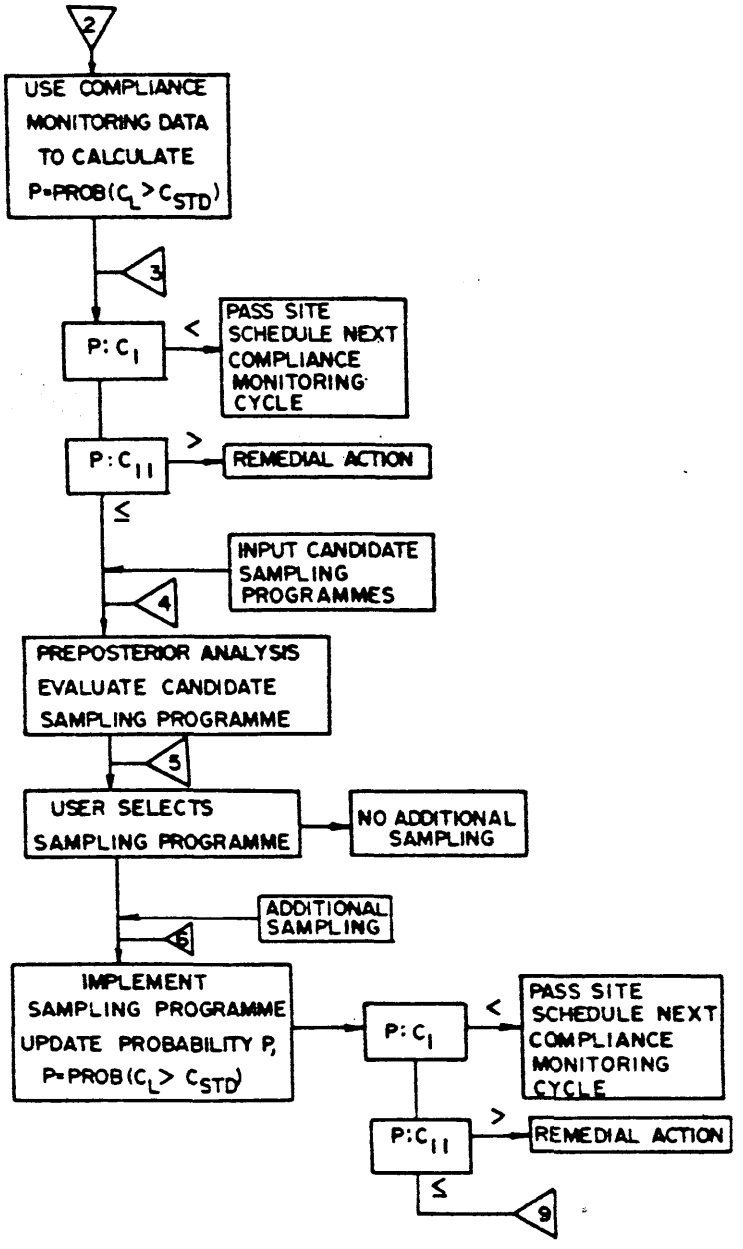

Figure II-2. Algorithm for the Sequential Decision-Analytic Framework (Existing Sites)

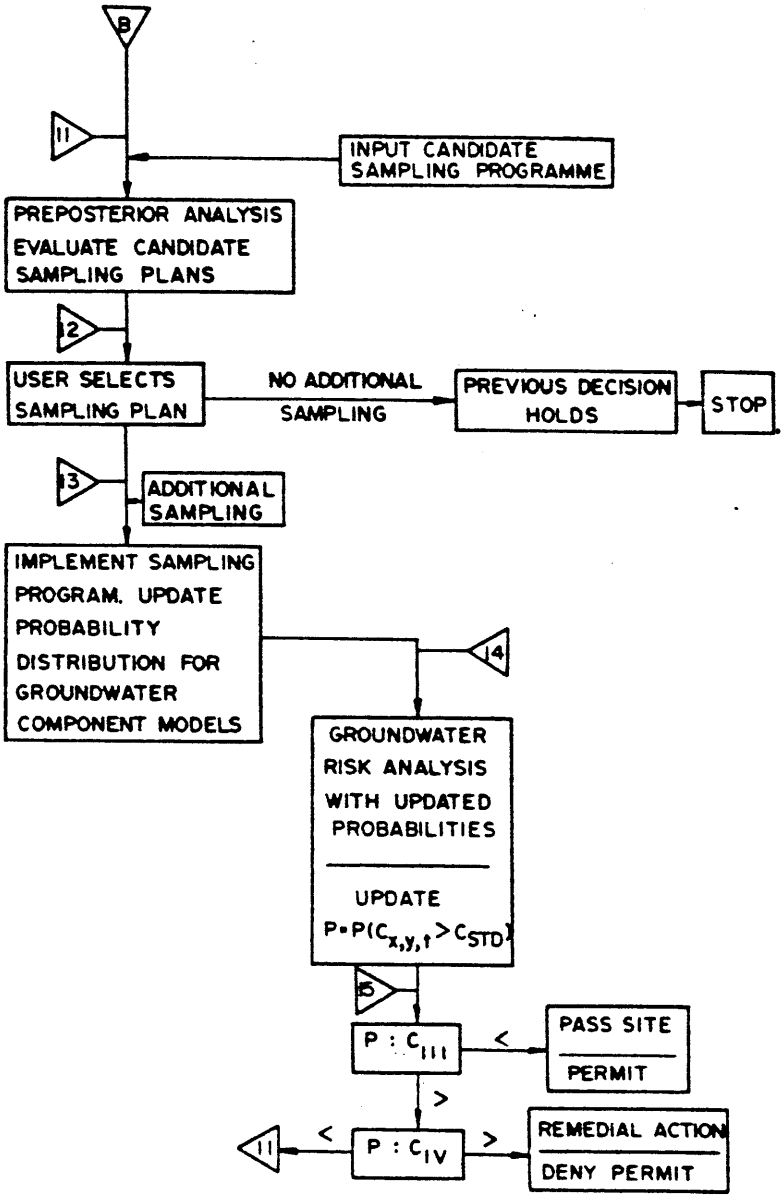

Figure II-2. Algorithm for the Sequential Decision-Analytic Framework (Additional Sampling)

STEP 4 Preposterior analysis uses the posterior probability distribution used to calculate p in step two, together with a sampling programme input by the user (number and type of samples, instrument measurement error), and calculates the average reduction in the variance of the posterior probability of the concentration and/or the likelihood of changing classification. The user can experiment similarly with alternative programmes. Eventually, the user must decide whether the benefit of the most efficient sampling scheme justifies its cost. Conceivably, criteria can be defined, which reflect agency priorities, that would make it possible to automate this juncture in future versions of the algorithm. The algorithm proceeds to step five.

STEP 5 A sampling recommendation is obtained from the user in step five. If no additional samples are taken, the algorithm proceeds to step nine. If sampling is recommended, then the algorithm proceeds to step six.

STEP 6 The additional data is combined with the posterior distribution in step two (now the prior) to obtain an updated posterior distribution for the concentration. The algorithm now proceeds to step seven.

STEP 7 In the seventh step, as in the third step, a site decision is made on the basis of the probability criteria adopted by the agency. If p, the updated probability calculated in step six, is less than the criteria I level, C_I, the site passes its routine compliance test and is scheduled for its next sampling cycle. If p exceeds the criteria II level, C_{II}, the site is recommended for remedial action. On the other hand, if $C_I \leq p \leq C_{II}$, then the site evaluation proceeds to step nine for a detailed groundwater risk analysis.

STEP 8 If the site in question is a proposed site, a preliminary screening analysis using LeGrand's (1980) ranking scheme is performed. If the site rank is less than the established rank criteria, the site passes inspection and is scheduled for routine compliance monitoring. If the site rank is greater than the established rank criteria, the algorithm proceeds to step nine for a detailed groundwater risk analysis.

STEP 9 Step nine performs a groundwater risk analysis using only currently available (prior) data. Probability models for leachate concentration, natural and parameter uncertainty in the hydraulic conductivity random field, and groundwater model error are included. Using Monte Carlo simulation, the groundwater risk analysis evaluates the probability distribution for the contaminant concentration at point x,y and time t, $P[C_{xyt}]=p$.

STEP 10 In the tenth step, as in the third step, a site decision is made on the basis of the probability criteria adopted by

the agency. If p, the probability calculated in step nine, is less than the criteria III level, C_{III}, the site passes its compliance test in the case of an existing site (is permitted in the case of a proposed site) and is scheduled for its next sampling cycle. If p exceeds the criteria IV level, C_{IV}, the site is recommended for remedial action in the case of an existing site (the permit is denied in the case of a proposed site). On the other hand, if $C_{III} \leq p \leq C_{IV}$, then the site evaluation proceeds to step eleven for consideration of additional sampling.

STEP 11 In step eleven, preposterior analysis is used to evaluate the potential benefit of alternative sampling plans for each of the component models in the risk analysis subroutine in step nine. Using the prior distributions of each of the component models, and a given user input sampling programme (number and type of samples, instrument measurement error), preposterior analysis is used to calculate the average reduction in the variance of the posterior probability of the concentration (relative to the posterior distribution for the concentration calculated in step nine) and/or the likelihood of changing classification (relative to the classification decision in step ten). The user can similarly evaluate alternative programmes. Eventually, the user must decide whether the benefit of the most efficient sampling scheme justifies its cost.

Conceivably, as before, criteria could be defined that would make it possible to automate this juncture in future versions of the algorithm. The algorithm proceeds to step twelve.

STEP 12 A sampling recommendation is obtained from the user in step twelve for each of the component models. If no additional samples are to be taken, the decision obtained in step ten, or alternatively in step fifteen, stands and the algorithm ends. On the other hand, if additional sampling is recommended, then the algorithm proceeds to step thirteen.

STEP 13 The additional data is combined with the prior distributions in each of the component models to yield updated posterior distributions for each of the component models. The algorithm now proceeds to step fourteen.

STEP 14 In step fourteen a groundwater risk analysis is performed as in step nine, except that the updated posterior distributions of each of the component models obtained in step thirteen are used instead. This results in an updated value of p. The algorithm proceeds to step fifteen.

STEP 15 In the fifteenth step, as in the tenth step, a site decision is made on the basis of the probability criteria adopted by the agency. If p, the updated probability calculated in step fourteen, is less than the criteria III level, C_{III}, the site

passes its compliance test in the case of an existing site (is permitted in the case of a proposed site) and is scheduled for its next sampling cycle. If p exceeds the criteria IV level, C_{IV}, the site is recommended for remedial action in the case of an existing site (the permit is denied in the case of a proposed site). On the other hand, if $C_{III} \leq p \leq C_{IV}$, then the site evaluation proceeds to step eleven for consideration of additional sampling. Once in the groundwater risk analysis loop, the algorithm can only end with a decision to stop sampling in step twelve.

2.3 Component Models of Risk Analysis

Concentration prediction calculations in a groundwater risk analysis mode consist of three linked stages : (1) analysis of the rate of contaminant leaching from the source into the aquifer; (2) statistical description of the parameters representing aquifer hydrology; and (3) simulation of groundwater transport from the source to a perimeter of compliance, given (1) and (2). The techniques required to implement these three stages may vary depending upon the type of contaminant source and the data requirements of the groundwater flow and mass transport models chosen.

In order to provide an example of a very thorough calculation of the uncertainties in concentration predictions, the probability models are linked in a Monte Carlo risk analysis with a groundwater solute transport model (Method of Characteristics, MOC) : applied in this section to the specific case of a lined hazardous waste landfill for which there is a certain probability of failure of the containment device and subsequent groundwater contamination. As noted earlier, such a detailed approach is not practical for every site review; however, it illustrates clearly the influence of uncertainty in the concentration predictions and the means by which this uncertainty can be quantified. The component models include: (1) a site reliability model, (2) a leachate concentration model, (3) a hydraulic conductivity random field model, and (4) the groundwater solute transport model, modified for Monte Carlo analysis.

Site Reliability - $P(t_f|p)$

Given that the probability that the landfill will fail in any year (alternative periods can be used without loss of generality) is p, then t_f, the year the landfill fails for the first time is geometrically distributed with parameter p :

$$\text{Prob}(t_f=t|p) = p(1-p)^{t-1} \qquad (2.1)$$

It is very likely that the value of p can be estimated only with limited precision. To reflect this uncertainty, we assume that the parameter p is a priori beta distributed with parameters a and b :

$$p \sim \text{Beta}(a,b) \tag{2.2}$$

Leachate Release Concentration - $P(C_L|t_f)$

Given that a failure has occurred, the probability of the amount/characteristics of the released point source contaminant, C_L, at time t_f is a priori normally distributed with mean u_c and variance v_c :

$$C_L|t_f \sim N(u_c, v_c) \tag{2.3}$$

Hydraulic Conductivity Random Field - $P(K|u_k,v_k)$

It is well documented that the spatial variability of hydraulic conductivity can have a significant effect on the field-length dispersion of contaminant plumes and that hydraulic conductivity is lognormally distributed (Freeze, 1975; Smith and Schwartz, 1980, 1981). A two level stochastic model is assumed to reflect both natural and parameter uncertainty in the hydraulic conductivity field distribution. For the case of m nodes, it is assumed that $\underline{K} = \ln(\underline{K}_0)$, the (mx1) vector of the natural logarithm of the hydraulic conductivity follows an m-dimension normal multivariate distribution with mean $u_k\underline{b}$ and covariance v_kB,

$$\underline{K} \sim N_m(u_k\underline{b}, v_kB) \tag{2.4}$$

where $\underline{b}=(1,1,\ldots,1)^T$, is an mx1 vector of ones, B is an mxm matrix whose diagonal elements are equal to one, and whose ijth off-diagonal elements are given by $\exp(-d_{ij}/d_0)$, where d_{ij} is the distance between the ith and jth point and d_0 is the correlation length. This model is similar to the one used by Hoeksema and Kitanidis (1985) in their statistical study of hydraulic conductivity properties. In addition, in order to reflect uncertainty about the parameters of the distribution, it is assumed that a priori u_k conditioned on v_k is normally distributed with mean M and variance v_k/r,

$$u_k | v_k \sim N(M, v_k/r), \tag{2.5}$$

and $(1/v_k)$ is gamma distributed with parameters c and d,

$$(1/v_k) \sim \text{Gamma}(c,d). \tag{2.6}$$

Groundwater Transport - $P(C(x,t) | C_L, t_f, \underline{K})$

Given a time to failure, t_f, a release concentration, C_L, and a log hydraulic conductivity field, $\underline{K}$, the contaminant concentration, $C(x,y,t)$, at point x,y and time t, is assumed *a priori* normally distributed with mean $G(x,y,t,\underline{K},t_f,C_L)$ and variance v_g.

$$C_{xyt} | \underline{K}, t_f, C_L \sim N(G(x,y,t,\underline{K},t_f,C_L), v_g). \tag{2.7}$$

where $G(x,y,t,\underline{K},t_f,C_L)$ is the output concentration from a deterministic groundwater model run using the values x, y, t, t_f, $\underline{K}$, and C_L; and v_g represents the model prediction error variance.

2.4 ERROR PROPAGATION

The groundwater component model presented in section 2.3 provides the probability distribution of the concentration, $C(x,t)$, given that the time to failure, t_f, the point source concentration, C_L, and the hydraulic conductivity were known precisely. In fact, as postulated above, all of these can be considered as random variables. If the uncertainty in each of these "inputs" is taken into account, then the resulting unconditional distribution,

$$P(C(xyt)) = \int\int\int\int\int\int \Big[P(C(xyt) | C_L, t_f, \underline{K}) P(C_L | t_f) P(t_f | p) P(p) \; P(K | u_k) P(u_k | v_k) P(v_k) \Big] dC_L dt_f dp dv_k du_k \tag{2.8}$$

will be characterized by a larger variance due to the uncertainty in each of its individual components. While it will not be possible, in general, to find an analytical solution to the integrals in Equation (2.8), Monte Carlo simulation can be used to obtain an approximation for the distribution for C(xyt) and for any analytical function thereof.

Monte Carlo Algorithm For Prior Analysis

Given the probability component models described above, the Monte Carlo algorithm used for performing the groundwater risk analysis outlined in step nine of the sequential algorithm is presented below:

STEP 1 Set I=1, specify coordinates x,y and time t, and NSIM the number of Monte Carlo simulations.

STEP 2 Generate time to failure, t_f.

2.1 Generate random variable p from a Beta(a,b) distribution.

2.2 Generate t_f from a Geometric distribution with parameter p.

STEP 3 Generate leachate concentration, C_L.

3.1 Generate random variable C_L from a Normal distribution with mean u_c and variance v_c.

STEP 4 Generate (mx1) vector of hydraulic conductivities, $\underline{K}_0$.

4.1 Generate random number $(1/v_k)$ from a Gamma(c,d) distribution.

4.2 Given the random number $(1/v_k)$ generated in 4.1, generate the random number u_k from a Normal distribution with mean M and variance v_k/r.

4.3 Given u_k and v_k above, generate an (mx1) vector $\underline{K}$ of random variables from a Normal distribution with mean $u_k\underline{b}$ and covariance v_kB.

4.4 Calculate $K_{0j} = \exp(K_j)$ for j=1,2,...,m

4.5 Set $\underline{K}_0=(K_{01}, K_{02},\ldots,k_{0m})^T$.

STEP 5 Generate $C(xyt)_I$.

5.1 Run groundwater model with conditions derived in steps one through five above for $(t-t_f)$ years for $(t-t_f)>0$.

5.2 Set $C(xyt)_I$ equal to the predicted concentration at coordinates x and y and time t if $(t-t_f)>0$, and equal to the background concentration otherwise.

STEP 6 Set I=I+1.

STEP 7 If I <= NSIM go to step 2, else go to step 8.

STEP 8 Perform statistical analyses on vector $C(xyt)_I$, i=1,2,...,NSIM.

8.1 Calculate sample mean, sample variance, skewness, etc., and sample cumulative distribution function.

8.2 Calculate, $Prob(C(xyt) > C_{std})$, the probability that the contaminant concentration at coordinates x and y at time t exceeds C_{std} (standard) using the cumulative distribution function calculated in 8.1.

Error Propagation With Additional Information

In general, the prior models presented in section 2.3 will be derived from regional or literature data. If additional site specific information were to be obtained for any given component, it would result in a reduction in the prediction uncertainty of the given component model and could ultimately result in a reduction in the error of the groundwater concentration.

The general principle underlying the process of updating prior information with additional data is embodied by Bayes' theorem (Raiffa, 1970). If the uncertainty in random variable A is described by the probability distribution P(A), and additional information, I_A, becomes available (e.g., through direct observation) whose uncertainty is characterized by the probability distribution $P(I_A|A)$, then Bayes'theorem states that the updated distribution of A, $P(A|I_A)$, after having observed the external information is given by

$$P(A|I_A) = \frac{P(I_A|A)\ P(A)}{\int P(I_A|A)P(A)\ dA} \qquad (2.9)$$

The probability distributions p(A) and $P(A|I_A)$ are known as the prior and posterior distributions for A, respectively.

Posterior analysis consists of two basic steps. First, update

the prior distributions (calculate the posterior distributions) to reflect the effect of the additionally collected data, and second, use the calculated posteriors to evaluate the effect of propagation error on the concentration predictions.

2.5 Compliance Monitoring and Evaluation of Alternative Sampling Programmes

Preposterior analysis is required in steps four and eleven of the sequential assessment algorithm. Each is treated separately. Step four involves only the leachate concentration. Step eleven, on the other hand, also involves the hydraulic conductivity and in addition requires the implementation of a groundwater simulation model. In the latter case, consideration could also have been given to obtaining additional information in the time to failure model. But as this information, at least as posed here, is beyond experimental control, its consideration was dropped from the preposterior analysis.

The essential idea behind preposterior analysis is that the distribution which currently summarizes the available information for a given quantity, the reference distribution, can in turn be used to evaluate the potential value of additional sample information without the need to explicitly obtain the additional information. Clearly, the reference distribution could be either a prior or a posterior distribution. Much of the future development of the advisory system will be devoted to compliance monitoring and the evaluation of alternative sampling schemes.

2.6 Results of Simulation Experiments

The component models described in Section 2.3 were utilized in a series of simulation experiments. The resulting distributions of contaminant concentrations provide insight into the process of error propagation. The groundwater flow and mass transport model chosen for the experiments is the Method of Characteristics (MOC) model (Konikow and Bredehoeft, 1978), described in detail in Chapter III. This two-dimensional model was modified for Monte Carlo simulation, to enable an analysis of the sensitivity of model predictions of contaminant concentrations to sources of uncertainty in the inputs and parameters of the model. Two of these concerned the variance in time to failure and the leachate concentration, while the other three concerned natural and parameter uncertainty and spatial clumping in the hydraulic conductivity field. The models were applied to a realistic aquifer situation, representative of the North Carolina coastal plain area.

In the first design only three factors were considered, with minus levels all set equivalent to zero variability. These factors were the variance in time to failure, variance in release concentration at the landfill, and the variance of lnK (natural log of the hydraulic conductivity). Because only three factors were considered a full factorial design was carried out in 8 runs, allowing identification of the interactive effects. It should be noted that, with r (degrees of freedom in the prior distribution for the lnK variance) held constant, the variance of lnK reflects both natural and parameter uncertainty. However, by allowing r to go to infinity the parameter uncertainty is eliminated. Additional runs were undertaken in this manner to contrast the contributions of natural and parameter uncertainty in the hydraulic conductivity distribution. Each simulation run consisted of 250 iterations. When the sample variance of lnK was set to 0 (- level), the value of lnK was adjusted accordingly to preserve the mean of K in normal space. One run in the design, with all variances set to zero, resulted in a deterministic outcome.

In the second set of simulations five factors were considered in the design, with plus and minus levels centered around observed values of variability. In addition to the three factors used in the first set of simulations, consideration was also given to two other factors determining the hydraulic conductivity field: r and d(0). Each simulation run consisted of 500 iterations. A complete factorial design in 5 factors would require 32 runs, which would consume considerable computing time. Therefore, following Box et al (1978), a design was constructed as a balanced quarter-fraction of the full design, requiring only 8 runs. This separates all of the main (single factor) effects, but leaves these effects subject to be mixed with higher order interactive effects, which are not specifically identified. In these runs lnK was fixed so that the median, rather than the mean K, was preserved.

Appropriate selection of parameter means and levels of variability is important to the successful interpretation of simulation results. As noted above, the minus levels of variability were simply set to zero for the first set of simulations, while the two factors not varied in these simulations (r and d(0)) were set to the mean of the levels used in the second simulations. Other parameters values are shown in Table II-1.

Observations of contaminant concentrations at a 25 year target period were made at 5 nodes along the main axis of flow leading from the landfill site. The first of these was beneath the site, while the other four were successively 500 feet further along the main flow axis. Background concentrations were set to a uniform 1 mg/l, so that some concentration was always observed. While the background concentrations were also subject to advection and dispersion, in this particular application of the model the concentrations always remained between 0.80 and 1.00 mg/l at the target year, unless

impacted by the contaminant plume from the landfill. The observed contaminant concentrations thus tended to follow a bimodal distribution, with a peak at 1.0 and a superimposed distribution resulting from the contaminant plume which tended to follow a log-normal distribution. The effect of the various treatments of each node was monitored in three ways: 1) the change in variance of contaminant distribution; 2) the change in probability of observed concentration ≤50 ppm; and 3) the change in probability of concentration ≤1 ppm, which represents the probability of not observing concentrations greater than the background level.

Table II-1. Parameter values used in the two experimental designs.

Parameter	Design 1		Design 2	
	+	-	+	-
1. Failure Time				
alpha	0.1	10 years	0.05	0.1
beta	0.1	(fixed)	0.15	0.1
2. Release Conc.	3500	3500	3500	3500
u(c) (ppm)	875	0	875	0
v(c)				
3. Hydraulic Conductivity				
mean lnK	-11.367	-10.911	-11.367	-11.367
sample var.	.913	0	1.140	.684
r (df)	18	18	23	13
d(0) (ft.)	36960	36960	55440	18480

First Simulation Experiment

In this set of simulations the (-) treatment levels were all set to 0 and the three factors investigated were variance in failure time, variance in release concentration and sample variance of ln K. Each run was composed of 250 iterations.

It is instructive first to compare the distributions obtained for each single source of variability with the deterministic solution. The sample concentration distributions for observation point 2 are shown in figure II-3(a)-(f). The effects of changes in the characterization of sources of variability are immediately evident. The first impression is the difference in the responses, relative to the deterministic solution, of the time to failure and release concentration effects versus the hydraulic conductivity effects. In the former case, as shown in Figures II-3(b) and II-3(c), the uncertainty in predictions is limited to a narrow range about the deterministic response. In the case of the release concentration variance the spread is fairly normal, reflecting the gaussian character of the release concentration distribution. In the time to failure case, however, the distribution manifests a bimodal character that reflects the exponential decay of the geometric time to failure distribution.

In contrast, the effect of variance in hydraulic conductivity results in more lognormal distributions with higher uncertainty as reflected by long right hand tails (see Figure II-3(e)). It is interesting to note, comparing Figure II-3(d) and II-3(e), the importance of parameter uncertainty in determining the extent of the right hand tail.

It is evident that in the first two instances (Figures II-3(b)-(c)), the extent of the uncertainty is limited by the absence of variability in the hydraulic conductivity which constrains the potential extent of plume migration. However, as evidenced in Figure II-3(f), the combination of all three sources of uncertainty magnifies the individual effects.

Finally, and more importantly, it is clear that while the incorporation of uncertainty has little effect on the mean concentration relative to the deterministic concentration profile (see Figures II-4(a)-(c)), uncertainty has a significant impact on the concentration variance, and hence the probability of violation. Further evidence is provided in Figure II-5, which shows the 5 and 95% quantiles of the concentrations at each of the five points due to uncertainty in the hydraulic conductivity. It is also worth noting that for the selected set of parameters, the variance decreases with increasing distance from the site. However, as is clear from Table II-2, the variance relative to the mean concentration remains large for points beyond 2. This is due to the fact that extension of the

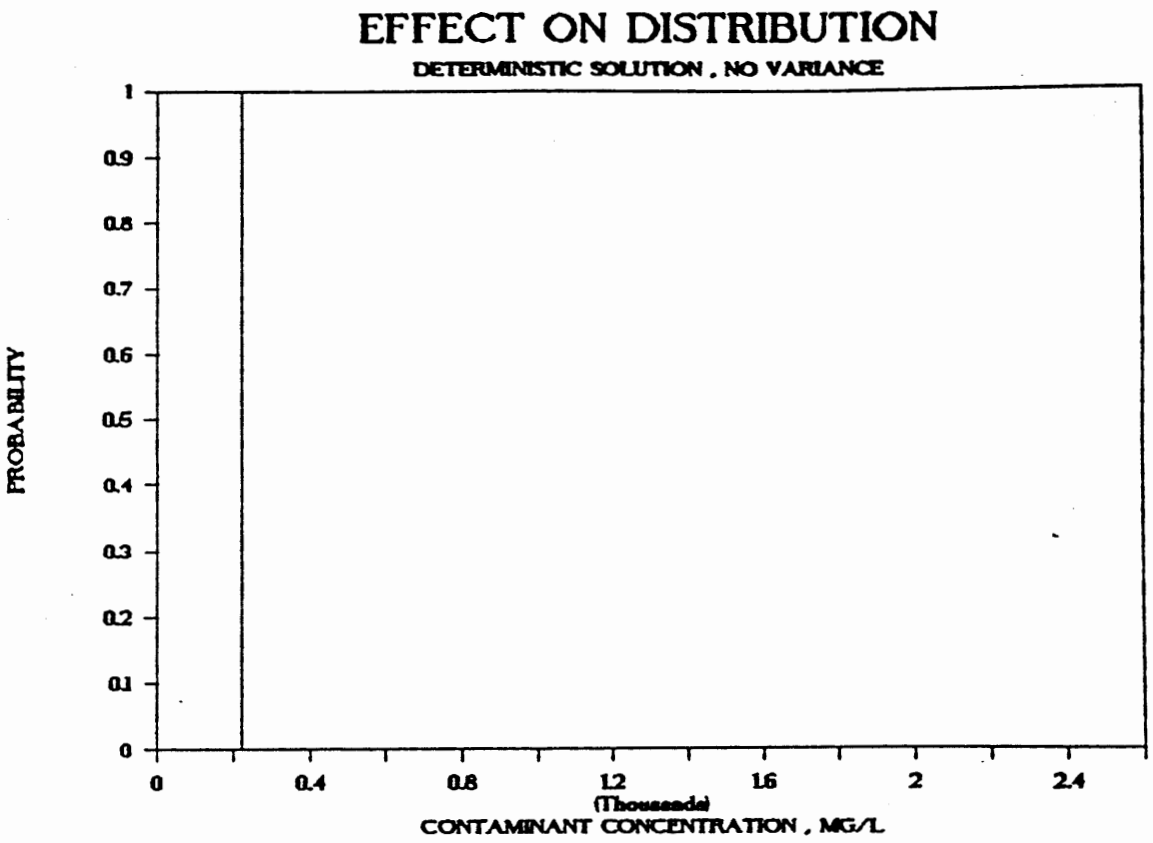

Figure II-3(a). Effect On Probability Distribution of Contaminant Concentration at a Point, Deterministic Solution With No Variance.

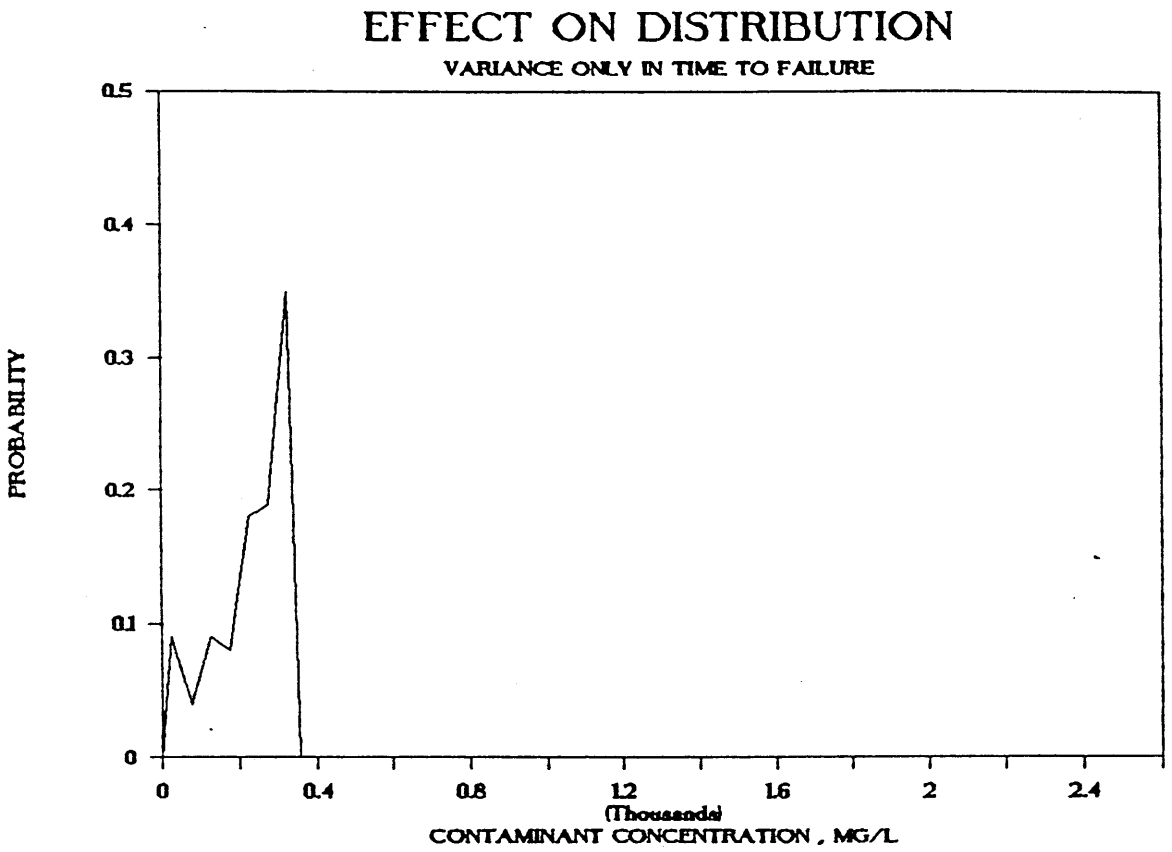

Figure II-3(b). Effect On Probability Distribution of Contaminant Concentration at a Point, Variance In Time To Failure Only

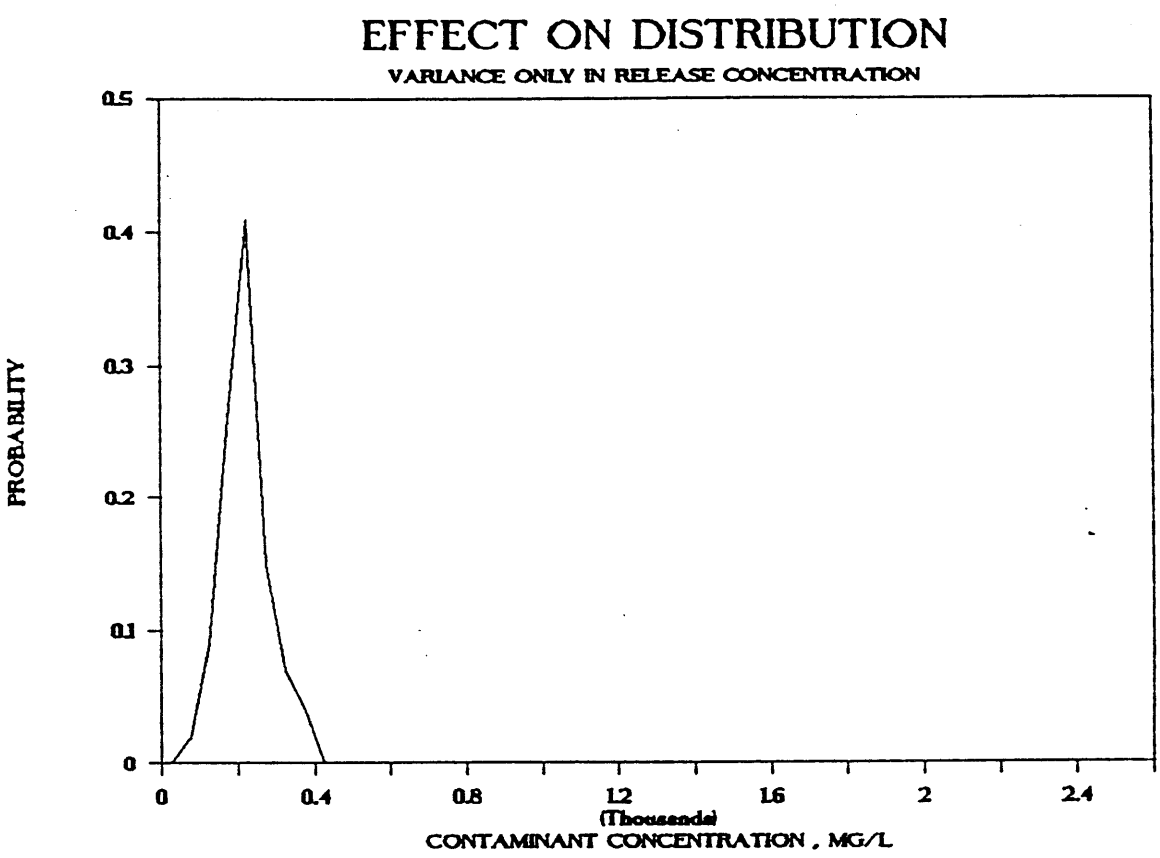

Figure II-3(c). Effect On Probability Distribution of Contaminant Concentration at a Point, Variance In Release Concentration Only

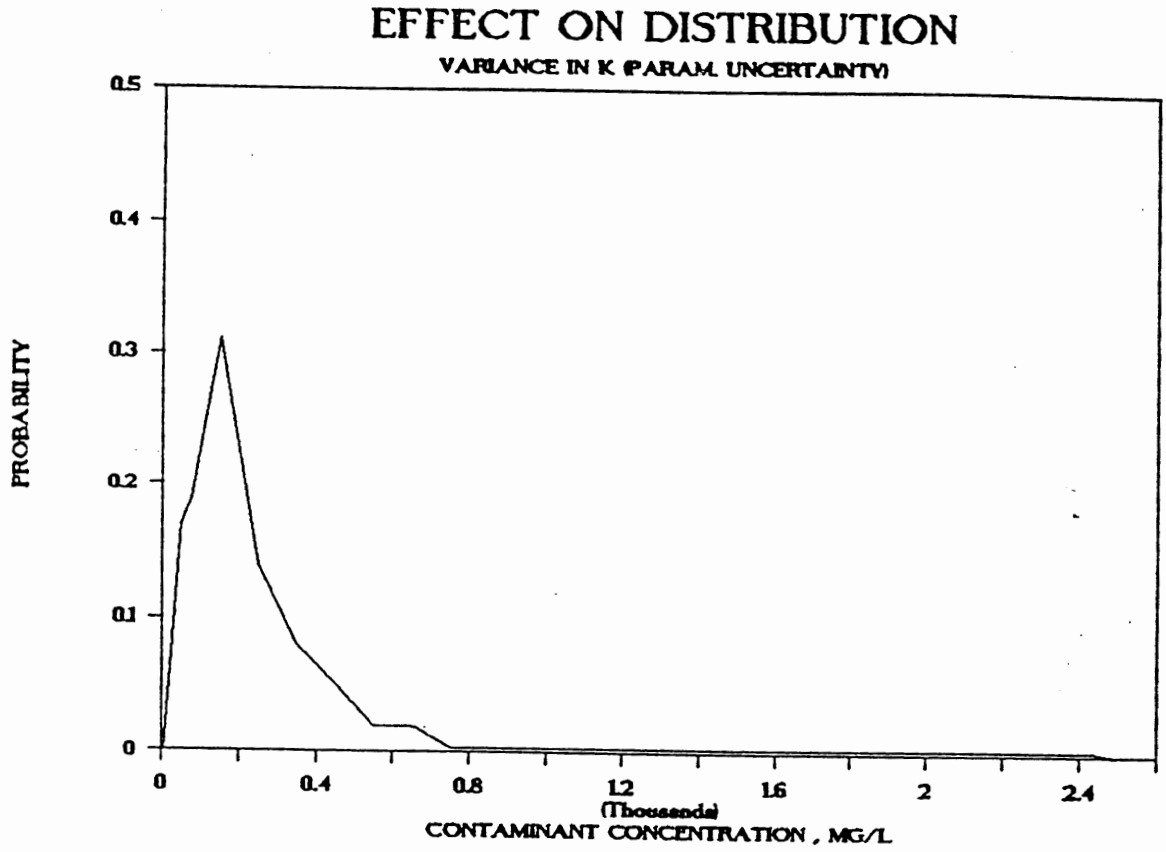

Figure II-3(d). Effect of Probability Distribution of Contaminant Concentration at a Point, Variance in Hydraulic Conductivity due to Parameter and Natural Uncertainty

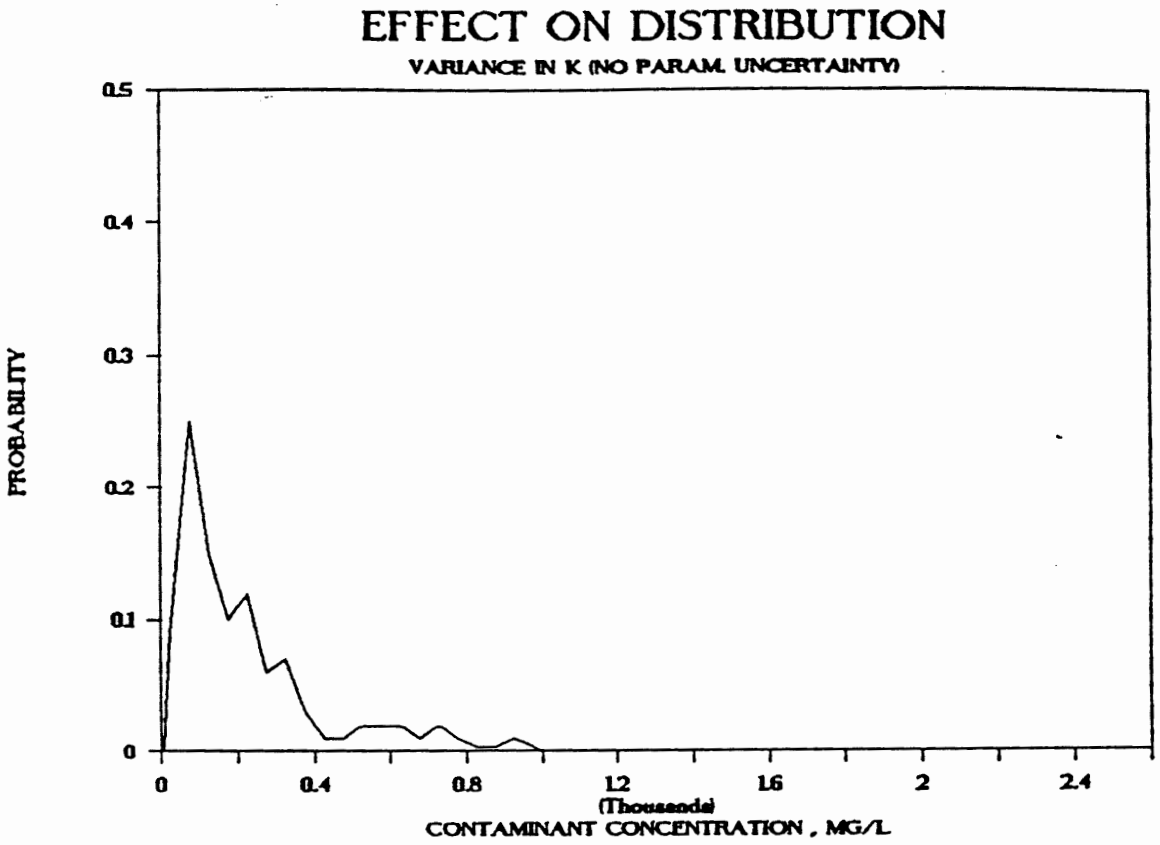

Figure II-3(e). Effect On Probability Distribution of Contaminant Concentration at a Point, Variance In Hydraulic Conductivity due to Natural Uncertainty

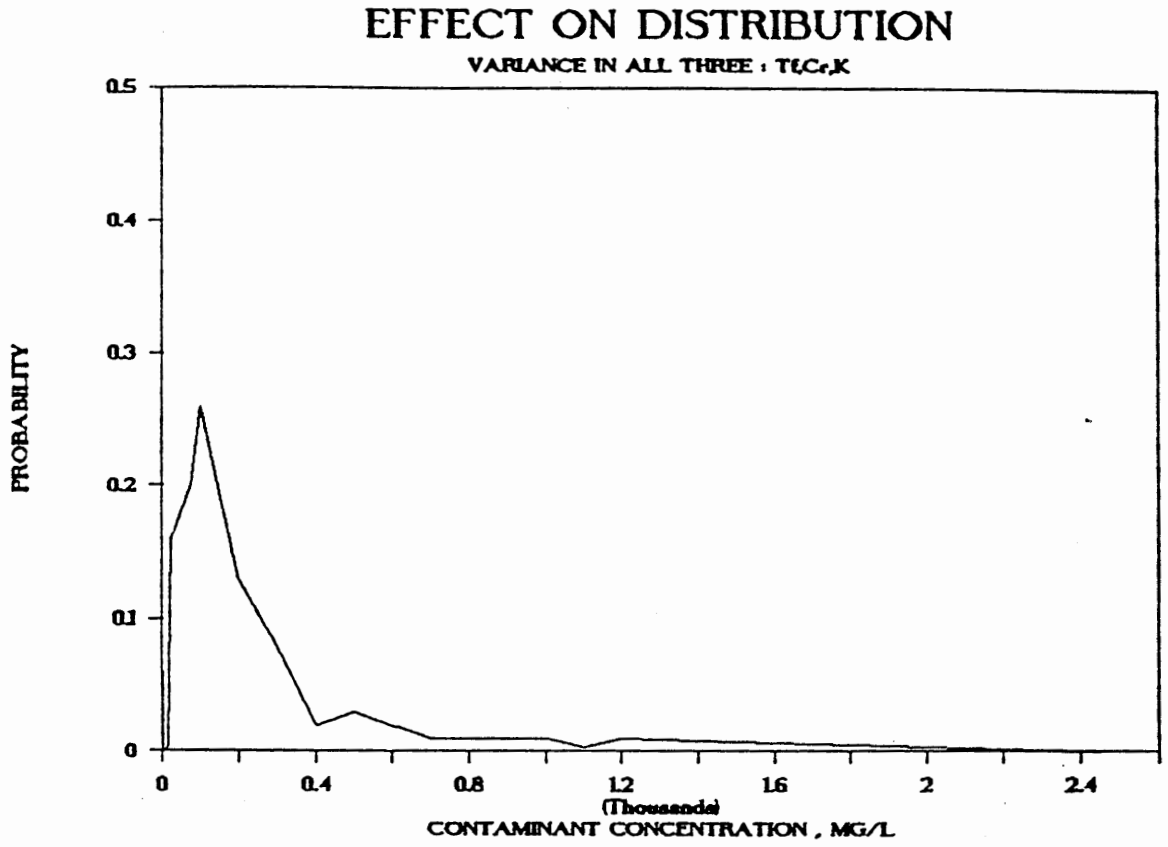

Figure II-3(f). Effect On Probability Distribution of Contaminant Concentration at a Point, Variance In Time To Failure, Release Concentration and In Hydraulic Conductivity

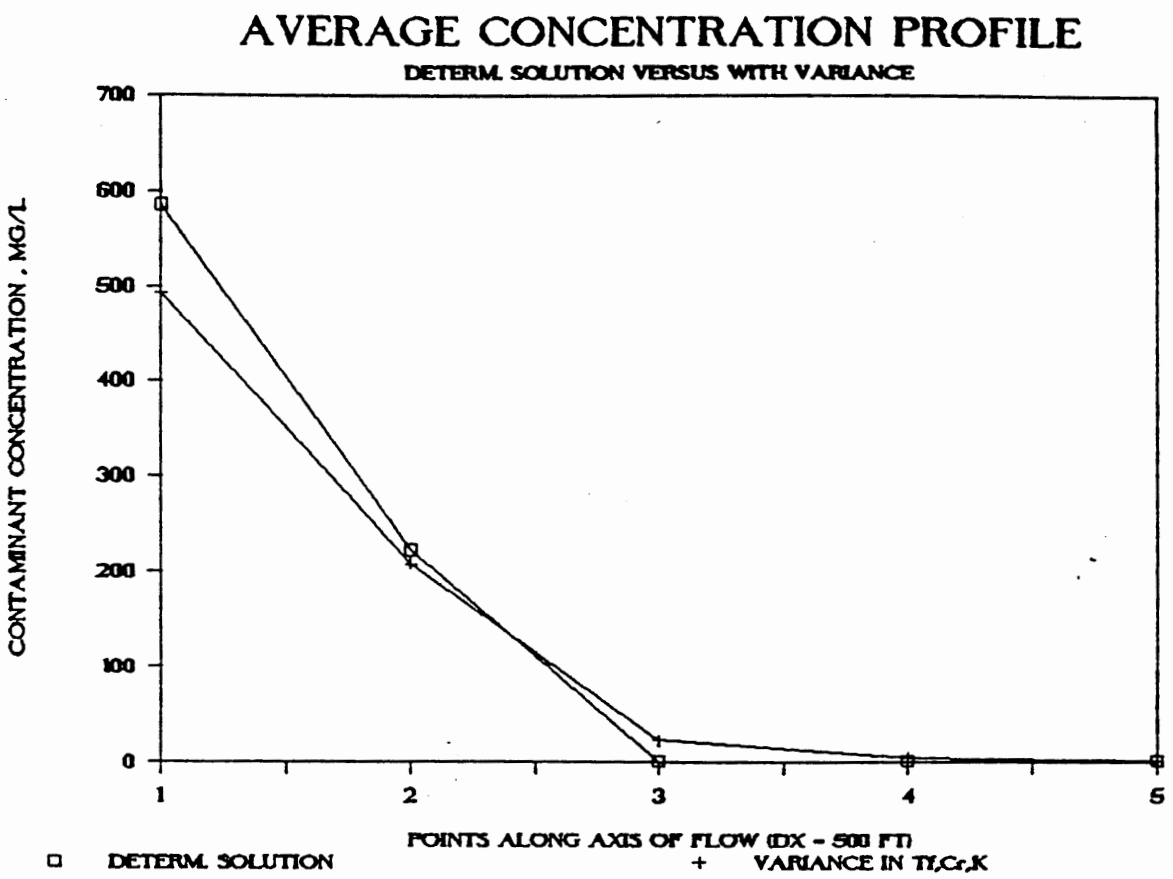

Figure II-4(a). Comparison of Average Concentration Profiles For Deterministic Solution and for Solution With Variance In Time To Failure, Release Concentration and Hydraulic Conductivity

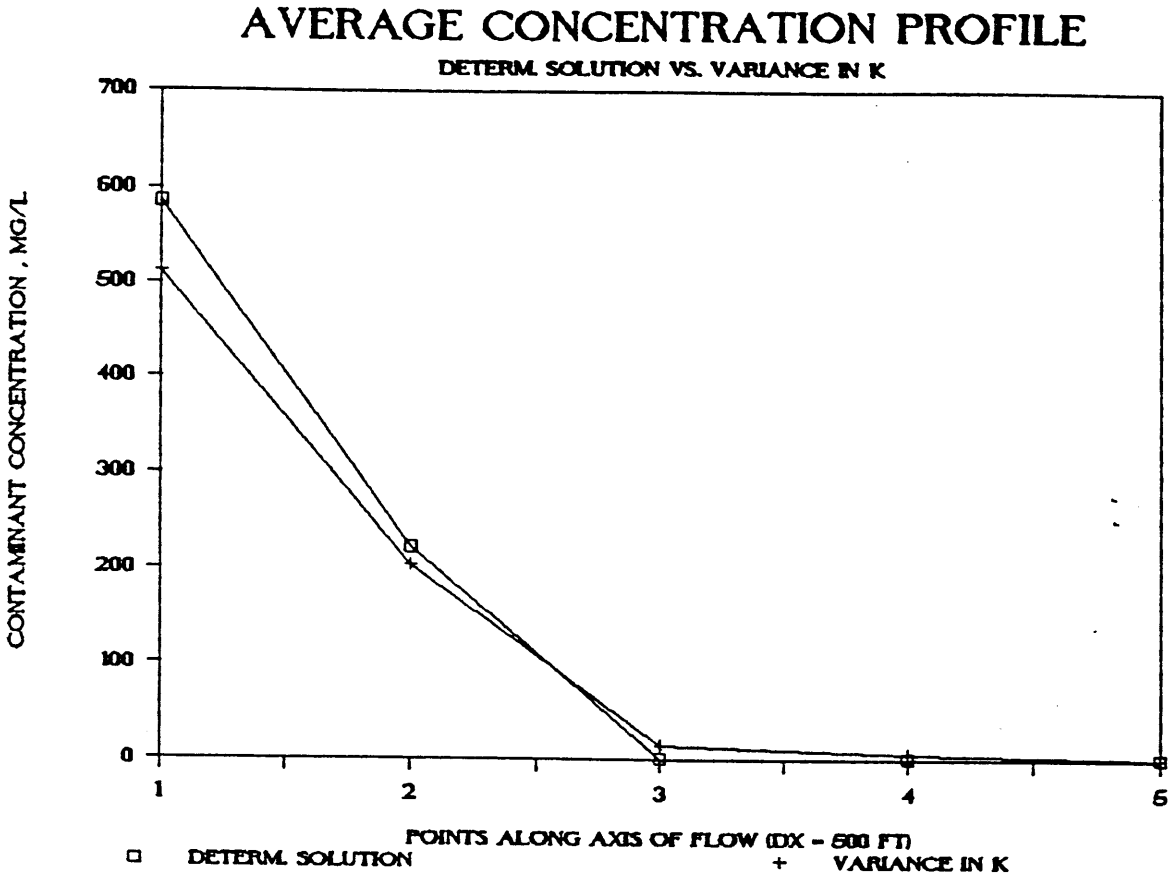

Figure II-4(b). Comparison of Average Concentration Profiles For Deterministic Solution and Solution With Variance Due To Natural and Parameter Uncertainty In Hydraulic Conductivity

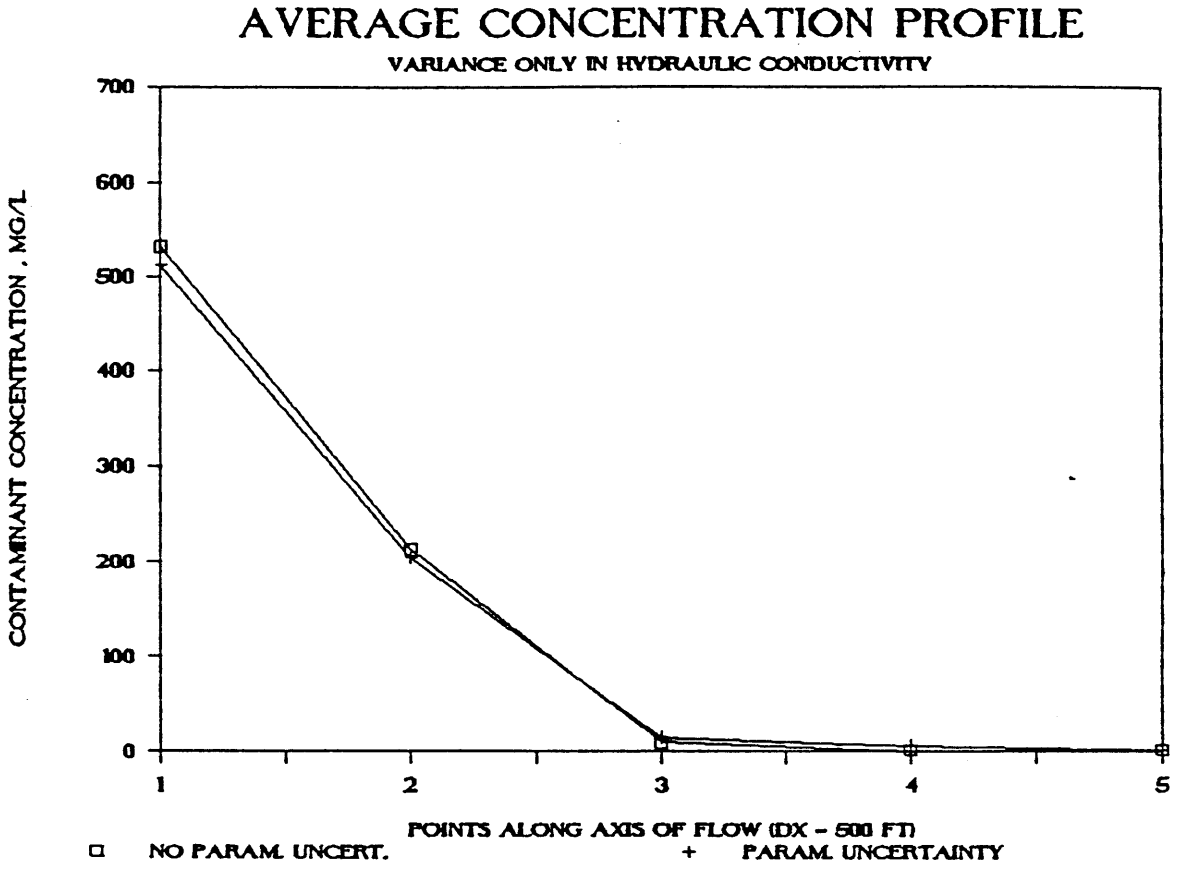

Figure II-4(c). Comparison of Average Concentration Profiles For Variance In Hydraulic Conductivity Due To Natural Uncertainty and Parameter Uncertain

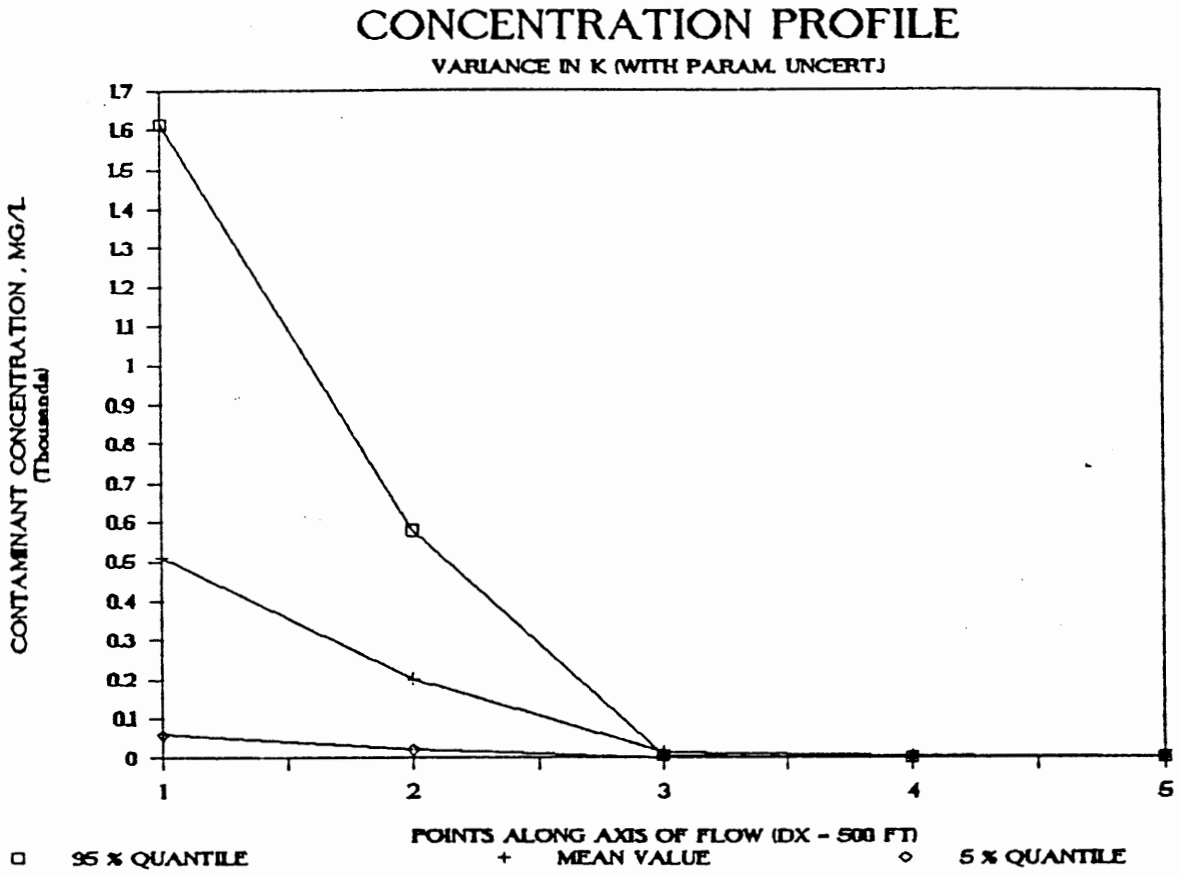

Figure II-5. Concentration Profile With 5, 95% QUANTILES, Variance Due To Natural and Parameter Uncertainty In Hydraulic Conductivity

plume past this point occurs, under this set of input conditions, only when there is variability in the hydraulic conductivity. This is evident from the long tails of the distribution in Figure II-3(d).

The full output of decoded results from the first simulations is given in Table II-2. This indicates that the dominant effect on variance of contaminant concentration at all points under the present input conditions is the variance of the hydraulic conductivity. This is due to two distinct effects. First, the effect of low conductivities which increases the variance of the left hand tail of the concentration distribution. This effect is more dominant near the waste site. Because the model introduces contaminant to the aquifer as a leakage process, low hydraulic conductivities at the landfill result in a low contaminant release rate, and thus a higher probability of nonexceedance. Second, the effect of high conductivities, which result in long right hand tails in the concentration distributions. This effect is more dominant over larger scales. High hydraulic conductivities result in higher release rates, which when combined with the propensity to form high velocity flow channels leading away from the landfill, leads to the long distribution tail effects observed at points further from the landfill.

Increased variance in time to failure has a similar effect near the landfill. At the (-) level in this design a failure always occurs at 10 years, while at the (+) level a certain probability (.056) of nonfailure is introduced which raises the probability of nonexceedance. Both variance in time of failure and variance in release concentration appear to have a relatively minor effect away from the landfill. Increasing the variance in the release concentration increases the variance at and near the landfill, but further away the effect is obscured because the plume only extends past point 2 when there is high variance in the hydraulic conductivity.

The second-order interactive effects all appear to have some significance in these simulations. To some extent this may reflect the background noise in the experimental design decoding process. However, we would expect that interactive effects should have some significance in any highly-interconnected simulation model. In particular, we would expect that both time-to-failure variance and release-concentration variance might interact nonadditively with the variance in hydraulic conductivity. Indeed, the 1x3 and 2x3 interaction terms are identical to the results for factors 1 and 2 after observation node 2, as the plume only reaches this extent when factor 3, the hydraulic conductivity variance, is at the (+) level.

Finally, we can compare the roles of natural and parameter uncertainty in the hydraulic conductivity field. The results here are rather complex. With no other sources of variability present, adding parameter uncertainty to natural uncertainty results in an

Table II-2. Results of first simulation design.

	Effects due to treatment factors								
	Change in Variance			Change in P<50 ppm			Change in P<1 ppm		
Factors:	1	2	3	1	2	3	1	2	3
Observ. Point									
1	.65E5	.16E5	.27E6	.069	-.007	.027	.056	0	0
2	.46E5	.52E5	.91E5	.043	-.053	.119	.056	0	0
3	.26E4	.90E3	.19E5	-.002	.020	-.058	.004	.024	-.076
4	.30E4	-.41E4	.66E4	-.002	.002	-.016	-.003	.019	-.059
5	.15E4	-.16E4	.17E4	0	-.003	-.006	.009	.002	-.025
	Interactive Effects								
	1x2	1x3	2x3	1x2	1x3	2x3	1x2	1x3	2x3
1	-.39E5	-.14E5	-.83E4	.009	.011	.003	0	0	0
2	-.21E5	.17E4	-.35E4	.045	.037	.029	0	0	0
3	-.62E4	.26E4	.90E3	.002	-.032	-.010	.002	-.026	-.006
4	-.40E4	.30E4	-.41E4	.004	-.002	.002	.001	-.033	-.011
5	-.16E4	.15E4	-.16E4	0	0	.002	.001	-.001	-.013

Identification of Factors:

1: Variance in time of failure
2: Variance in release concentration
3: Sample variance of mean ln$\underline{K}$

increase in contaminant concentration variance of from 14-86%, but with a corresponding increase in the nonexceedance probabilities (decrease in number of violations). The increase in variance results because there are fewer, but more severe violations. With the other two sources of variability present (+ level) the opposite effect is observed. That is, addition of parameter uncertainty results in a reduction of contaminant concentration variance of as much as 57%, but with a decrease in the nonexceedance probabilities (increase in violations) and an increase in the mean.

Second Simulation Experiment

As noted above, the second simulation experiment considered 5 factors, with variations set at more realistic levels around the means. An important difference from the first simulations is that the mean $\ln K$ was kept constant, so that the median, rather than the mean of the K distribution is preserved between the (+) and (-) levels.

Effects of the treatments in the second simulation experiment are decoded similarly to those in the first experiment, except that, because this is a quarter fraction, the higher order interactions can no longer be decoded or separated from the main effects. The results are summarized in Table II-3.

The effects observed here are generally in line with those observed in the first simulation experiment. Once again, $s^2(K)$, which has here been separated from the effect of parameter uncertainty by the introduction of r as a factor, produces the most notable effect on both variance and nonexceedance probabilities. Also, increasing $s^2(K)$ results in an increase in the 50 ppm (mg/l) nonexceedance probabilities at the first two observation points, and a decrease thereafter. This can be identified as primarily the result of the natural variability of K.

Consideration of r as a treatment now allows explicit analysis of the role of parameter uncertainty on K , and conversely of the value of additional information. We see that increasing r from 13 to 23, as might occur as a result of additional sampling of the hydraulic conductivity field, results in a consistent reduction in contaminant concentration variance, which is on the order of 2-15%. Still this effect tends to be an order of magnitude smaller than the increase resulting from augmenting $s^2(K)$.

Increasing the third hydraulic conductivity parameter, d(0), results in a consistent, but relatively minor increase in concentration variances. The increase in variance is expected as increasing d(0) increases the spatial correlation of the conductivity

Table II-3: Results of second simulation design.

1) Change in Variance

Observ. Point	Treatment Factor 1	2	3	4	5
1	.59E5	.40E5	.17E5	-.80E4	.20E6
2	.40E5	.39E4	.16E5	-.11E5	.11E6
3	.43E4	-.29E4	.72E4	-.61E4	.39E5
4	.19E4	-.14E4	.19E4	-.46E4	.20E5
5	.12E4	-.89E3	.11E4	-.23E4	.40E4

2) Change in non-exceedance probabilities

	P<50					P<1				
	1	2	3	4	5	1	2	3	4	5
1	.004	.002	-.002	-.013	.023	.010	.006	0	.004	0
2	-.008	.024	-.008	-.031	.048	.010	.006	0	.004	0
3	-.007	.012	.006	.007	-.055	0	.009	.027	.008	-.074
4	-.012	.001	-.002	.007	-.022	-.009	.010	.006	.008	-.056
5	-.004	0	-.003	.003	-.008	-.011	.001	.001	.008	-.045

Identification of treatment factors:

1: Variance of failure time
2: Variance of release concentration
3: d(0)
4: r (df)
5: Sample variance of ln$\underline{K}$

values, resulting in a more heterogenous medium. However, d(0) seems to have surprisingly little effect on the observed nonexceedance probabilities.

Effects due to failure time variance and release concentration variance seem to be similar to those observed in the first simulation experiment. However, the role of failure variance in decreasing nonexceedance near the landfill is no longer evident, primarily because the (-) level is no longer zero variability and the difference in actual number of nonfailures between the (+) and (-) levels is considerably reduced from that found in the first simulations.

CHAPTER III

COMPONENT MODELS OF THE ADVISORY SYSTEM

A sequential decision-analytic framework (presented in Chapter II) controls the application of the predictive flow and mass transport models. This chapter describes primarily the theoretical mathematical basis for the predictive models. Although a users' manual is provided in Chapter IV, the reader should become familiar enough with the mathematical details in this chapter to appreciate the limits of application to field problems. Mathematical models are merely abstractions of the physical and bio-chemical processes, even when the latter are well understood.

3.1 ALGORITHM TO GUIDE MODEL SELECTION: CHOICE

In order to assist less experienced users, an algorithm has been developed in an interactive mode to provide guidelines for proper predictive model selection. These predictive models are based upon analytical, semi-analytical or numerical solutions to the governing differential equations of flow and mass transport. CHOICE is not a predictive model, but rather a screening model : it responds with recommendations based upon replies by the user to queries with regard to the proposed application. For example, the algorithm checks whether a particular solution applies : if the user responds in the affirmative that flow in the region is strongly affected by pumping wells, then semi-analytical (complex velocity potential) methods or complete numerical methods would be indicated as more appropriate than models based upon analytical solutions. The algorithm requests information about the means of waste disposal (e.g., lagoons, landfills, rotary distributors, spray irrigation devices, etc.), the nature of the aquifer, the perimeter of compliance, penetration, type of waste and many other factors. Because this model is primarily a user-oriented tool, the complete flow chart and details are presented in Chapter IV. Users can by-pass this algorithm (e.g., experienced modelers), or choose a particular model for other compelling reasons.

3.2 LEGRAND METHOD FOR PRELIMINARY SITE SCREENING, LGRD

For the purposes of preliminary site analysis we have included in the System the standardized evaluation method developed by LeGrand (1983). The LeGrand method is not a contaminant transport model, but rather a tool for the preliminary assessment of a site given certain commonly available information on the site and its situation. The system offers a concise screening mechanism for evaluating the contamination potential of waste sites, as well as a management-control procedure that can be used by regulatory agencies and owner/operators

of waste facilities during planning and operational stages of contaminant handling.

The LeGrand method focuses on weighting the key characteristics of a site in a standardized manner in order to form a preliminary evaluation of contamination potential. Each key characteristic is assigned a numerical value. The systems consists of the quantification of parameters, evaluated in a logical sequence, with the results presented in a standardized form. The numerical rating system is divided into ten steps within four stages:

1. Standard hydrogeological description of the site.

2. Determination of the degree of seriousness of the hazard potential in a matrix by identifying the degree of of aquifer sensitivity and the degree of contaminant severity.

3. Description of the relative probability of contamination by comparing the site's numerical value with a standard value that is derived from an integration of aquifer sensitivity and contaminant severity.

4. Reassessment of the site, with consideration given to engineering modifications.

Stage I: Numerical Description of Site Hydrogeology

The numerical rating system first provides a description of the site hydrogeology. This is based primarily on four key characteristics: a) Distance on the ground from a source of contamination to the nearest well, surface stream or property boundary; b) Depth of the water table below the waste or contamination source; c) Approximate slope of the water table; and d) Character of the soil materials through which the contaminant is likely to pass, expressed in terms of permeability and sorption. The method used to describe site hydrogeology assigns a "0" value to the most favorable setting of each hydrogeological factor, and a "9" value to the least favorable. Intermediate numerical values are defined by interpolating conditions between the two extremes. For each site the estimated numerical or point value for each of the four factors is added and the total expressed as a number between 0 and 32 that characterizes the site.

This stage consists of seven steps. The first four steps involve the recording of estimated values for each of the four key hydrogeological parameters. These four steps represent the core of the description method:

a) Distance: A great distance between a contamination source and a water supply (or perimeter of regulatory compliance) is generally considered a favorable factor, especially in loose, granular mater-

ials with some sorption capacity. It is a less significant factor in fractured materials or cavernous rock, where contamination is likely to reach greater distances. To distinguish one situation from the other an identifying letter is introduced in Step 6.

b) Depth to the water table: Many contaminants attenuate in the unsaturated zone above the water table. Therefore, it is generally beneficial to have a deep water table. The depth to the water table is defined here as the distance from the ground surface to the surface of water standing in an unpumped well (pumped wells will lower the water table locally). The points assigned increase with shorter distance to the water table. The scale is not a simple arithmetic progression in order to account for the increased sensitivity at smaller depths to the water table.

c) Water table gradient. This factor establishes whether the contaminant is moving toward or away from the water supply (or perimeter of interest). Since the exact gradient is difficult to estimate unless current water table maps are available, only 5 points are spread across this scale.

d) Permeability and sorption. The scale for the permeability-sorption factor extends from 0, representing the low permeability and high sorption characteristic of clay, to 9, representing the high permeability and low sorption of clean gravel. The sites are also classified using a letter qualifier. The letter attached to each digit in the matrix of permeability-sorption is for specific identification of the characteristics of a site (see table IV-1).

Steps 5 and 6 provide for the addition of letter identifiers that identify special features with respect to the site. In step 7 the separate ratings and identifying letter suffixes are recorded and the values added to achieve a total description.

A site description from the LeGrand method is a compound of four separate digits, representing values from the first four steps, and four or more letters derived from steps 4, 5 and 6. The first letter identifier is derived from the permeability sorption matrix (Step 4). The second letter (A, B or C) assigns a level of confidence to the overall values derived from Steps 1 to 4 (Step 5). The third letter indicates whether the distance from a contamination source is to a well, spring, perennial stream or specified boundary. The fourth letter identifier is selected from the most appropriate characteristic listed with the letter identifiers in Step 6; an additional letter identifier from this list may also be added.

Step 7 is the completion of the site numerical description. It is accomplished by adding the separate point values determined in the first four steps and writing the sum with the appropriate number value and letter suffixes. At this stage the site can be rated in terms of relative hydrogeological conditions, but not necessarily

with respect to the possibility of contamination. The site is assigned a grade based on its critical hydrogeological parameters as assessed in Steps 1-6.

Stage II: Evaluation of Degree of Seriousness

The total hazard potential has two components: degree of seriousness and probability of contamination. The degree of seriousness is somewhat independent of the site description obtained in Stage I, but is an essential part of any groundwater contamination evaluation. The analysis performed at this level is made with a matrix considering the sensitivity of the aquifer to contamination and the severity of the contaminant. These factors are defined as follows:

a) Aquifer sensitivity: This term is used to indicate likelihood and degree of groundwater contamination at a given site. The aquifer's areal extent and importance as a ground water source are also considered in this definition. For use in this rating system, aquifers are divided into three categories: sensitive, moderately sensitive and insensitive. Permeability is the key factor in considering aquifer sensitivity. Additional factors are the thickness of the saturated part of the aquifer and the quality of water with respect to its acceptability for use.

b) Contaminant severity. This term includes qualitative weighting of toxicity, concentration and volume, mobility in the groundwater and persistence. The contaminant severity scale ranges from the effluent of a single septic tank at the low end to large volumes of high-level radioactive wastes at the high end.

The overall degree of seriousness is determined by the intersection between "contaminant severity" and "aquifer sensitivity". The overall degree of seriousness is divided into nine categories, ranging from "relatively small" to "extremely high".

Stage III: Evaluation of Probability of Contamination

The matrix of contaminant severity and aquifer sensitivity is used again in stage III to grade a situation more specifically. For each intersection of these two parameters a standard situation rating is defined. The standard situation rating represents the approximate numerical value which a site's description should not exceed to prevent serious contamination of groundwater. These PAR values (Protection of Aquifer Ratings) were derived from extensive studies of a large number of situations of varying aquifer sensitivities and contaminant severities, including cases where contamination has or has not occurred. These values, empirical in nature, are then compared with the hydrogeological numerical grade for the site obtained in stage I. Based on this comparison we obtain a situation rating, from

which the probability of contamination, degree of acceptability and situation grade are derived for the site under consideration. Stage III consists of steps 8 and 9. Step 8 evaluates the probability of contamination and degree of acceptability for a natural site, and step 9 performs this evaluation for a modified site.

Stage IV: Engineering Improvements and Final Acceptance

Generally, the areas around potential contaminant sites are heavily influenced by human modifications which result in changes in the subsurface hydrological regime. Engineering modifications to limit contamination are common and should be evaluated. Stage IV provides a means to rate sites that are modified by human action. These changes result in aquifer sensitivity and/or contaminant severity modifications. In stage IV the effect of the modified properties is reassessed and the new PAR values are evaluated. This results in a new situation rating, giving new probability of contamination, degree of acceptability and situation grade. This stage provides a simple method to predict the impact of human action on the contamination potential of a site, and establish a preliminary evaluation of the cost/benefit ratio.

Full details of data input for the LeGrand model are given in section 4.2.1.

3.3 ANALYTICAL ONE-DIMENSIONAL CONTAMINANT TRANSPORT MODEL, ODAST

The model ODAST, documented in Javandel et al. (1984), provides an analytical solution of the one-dimensional convective-dispersive transport equation, and is adapted from the set of one-dimensional solutions published by Van Genuchten and Alves (1982).

For the derivation of the model we consider a one-dimensional system consisting of an infinitely long homogeneous isotropic porous medium with a steady state uniform flow with seepage velocity v. A dissolved constituent is injected from one end of the model for a period of time t_0, such that the input varies as an exponential function of time. The governing equation for this situation, in a confined homogeneous isotropic aquifer and ignoring the dependence of dispersion on space and time, is:

$$D \frac{\delta^2 C}{\delta x^2} - v \frac{\delta C}{\delta x} - \lambda RC = R \frac{\delta C}{\delta t} \qquad (3.1)$$

where D is the dispersion coefficient, lambda is a radioactive decay constant, and R is the retardation coefficient. This is to be solved

subject to initial and boundary conditions:

$$C(x,t) = 0 \qquad t = 0 \tag{3.2}$$

$$\frac{\delta C\ (x,t)}{\delta x} = 0 \qquad x = \infty \tag{3.3}$$

$$\left[-D\frac{\delta C}{\delta x} + vC\right]\Big|_{x=0} = vf(t) \tag{3.4}$$

$$f(t) = c_0 \exp(-\alpha t) \qquad 0 < t \leq t_0 \tag{3.5}$$

$$f(t) = 0 \qquad t > t_0 \tag{3.6}$$

where C_0 and α are constants.

Using the Laplace transform technique, Van Genuchten (1982) solved this set of equations, obtaining:

$$\begin{aligned} C(x,t) &= A(x,t) \qquad 0 < t \leq t_0 \\ C(x,t) &= A(x,t) - A(x,t-t_0)\exp(-\alpha t_0) \qquad t > t_0 \end{aligned} \tag{3.7}$$

where:

$$\begin{aligned} A(x,t) &= C_0 \exp(-\alpha t)A_1(x,t) \qquad a \neq \lambda \\ A(x,t) &= C_0 \exp(-\alpha t)A_2(x,t) \qquad a = \lambda \end{aligned} \tag{3.8}$$

$$\begin{aligned} A_1(x,t) = {} & \frac{v}{v+U}\exp\left[\frac{x(v-U)}{2D}\right]\operatorname{erfc}\left[\frac{Rx-Ut}{2\sqrt{DRt}}\right] \\ & + \frac{v}{v-U}\exp\left[\frac{x(v+U)}{2D}\right]\operatorname{erfc}\left[\frac{Rx+Ut}{2\sqrt{DRt}}\right] \\ & + \frac{v^2}{2DR(\lambda-\alpha)}\exp\left[\frac{vx}{D} + (\alpha-\lambda)t\right]\operatorname{erfc}\left[\frac{Rx+vt}{2\sqrt{DRt}}\right] \end{aligned} \tag{3.9}$$

$$U = \left[v^2 + 4DR(\lambda-\alpha)\right]^{\frac{1}{2}} \tag{3.10}$$

$$\begin{aligned} A_2(x,t) = {} & \frac{1}{2}\operatorname{erfc}\left[\frac{Rx-vt}{2\sqrt{DRt}}\right] + \left[\frac{v^2t}{\pi DR}\right]^{\frac{1}{2}}\exp\left[-\frac{(Rx-vt)^2}{4DRt}\right] \\ & - \frac{1}{2}\left[1 + \frac{vx}{D} + \frac{v^2t}{DR}\right]\exp\left[\frac{vx}{D}\right]\operatorname{erfc}\left[\frac{Rx+vt}{2\sqrt{DRt}}\right] \end{aligned} \tag{3.11}$$

The model can then be adapted for Monte Carlo simulation by treating D and v as random variables. The velocity (v) is not however directly generated, but is assumed to result, via Darcy's law, from gradient, porosity and hydraulic conductivity. Hydraulic conductivity may be generated directly for the simulation via a log-normal distribution. However, this method does not take into account the known relationship between the hydraulic conductivity and other parameters. Therefore the option is also provided to generate a distribution of hydraulic conductivities from the underlying variables of mean particle size and porosity, via the Karmen-Cozeny relationship, using the techniques described by Mulkey and Brown (1985). This is the approach most appropriate for preliminary analysis of contamination risk when there is considerable uncertainty regarding the hydrogeology. The underlying variables of gradient and mean particle size are generated for Monte Carlo simulation in the manner described for the model EPAGW (section 3.7). The data input requirements, and the limitations of this approach, are described in more detail in section 4.2.2.

3.4 ANALYTICAL TWO-DIMENSIONAL CONTAMINANT TRANSPORT MODEL, TDAST

The model TDAST provides an analytical solution to steady state flow in a two-dimensional Cartesian coordinate system, and is documented in Javandel et al. (1984). If the flow is coincident with the x axis, and the longitudinal and transverse components of the dispersion tensor are assumed independent of position and designated by D_L and D_T, the general governing equation for a confined, homogeneous, isotropic aquifer can be written as:

$$D_L\frac{\delta^2 C}{\delta x^2} + D_T\frac{\delta^2 C}{\delta y^2} - v\frac{\delta C}{\delta x} - \lambda RC = R\,\frac{\delta C}{\delta t} \qquad (3.12)$$

where lambda represents decay and R is the retardation coefficient.

For a particular solution we first assume that the medium is initially free of the solute, and that at a certain time a strip type source of length 2a, orthogonal to the flow direction, is introduced along the y axis. If the source concentration diminishes exponentially with time, the initial and boundary conditions are:

$$\begin{aligned} &C(0,y,t) = C_0 e^{-\alpha t} && -a \le y \le a \\ &C(0,y,t) = 0 && |y| > a \\ &\lim_{y\to\pm\infty}\frac{\delta C}{\delta y} = 0 \\ &\lim_{x\to\infty}\frac{\delta C}{\delta x} = 0 \end{aligned} \qquad (3.13)$$

Where the source "strip" is arranged orthogonal to the direction of flow, an analytical (but not closed form) solution is presented by Cleary and Ungs (1978) as:

$$C(x,y,t) = \frac{C_0 x}{4\sqrt{\pi D_L}} \exp\left[\frac{vx}{2D_L} - \alpha t\right] \cdot \int_0^{t/R} \exp\left[-\left(\lambda R - \alpha R + \frac{v^2}{4D_L}\right)\tau - \frac{x^2}{4D_L\tau}\right] \tau^{-3/2} \cdot \left[\operatorname{erf}\left(\frac{a-y}{2\sqrt{D_T\tau}}\right) + \operatorname{erf}\left(\frac{a+y}{2\sqrt{D_T\tau}}\right)\right] \delta\tau \qquad (3.14)$$

This model can be adapted for Monte Carlo simulation in a manner analogous to ODAST, except that here the variable D_T must also be generated. Full details of data input are given in section 4.2.3.

3.5 ANALYTICAL TWO-DIMENSIONAL POINT SOURCE CONTAMINANT TRANSPORT MODEL, PLUM2D

The model we refer to in the system as PLUM2D, properly named PLUME 2D, was developed to provide an analytical solution for multiple, fully penetrating point sources in a homogeneous, non-leaky confined aquifer with uniform regional flow, with the flow coincident with the x axis. The solution is documented in van der Heijde (1985). Sources are conceived as fully penetrating wells. In this case, the general governing equation for a solute subject to radioactive decay and adsorption described by a linear, equilibrium relationship can be written as:

$$R_d \frac{\delta C}{\delta t} = D_x \frac{\delta^2 C}{\delta x^2} + D_y \frac{\delta^2 C}{\delta y^2} - \bar{V} \frac{\delta C}{\delta x} - \lambda R_d C \qquad (3.15)$$

where the dispersion coefficients may be written as:

$$D_x = \alpha_x \bar{V}$$

$$D_y = \alpha_y \bar{V}$$

$$\bar{V} = v/n$$

where v is the Darcy velocity, n is the porosity, α_x and α_y are the dispersivity in the x and y direction, R_d is the retardation coefficient, and lambda = $\ln 2/\tau$, with τ being the half-life time.

For an infinite two-dimensional porous medium in the x,y plane with mass per unit length in the z-direction M_2 instantaneously injected along the vertical z-axis, the solution is given by:

$$C(x,y,t) = \frac{M_2}{4\pi nt\sqrt{D_x D_y}} \exp\left[- \frac{\left(x - \frac{\bar{V}t}{R_d}\right)^2}{4D_x\, t/R_d} - \frac{y^2}{4D_y t/R_d} - \lambda t \right] \quad (3.16)$$

The solution may be written by analogy to Hantush's leaky well function, W(u, r/B), following Wilson and Miller (1978), as:

$$C(x,y,t) = \frac{f_2 \exp\left(\frac{x}{B}\right)}{4\pi n\sqrt{D_x D_y}} W\left(u, \frac{r}{B}\right) \quad (3.17)$$

where:

$$B = \frac{2\, D_x}{\bar{V}}$$

$$r = \left[\left(x^2 + \frac{D_x}{D_y} y^2 \right) \gamma \right]^{\frac{1}{2}}$$

$$\gamma = 1 + \frac{2B\lambda\, R_d}{\bar{V}}$$

$$u = \frac{R^2\, R_d}{4\gamma D_x t}$$

$$W\left(u, \frac{r}{B}\right) = \int_u^\infty \frac{1}{\theta} \exp\left[-\left(\theta + \frac{r^2}{4B^2\theta} \right) \right] d\theta$$

Here, B forms the mixing scale <u>equivalent</u> of the Hantush leakage factor, which accounts for the effects of dispersion in the transport model.

Because of the nature of the solution, various sources may now be superimposed to estimate the result of contamination from multiple point sources, which may have been operational for varying lengths of time. The solution used in the program is obtained by use of an accurate analytical approximation of the Hantush leaky well-function, given by Walton (1983). The model may then be adapted for Monte Carlo simulation in a manner similar to that for other analytical solutions

derived here. Full details of data input for Monte Carlo simulation, as well as limitations of the solution method, are discussed in section 4.2.5.

3.6 LATERAL AND VERTICAL DISTRIBUTION OF CONTAMINANT PLUME UNDER FREE WATER SURFACE CONDITIONS, DUPVG

The model we refer to as DUPVG was developed to address the problem of solute transport in an unconfined aquifer, where the water table surface may be moving in response to input from a source (Guvanasen and Volker, 1982; Volker and Guvanasen, 1987). The equations governing flow and transport in the saturated zone of unconfined aquifers are subject to the non-linear moving free-surface boundary. Where the movement of this free surface is a significant component of the flow regime analytical solutions based on the assumption of a confined aquifer are no longer appropriate. The model of Volker and Guvanasen provides an approximate analytical solution for such cases.

Consider a case in which an infinitely long (in y) unconfined aquifer is being recharged through an infinitely long recharge basin of width 2L. A symmetrical setting is assumed, and the aquifer is bounded by a drain of constant head on each side (in x) at distance B from the center of the recharge basin. The basin is recharging the aquifer at rate P_0. The medium is assumed homogeneous and uniform with effective porosity θ_e, hydraulic conductivity K and initial saturated depth a_0. Flow is assumed to arise only as a result of the recharge (R), which results in a spatially varying head-rise of s.

By symmetry, the solution need be sought only in the $x>0$ segment. The procedure adopted by the authors is first to solve the flow equations, governing the velocity distribution, then apply these to the transport equation. The rise of the free surface above the initial saturated depth, s, is first obtained by applying the Dupuit-Forcheimer assumption. The resulting equation is then linearized under the assumption that $s/a_0 \ll 1$, which will be true for small infiltration rates. The equation governing flow is then:

$$\frac{Ka_0}{\theta_e}\frac{\delta^2 s}{\delta x^2} = \frac{\delta s}{\delta t} - \frac{R}{\theta_e} \qquad (3.18)$$

subject to boundary conditions:

$s=0$,	$t=0,\ 0\le x\le B$
$\delta s/\delta x=0$,	$x=0$
$s=0$,	$x=B$
$R=P_0$,	$0\le x\le L$
$R=0$,	$L<x\le B$

A solution to this equation can be obtained through the eigen-

function expansion method, defining the position of the upper boundary of the saturated flow domain. However, the Dupuit-Forcheimer assumption implies a horizontal flow beneath the basin, where a vertical flow component may actually predominate.

To obtain a more accurate representation of the flow field the authors first assume that the flow pattern at any time t can be described as a function of the steady state velocity:

$$u_i(x,z,t) = u_i(x,z,\infty)\ f(t) \tag{3.19}$$

where f(t) is the scale function dependent on time. The velocity distribution is then sought by transforming the free-surface flow domain to rectangular coordinates:

$$X \equiv x, \qquad Z \equiv za_0/(s + a_0) \tag{3.20}$$

Given the assumption that $s/a_0 \ll 1$, it can be further assumed that the unsteady free surface can be approximately described by a streamline, that streamline and equipotential functions change little with time, and that further away from the source the velocity is essentially horizontal and its spatial variation is negligible. Based on these assumptions, only the steady-state velocity pattern in the transformed domain need be sought, and the downstream end can be extended to infinity. The flow equation and associated boundary conditions are simplified to:

$$K\left(\frac{\delta^2 h}{\delta X^2} + \frac{\delta^2 h}{\delta Z^2}\right) = 0, \quad 0 \le X \le \infty, \ 0 \le Z \le a_0 \tag{3.21}$$

$$K\frac{\delta h}{\delta Z} = P_0, \quad 0 \le X \le L, \ Z = a_0 \tag{3.22}$$

Solutions are then obtained by the Schwarz-Christoffel transformation method in terms of the relationships between X, Z, and the equipotential and stream function, yielding:

$$X = \frac{a_0}{\pi} \ln\left(\sqrt{\xi} + \sqrt{(1+\xi)}\right) \tag{3.23}$$

$$Z = \frac{a_0}{\pi} \cos^{-1}\left(\gamma_1/\cosh(\pi X/a_0)\right) \tag{3.24}$$

$$\phi = \frac{Q}{\pi} \ln\{\sqrt{\upsilon} + \sqrt{(1+\upsilon)}\} \tag{3.25}$$

$$\psi = \frac{Q}{\pi} \cos^{-1}\left(\lambda_1/\cosh(\pi\phi/Q)\right) \tag{3.26}$$

where:

$$\gamma_1 = \epsilon_1 \cosh(\pi\phi/Q)\cos(\pi\psi/Q) + \epsilon_2$$

$$\gamma_2 = \epsilon_1 \sinh(\pi\phi/Q)\sin(\pi\psi/Q)$$

$$\xi = \frac{1}{2}\left\{ (\gamma_2^2+\gamma_1^2-1) + \sqrt{(\gamma_2^2+\gamma_1^2-1)^2 + 4\gamma_2^2} \right\}$$

$$\epsilon_1 = -\frac{1}{2}\left\{ 1 - \cosh(\pi L/a_0) \right\}$$

$$\epsilon_2 = -\frac{1}{2}\left\{ 1 + \cosh(\pi L/a_0) \right\}$$

$$\lambda_1 = \frac{1}{\epsilon_1}\cosh(\pi X/a_0)\cos(\pi Z/a_0) - \epsilon_2/\epsilon_1$$

$$\lambda_2 = \frac{1}{\epsilon_1}\sinh(\pi X/a_0)\sin(\pi Z/a_0)$$

$$\upsilon = \frac{1}{2}\left\{ (\lambda_2^2+\lambda_1^2-1) + \sqrt{(\lambda_2^2+\lambda_1^2-1)^2 + 4\lambda_2^2} \right\}$$

The steady state velocity along streamlines is then given by:

$$\upsilon(\phi,\psi;t\to\infty) =$$

$$\frac{Q}{\epsilon_1 a_0} \frac{[(\gamma_1^2+\gamma_2^2-1)^2+4\gamma_2^2]^{\frac{1}{4}}}{\sqrt{\cosh^2(\pi\phi/Q)\sin^2(\pi\psi/Q)+\sinh^2(\pi\phi/Q)\ \cos^2(\pi\psi/Q)}} \qquad (3.27)$$

By assumption:

$$u_\phi(t) = u_\infty\ f(t), \quad \text{and} \quad f(t) = 1 - \exp\left\{ \frac{-Ka_0\pi^2}{\phi_e 4B^2}\ t \right\} \qquad (3.28)$$

The transformation of the domain is then applied to the transport equation, with the additional transform of time:

$$\tau = \int_0^t f(t)d(t) \qquad (3.29)$$

With the assumptions that $s/a_0 \ll 1$, the slope of the free surface is small, the rate of rise of the free surface is very small, and there is no dispersion across streamlines, the transport equation can be expressed in the curvilinear equipotential-streamline coordinate system as:

$$\frac{\delta C}{\delta \tau} + u_\infty^2 \frac{\delta C}{\delta \phi} = u_\infty^2 \frac{\delta}{\delta \phi}\left(D_L \frac{\delta C}{\delta \phi} \right) \qquad (3.30)$$

For use in the Advisory System we follow Solution S1 as given by Guvanasen and Volker (1982). The reduced governing transport equation is solved subject to the following conditions:

1) The boundary condition upstream is equivalent to:

$$C(\phi=0,\tau) = C_0$$

which implies a concentration gradient across the boundary approaching zero.

2) At the vertical downstream end, with $\phi=\phi_B$:

$$\frac{\delta C}{\delta \phi} = \frac{C}{2D_L}$$

which is an approximation true for lower values of C.

3) The velocity along streamlines at steady state is assumed to be uniform and equivalent to:

$$u_\infty(\phi\rightarrow\infty) = v_\infty = P_0 L/(\phi_t a_0)$$

which assumes that D_L can be taken outside the differentiation, and is thus independent of position.

4) Initial condition:

$$C(\phi,\tau=0) = 0.$$

By Laplace transform methods, Volker and Guvanasen show that the solution under these conditions can be written in the following form:

$$C(\phi,\tau) = C_0 \exp\left(\frac{\phi}{2D_L}\right) \sum_{n=-\infty}^{\infty} \left(\frac{-1}{2}\right)^n \left\{ \exp\frac{(-\phi+2n\phi_B)}{2D_L} \cdot \right.$$

$$\left. \operatorname{erfc}\frac{(\phi-2n\phi_B-v_\infty^2\tau)}{2v_\infty\sqrt{D_L\tau}} + \exp\left(\frac{\phi-2n\phi_B}{2D_L}\right) \cdot \operatorname{erfc}\frac{(\phi-2n\phi_B+v_\infty^2\tau)}{2v_\infty\sqrt{D_L\tau}} \right\} \qquad (3.31)$$

Several approximations can be derived for this solution given

certain simplifying assumptions. Volker and Guvanasen provide two such approximations, of which we have employed the first (their S1). This is obtained by noting that as B, the distance to the constant head boundary, goes to infinity, a good approximation to equation (3.31) is provided by:

$$C = \frac{C_0}{2}\left\{\operatorname{erfc}\frac{(\phi - v_\infty^2 \tau)}{2v_\infty\sqrt{D_L \tau}} + \exp\left(\frac{\phi}{2D_L}\right)\ \operatorname{erfc}\frac{(\phi + v_\infty^2 \tau)}{2v_\infty\sqrt{D_L \tau}}\right\} \quad (3.32)$$

This approximation is the solution provided in the system. Note that this may not be a particularly good approximation when the distance to the constant head boundary is small relative to distance from the source. However, the approximation is only involved in solution of the transport equation, and not in the solution of the velocity equation. Thus the error should not affect the computed average position of the front. A discussion of the relative performance of the various approximate solutions is provided in Volker and Guvanasen (1987).

3.7 Modified EPA Model for Monte Carlo Analysis of Impact On Groundwater, EPAGW

This groundwater model accounts for most of the major physical and chemical processes that affect movement and transformations of chemicals in simple, homogeneous and isotropic porous media under steady flow conditions (U. S. EPA, 1986). The mechanisms considered include advection, hydrodynamic dispersion in the longitudinal, lateral and vertical dimensions, adsorption and chemical degradation. Major assumptions made by the transport model are :

(1) groundwater velocity is uniform, one-dimensional and steady-state, in a saturated aquifer;

(2) the porous medium is homogeneous and isotropic;

(3) mass transport is also in a steady state;

(4) the aquifer is semi-infinitely large in the direction of groundwater flow and infinitely large in the transverse direction;

(5) the contaminant source is sufficiently large in mass such that the down-gradient concentration will be maintained once it is reached;

(6) the distribution of contaminant concentration at the source boundary is Gaussian;

(7) degradation of chemicals is caused only by hydrolysis;

(8) equilibrium, reversible speciation, and sorption are appropriate -- in order to utilize an equilibrium partition coefficient.

The advection-dispersion equation for the transport of a non-conservative contaminant in an adsorbing homogeneous and isotropic porous medium with fully-saturated flow may be written as follows :

$$D_{xx} \frac{\delta^2 C}{\delta x^2} + D_{yy} \frac{\delta^2 C}{\delta y^2} + D_{zz} \frac{\delta^2 C}{\delta z^2} -$$

$$\frac{V}{R_f} \frac{\delta C}{\delta x} = \frac{\delta C}{\delta t} + \lambda C + IC \qquad (3.33)$$

where x,y,z = spatial coordinates in the longitudinal, lateral and vertical directions, respectively, (L);

C = dissolved concentration of chemical, (M/L^3);

D_{xx}, D_{yy}, D_{zz} = retarded dispersion coefficients in the x,y and z directions, respectively, (L^2/T);

V = groundwater seepage velocity, assumed to be in the x direction, (L/T);

R_f = retardation factor;

t = elapsed time, (T);

θ = volumetric water content of the porous medium;

I = net recharge due to precipitation, (T^{-1}).

The retardation factor and the effective reaction rate constant are defined as follows:

$$R_f = 1 + \frac{\rho_b K_d}{\theta} \tag{3.34}$$

$$\lambda = \frac{\lambda_1 \theta + \lambda_2 \rho_b K_d}{\theta + \rho_b K_d} \tag{3.35}$$

where ρ_b = bulk density of the porous medium, (M/L^3);

K_d = distribution coefficient, (L^3/M);

θ = volumetric water content;

λ_1 = rate coefficient for dissolved phase, (T^{-1});

λ_2 = rate coefficient for sorbed phase, (T^{-1}).

The three dimensional region of interest is regarded as semi-infinite in the x-direction ($0 \leq x < \infty$), infinite in the y-direction ($-\infty < y < \infty$), and finite in the z-direction ($0 \leq z \leq B$), where B is equal to the saturated zone thickness. The above partial differential equation is solved analytically. The solution treats the source concentration as a Gaussian distribution in the lateral direction (along the y-axis corresponding to the leading, down-

gradient edge of the unit), and a uniform distribution over the vertical mixing or leachate penetration depth, H. The maximum dissolved concentration of contaminant, C_o, occurs at the center of the Gaussian distribution, y_o. This distribution is defined by its standard deviation, σ, which is measured in terms of distance (in meters) and is related to the width of the disposal unit. The initial and boundary conditions necessary to solve the equation may be written as follows:

$$C(x,y,z,0) = 0 \tag{3.36}$$

$$C(0,y,z,t) = C_o\, e^{-y^2/2\sigma^2}\, U(Z) \tag{3.37}$$

$$C(x,\infty,z,t) = 0 \tag{3.38}$$

$$C(x,-\infty,z,t) = 0 \tag{3.39}$$

$$C(\infty,y,z,t) = 0 \tag{3.40}$$

$$\frac{\delta C}{\delta x}\,(x,y,0,t) = 0 \tag{3.41}$$

$$\frac{\delta C}{\delta x}\,(x,y,B,t) = 0 \tag{3.42}$$

where C_0 is the peak concentration at the source, σ is the standard deviation of the Gaussian distribution centered at $x = y = 0$, and $U(z)$ is a unit step function defined as

$$U(z) = 1 \quad , \quad H_1 \le z \le H_2$$

$$U(z) = 0 \quad , \quad z > H_1 \text{ or } z > H_2$$

A steady-state analytical solution can be obtained by direct solution of the steady-state version of equation (3.33), which implies removal of the time-derivative term. Details of the solution procedure are contained in a U.S. EPA report (1985). The solution is:

$$c_p\ (x,y,z) = \frac{H}{B}\ c_f\ (x,y) + \Delta c_p\ (x,y,z) \qquad (3.43)$$

where

$$c_f(x,y) = \xi' \int_{-\infty}^{\infty} \frac{\exp(-y'^2/2\sigma^2)}{\left\{x^2 + (y'-y)^2\ D_x/D_y\right\}^{\frac{1}{2}}}$$

$$\cdot\ K_1\left\{\left[\frac{\eta x^2}{D_x} + \frac{\eta(y'-y)^2}{D_y}\right]^{\frac{1}{2}}\right\}\ dy' \qquad (3.44)$$

$$\Delta c_p(x,y,z) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n}\ \sin\left(\frac{n\pi H}{B}\right)\ \cos\left(\frac{n\pi z}{B}\right)$$

$$\cdot\ \xi' \int_{-\infty}^{\infty} \frac{\exp(-y'/2\sigma^2)}{\left\{x^2 + (y'-y)^2\ D_x/D_y\right\}^{\frac{1}{2}}} \cdot K_1\left\{\left[\frac{\beta_n x^2}{D_x} + \frac{\beta_n(y'-y)^2}{D_y}\right]\right\}\ dy' \qquad (3.45)$$

in which y' is a dummy variable of integration, and ξ' is a constant:

$$\xi' = \frac{xc_0}{\pi}\ \sqrt{\frac{B_n}{D_y}}\ \exp\left(\frac{V_s x}{2D_x}\right)$$

$$\eta = \frac{V_s^2}{4D_x} + \lambda + I$$

$$\beta_n = n + \frac{n^2\pi^2 D_z}{B^2}$$

and $K_1(\cdot)$ is the modified Bessel function of the second kind and of first order. The solution given assumes that the source extends from the top of the aquifer through the thickness H, so that H_1=0 and H_2=H.

To obtain the steady-state concentration distribution along the x (flow) axis, the solution can be reduced to:

$$c_p\ (x,0,0) = \frac{H}{B}\ c_f(x,0) + \Delta c_p\ (x,0,0) \qquad (3.46)$$

where:

$$c_f(x,0) = \xi^* \int_0^\infty \exp\left\{-\left[\frac{\sigma^2\ \xi^2}{2} + x\sqrt{\frac{\xi^2 D_y}{D_x} + \frac{n}{D_x}}\ \right]\right\}\ d\xi \qquad (3.47)$$

$$\Delta c_p(x,0,0) = \frac{2}{\pi} \sum_{n=1}^{\beta} \frac{1}{n} \sin\left(\frac{n\pi H}{B}\right)\ \cos\left(\frac{n\pi z}{B}\right)$$

$$\cdot\ \xi^* \int_0^\infty \exp\left\{-\left[\frac{\sigma^2\xi^2}{2} + x\sqrt{\frac{\xi^2 D_y}{D_x} + \frac{\beta_n}{D_x}}\ \right]\right\}\ d\xi \qquad (3.48)$$

$$\xi^* = \frac{2c_0\sigma}{\sqrt{2\pi}} \exp\left(\frac{V_s x}{2D_x}\right)$$

El-Kadi et al. (1987) applied this model to six waste disposal sites in different regions of the United States. The model was tested against a three-dimensional finite element model (CFEST) and was found to generally underestimate the contaminant concentrations : they recommend using a factor of safety of one order of magnitude for a conservative permit denial decision. It should be emphasized that the "exact" results were taken to be those produced by the numerical model. Overestimation of concentrations resulted when the model was applied to a site where radial flow existed. With appropriate choice of parameters, analytical solutions are especially suitable for management purposes when combined with sensitivity analysis and/or uncertainty analysis (e.g., Monte Carlo simulation).

MONTE-CARLO SIMULATION

Input data for all model parameters must be identified in order to use the EPAGW model. In general, however, the behavior of a specific constituent in the environment is highly dependent on both the environmental setting and the properties of the constituent. The assignment of specific values to describe the behavior of the modeled system is further complicated by uncertainty about how to specify a single value for each model parameter which represents a "worst case" (obtained from the steady-state solution along the x-axis).

As an alternative to identifying reasonable worst-case values for each model, a Monte Carlo simulation technique is used. It involves a large number of computer runs with values for each input

parameter drawn from data sets describing ranges of possible values and the distribution of values within the range. Where parameters are correlated, and therefore dependent, the relationships are properly defined in the Monte Carlo routine. The Monte Carlo process in EPAGW (and in general) proceeds as follows:

1. Values from each input distribution are selected at random.

2. The model is run with a set of randomly-generated parameters to give a set of output variables.

3. The input selection and computation steps are repeated a large number of times (1000 to 5000) to produce a well-defined distribution of outputs.

4. The output values are analyzed for presentation as a distribution.

The groundwater model parameters and input data requirements include the following: groundwater velocity, porosity of the saturated media, dispersivity of the aquifer, distance to the measurement point, standard deviation of the Gaussian source, penetration depth of leachate into the aquifer, thickness of aquifer, fraction of organic carbon content of the soil, pH and temperature of groundwater, acid, neutral and base hydrolysis rates. Relationships between these environmental parameters must be determined in order to apply the Monte Carlo analysis properly. All the parameters and input data previously mentioned are in some extent linked or dependent on at least one of the others. In some cases an independent seed distribution can be generated to which other variables are correlated. Such is the case of temperature, which is not a function of any of the other parameters, but influences the values of some of them (e.g., hydrolysis rate coefficients). Dependent data sets can be developed as empirical, joint or multivariate distributions, theoretical distributions, or from functional dependencies among the variables and parameters. The parameters and variables to be generated independently are as follows:

a. Thickness of the saturated zone, B
b. Fractional organic carbon content, FOC. The fractional organic carbon content is used to determine the distribution coefficient, K_D, from the following relationship:

$$K_D = (f_{oc})\ (K_{oc})$$

where K_{oc} = distribution coefficient normalized to organic carbon.

c. Groundwater pH, assumed to be independent of contaminant concentration and temperature.
d. Groundwater temperature, T.
e. Leachate penetration into the saturated zone, H, probably

related to the relative differences in the leachate and groundwater velocities. A simple, independent, uniform distribution ranging from a fixed minimum to a fixed maximum is used to represent this variable.

f. Net recharge, I. It is the amount of water that enters an aquifer system. Since the groundwater model assumes that the porous media is uniform, the effect of recharge causes the groundwater to rise and fall uniformly. There is thus no change on the gradient or groundwater velocity. I is estimated as follows:

$$I = q' / H$$

where q' = net infiltration, m/year

H = leachate penetration depth, m .

The remaining input parameters and variables are dependent and cannot be generated without properly matching each value with other related values. Dependencies are considered with the objective of avoiding unrealistic or impossible sets of data, that is, to provide consistent sets of data. In general, precise functional relationships among all the dependent variables or parameters do not exist. Similarly, observed data for all values taken in sets do not exist or are inadequate in number to permit statistical representation of these dependencies. However, equations do exist in the engineering and scientific literature to permit generation of sets of possible combinations of input data. The parameters and variables to be generated as dependent values are as follows:

$\alpha_L, \alpha_T, \alpha_V$ = dispersivities in the longitudinal, lateral and vertical directions assumed to be largely dependent on distance, x.

θ = porosity of the soil or porous media, assumed to be largely dependent on soil properties and parent material.

ρ = bulk density of the soil or porous media, largely dependent on soil properties including porosity.

V = groundwater flow velocity, largely dependent on soil properties including hydraulic conductivities, porosity, bulk density and hydraulic gradient.

σ = standard deviation of the gaussian distribution representation of the source concentration, related via mass balance principles to leachate volumes, groundwater velocity, porosity, and depth of leachate penetration into the saturated zone.

K_a, K_n, K_b = hydrolysis rate constants, dependent on groundwater pH and temperature, and on specific chemical properties.

K_D = effective distribution coefficient for each specific chemical. It is assumed to be dependent on the organic carbon content of the soil, and in some cases on the pH and specific chemical properties of the pollutant.

The relationships used for the generation of these parameters and variables are discussed below.

g. Dispersivity. Guven et al. (1984) reported a simple, linear dependency on the travel distance for the longitudinal dispersivity, of the form:

$$\alpha_L = 0.093\ X + 0.007$$

where X = mean travel distance, m.

Transverse dispersivity, α_T, has been studied to a lesser degree but its magnitude is known to be less than the longitudinal dispersivity while maintaining scale dependency (Sudicky et al., 1983). Typically, α_T is related to α_L by a simple ratio leading to the expression:

$$\alpha_L / \alpha_T = LTR$$

where LTR = longitudinal/transverse dispersivity ratio.

However, such ratios are often assumed quite arbitrarily. The actual relationship is the subject of current research. A range of LTR has been reported that appears to center around a value of 3.0, which has been selected for the Monte Carlo analysis. For multidirectional flow in the longitudinal direction the vertical dispersivity, α_V, is quite low. Using the ratio α_L/α_V to describe vertical dispersivity, Gelhar et al (1985) reported a range of 30-1860, with an average of 400. Because of the uncertainty surrounding proper specification of values for vertical dispersivity, it is varied uniformly from 40 to 400 in the Monte Carlo routine.

The data generation approach for dispersivity can be summarized by the following equations:

$$\alpha_L = 0.093\ X + 0.007$$

$$\alpha_T = 0.0333\ X$$

$$\alpha_V = 0.0025\ X - 0.01\ X$$

where X is the downgradient exposure point distance selected for the implementation of the decision rule.

h. Porosity, θ. This is the ratio of the volume of voids of a given soil to the total volume of soil. It is largely a function of particle size. For small particle size like clay, porosity increases to a maximum of about 0.5. Porosities of coarse media (e.g. gravel) decrease to a minimum of about 0.3. These measured ranges suggest a

strong correlation with mean particle diameter, d. Data reported by Davis (1969) were used to develop a regression equation relating porosity to mean particle size as follows:

$$\theta = 0.261 - 0.0385 \ln (d)$$

where ln (d) = natural logarithm of the mean particle diameter.

The distribution for porosity is generated from a seed distribution for particle size diameter. After a uniform and a log-uniform distribution for the particle size diameter were investigated, the log-uniform distribution was selected because it more heavily weights the influence of smaller particle sizes and because the related velocity distribution is more consistent with observed data.

i. Bulk density is defined as the mass of dry soil divided by its total or bulk volume. According to Freeze and Cherry (1979):

$$\theta = 1 - \frac{\rho_b}{\rho_p} \qquad (3.49)$$

where ρ_p = particle size density, g/cm^3 ;

ρ_b = bulk density, g/cm^3 .

The particle density of soil materials varies over a very narrow range, with an average 2.65 g/cm^3. Substituting this value in equation (3.49), the bulk density may be calculated as a function of porosity as follows:

$$\rho_b = 2.65 \ (\ 1 - \theta \ ) \qquad (3.50)$$

j. Velocity, V. The velocity of groundwater is a major determinant of the transport of solutes in subsurface systems. In uniform porous media it is the dominant factor and must be properly specified in the Monte Carlo process. Dependencies among its input data must be preserved while generating realistic values of velocity.

Velocities are related to soil properties and other site-specific factors through Darcy's Law. Assuming steady flow in uniform, saturated media, Darcy's Law states (in simplified form):

$$V = \frac{K_s \, S}{\theta} \tag{3.51}$$

where K_s = saturated hydraulic conductivity, cm/sec
S = hydraulic gradient.

The saturated hydraulic conductivity is a measure of the ease with which water flows though porous media. For any given fluid, it is a function of the medium properties including particle size, grain shape, connectivity and tortuosity. Several approximate functional relationships to estimate the value of K_s have been proposed. The most notable among them is the Karmen-Cozeny equation (Bear, 1979) :

$$K_s = 478\left[\frac{\theta^2}{(1-\theta)^2}\, d^2\right] \tag{3.52}$$

where θ = porosity;
d = mean particle diameter.

The hydraulic gradient, S, is a function of the local topography, groundwater recharge volumes and locations, and the influence of withdrawals, and it is indirectly related to porous media properties. Since there is no functional relationship to express these dependencies, another independent seed distribution is required to generate this variable. To prevent unrealistic conditions due to very large values of the velocity caused by high values of both K_s and S, the velocity field has been bounded such that a fixed maximum is not exceeded. An observed value of 9250 m/year was selected for this purpose.

h. Standard deviation of the Gaussian distribution for the source concentration, σ. This parameter reflects the nature and extent of the leachate interaction with the groundwater. From mass balance principles it may be stated that

$$\sigma = \frac{q \, A_w \, C_L}{\sqrt{2\pi} V \, \theta \, H \, C_0} \tag{3.53}$$

where q = unit areal flux of leachate through the land disposal facility, m/year;
A_w = area of disposal facility, m^2;
V_w = groundwater velocity, m/year;
θ = saturated zone porosity;
H = leachate penetration into the saturated zone, m;
C_L = contaminant concentration in the leachate;
C_o = contaminant concentration in the mixing zone beneath the facility.

Assuming that the leachate concentration is the same as the maximum concentration of the Gaussian concentration distribution, σ can be calculated directly from equation (3.53) given the other variables. This assumption implies that the leachate displaces the groundwater and dilution begins after advective transport has been initiated. Values for the chemical flux, q, and the area term, A_w, were generated by independent seed distributions. For mathematical reasons (boundary effects) the constraint that the ratio H/B is less than 0.5 must also be made. The minimum saturated thickness is set to 3 meters.

1. Hydrolysis rates. Hydrolysis rates depend on the chemical nature of the pollutant and have to be taken from the literature or measured experimentally in the laboratory. Acid- and base- catalyzed hydrolysis rates depend on groundwater pH, and acid-, base- and neutral hydrolysis rates are a function of temperature. The temperature dependency has been described using the Arrhenius equation. Using the generic activation energy recommended by Wolfe (1985) of 20 kcal/mole, the temperature correction factor can be written as :

$$\frac{K^T_{a,n,b}}{K^{Tr}_{a,n,b}} = \exp\left[10^4\left(\frac{1}{Tr} - \frac{1}{T}\right)\right] \qquad (3.54)$$

where $k^T_{a,n,b}$ = second-order hydrolysis rate constant for acid, neutral, or base conditions at temperature T;
$k^{Tr}_{a,n,b}$ = second-order hydrolysis rate constant for acid neutral or base conditions at reference temperature T_r;
T = temperature, °K;
T_r = reference temperature, °K.

m. Distribution Coefficient. In most cases, the sorption process is dominated by hydrophobic binding. It is possible then to relate the distribution coefficient directly to the soil organic carbon. As stated earlier, the dependency is given by:

$$k_D = (k_{oc})\ (f_{oc}) \qquad (3.55)$$

where k_{oc} = distribution coefficient normalized to organic carbon;
f_{oc} = fractional organic carbon.

The values for fractional organic carbon are generated as an independent parameter. For other binding mechanisms, as those presented by polar or ionizable compounds, adjustments are made on a case-by-case basis (Karickhoff, 1985). In cases where reliable relationships do not exist, measurements are required.

3.8 MODIFIED EPA MODEL FOR ANALYSIS OF IMPACT ON SURFACE WATER, EPASF

As part of recently proposed rules for land disposal restrictions, the U.S. Environmental Protection Agency (1986) developed models for the back-calculation of screening levels of constituents in land disposal systems under conditions of uncertainty. The models developed for this purpose considered the impacts of hazardous constituents both in groundwater and in surface waters contaminated via migration through groundwater. These models have been modified for down-gradient calculation of concentrations under uncertainty and have been included in the Advisory System under the acronyms EPAGW and EPASF. EPASF addresses the contamination scenarios concerned with impacts in and through surface waters. These are:

Scenario 2A: Violation of an environmental standard in surface water contaminated by leachate. This scenario involves failure of the waste container, followed by transport in groundwater and mixing with uncontaminated stream water.

Scenario 2B: Exposure of humans through drinking water coming from surface water contaminated by leachate. This continues the previous scenario with downstream transport, intake by water treatment plant, and exposure of humans to the contaminant via drinking water.

Scenario 3: Exposure of humans through consumption of fish from surface waters contaminated by leachate carried through groundwater. This proceeds as in Scenario 2A, followed by uptake of contaminant by fish (bioconcentration and/or biomagnification), and human exposure via fish consumption.

All three of these scenarios require calculation of diluted in-stream concentrations. This may then be equated to standards of human exposure through drinking water and human exposure through consumption of fish by appropriate assumptions regarding daily water intake and daily average fish consumption. For instance, the pathway analysis through fish consumption is based on an average consumption rate of 6.5 grams of fish per day.

The actual process of surface water contamination through land disposal sites includes a large number of complex phenomena, which may vary greatly from site to site. In the course of a site permitting analysis sufficient hydrogeologic data is usually not available to make a detailed and accurate analysis of mass loading to surface water through groundwater transport. Therefore, the regulations proposed by EPA involve a generalized analysis with the incorporation of a Monte Carlo uncertainty analysis. This appears to be the only practical route available for preliminary analysis of potential surface water impacts in the site permitting process. If such an analysis

does suggest potential problems it may then be necessary to proceed to more specific modeling of the ground water-surface water interaction. EPASF thus serves as a flag to potential surface water problems. Where such are indicated by EPASF the finding should place a burden on the applicant to provide sufficient hydrogeologic data for more detailed modeling of the interaction.

To derive an approximate solution we first assume that the average concentration at the ground water outlet to the surface water, C_g, can be related linearly to the leachate concentration, C_L, as:

$$C_g = z_g C_L \tag{3.56}$$

where z_g is a ground water attenuation factor.

It is assumed that the saturated zone transport has reached steady-state. The contaminant mass flux leaching from the site into the groundwater system, m_L, is given by:

$$m_L = Q_L C_L \tag{3.57}$$

where Q_L is the volumetric rate of leaching from the site, and C_L is the leachate concentration. Transport in ground water from the site to the stream results in a plume that intercepts the stream over an area A_g with an average concentration C_g. C_g corresponds to the average of the actual point concentration, which is assumed to be a Gaussian distribution over the effective flow area. If the ground water steady-state seepage velocity is represented by V_g, the contaminant mass flux from the ground water system into the surface water system, m_g, is given by:

$$m_g = V_g A_g C_g = Q_g C_g \tag{3.58}$$

where Q_g is the contaminated ground water discharge rate.

At steady state, m_g is related to m_L by:

$$m_g = f_H m_L \tag{3.59}$$

where f_H is the fraction of the contaminant mass not transformed by hydrolysis or initial speciation in the groundwater (as, at steady state, lateral dispersion of the plume does not affect the total mass loading to the stream).

Combining these equations gives an expression for the concentration dilution factor due to transport in groundwater:

$$\frac{C_g}{C_L} = \frac{f_H Q_L}{Q_g} = z_g \qquad (3.60)$$

The parameters Q_L and f_H are estimated in the simplest case from:

$$Q_L = P(1-f_R)A_w/(86400 \cdot 365.25) \qquad (3.61)$$

and

$$f_H = e^{(-K_g \tau_g)} \qquad (3.62)$$

where:
Q_L=rate of percolation through the land disposal unit, m^3/sec.
P=average annual precipitation rate, m/year.
f_H=runoff fraction.
A_w=surface area of the waste site, m^2.
K_g=total effective decay constant in ground water, 1/yrs.
τ_g=time taken by the contaminant to travel from the land disposal unit to the stream entry point, years.

The factor K_g is estimated exactly as in the model EPAGW. Similarly, the travel time of the constituents in ground water is given, in the one-dimensional case without dispersion, by:

$$\tau_g = \frac{X_g}{V_g f_{Dg}} \qquad (3.63)$$

where:
X_g=distance from site to stream, m.
V_g=ground water seepage velocity, m/yr.
f_{Dg}=fraction of compound that is dissolved, calculated as in the model EPAGW.

When the contaminated ground water enters the stream it mixes with surface water supplied by the upstream watershed. Assuming that the downstream end of the plume entry is given by x=0, and that lateral concentration gradients disappear due to mixing, the laterally averaged concentration, C_x increases with x reaching a maximum near the downstream end of the impacting plume (x=0).

From mass balance considerations, at x=0,

$$C_s = \frac{Q_g}{Q^B_s} C_g = z_s C_g \tag{3.64}$$

where Q^B_s is the stream base flow at x=0, given by:

$$Q^B_s = P(1-F_R)A_s/(86400 \cdot 365.25) \tag{3.65}$$

where A_s is the surface area of the upstream watershed and it is assumed that the average annual precipitation rate, P, and the average runoff coefficient, f_R are the same for the waste site and the entire watershed. Combining equations then yields the laterally averaged concentration at the downstream edge of the ground water plume, C_s, as:

$$C_s = \frac{f_H A_w}{A_s} C_L \tag{3.66}$$

The steady-state laterally averaged value of concentration downstream may then be approximated through an attenuation factor, $z_T = e^{-\beta}$, where $\beta = K \cdot x/U$, K = decay rate constant, sec^{-1}, and U = mean downstream velocity, m/sec. In stream decay processes include sorption, hydrolysis and volatilization. Hydrolysis is calculated dependent on pH and organic carbon fraction of the suspended sediment, in a manner analysis to that employed for hydrolysis in ground water used in EPAGW.

As programmed, the model provides considerable flexibility through the determination of f_H, the mass loading factor, and τ_g, the time taken by the contaminant to travel from the land disposal unit to the stream entry point. The situation described above demonstrates the one-dimensional flow case without dispersion. Options are also included to derive f_H and τ_g with the inclusion of dispersion, using a one-dimensional advection-dispersion solution, and by use of a three-dimensional transport equation. For the latter case, the ground water transport equation used in determination of f_H is the same as is documented for the model EPAGW.

3.9 EVALUATION OF ROTARY DISTRIBUTOR SYSTEMS FOR PERMITTING, LTIRD

The advection-dispersion equation for plane radial flow (Bear, 1979) may be written as:

$$\frac{1}{r}\frac{\delta}{\delta r}\left[Dr\frac{\delta C}{\delta r}\right] - V\frac{\delta C}{\delta r} = \frac{\delta C}{\delta t} \qquad (3.67)$$

For steady plane radial flow (but transient mass transport), replacing the dispersion coefficient D by $\alpha_L V$, the following expression is obtained (Javandel et al., 1984):

$$\alpha_L V\frac{\delta^2 C}{\delta r^2} - V\frac{\delta C}{\delta r} = \frac{\delta C}{\delta t} \qquad (3.68)$$

Consider a confined aquifer with thickness b being recharged through a fully penetrating well at a constant rate Q. If the concentration of a chemical in the recharge fluid is C_0 (and the concentration of that chemical in the aquifer water was originally zero), equation (3.68) may be rewritten as:

$$\frac{1}{r_D}\frac{\delta^2 C_D}{\delta R_D^2} - \frac{1}{r_D}\frac{\delta C_D}{\delta r_D} = \frac{\delta C_D}{\delta t_D} \qquad (3.69)$$

where:

$$r_D = r/\alpha_L$$

$$t_D = \frac{Q\,t}{2\pi bn\alpha_L^2}$$

$$C_D = C/C_0$$

Initial and boundary conditions for this problem are:

$$C_D\,(r_D,\ t_D) = 0, \quad t_D=0 \qquad (3.70)$$

$$C_D\,(r_{D_w},\ T_D) = 1 \qquad (3.71)$$

$$\lim_{r_D\to\infty} C_D\,(r_D,\ T_D) = 0 \qquad (3.72)$$

where r_{Dw} is the dimensionless well (source) diameter. The solution in Laplace transform domain, in terms of Airy functions, is:

$$L_D = \frac{1}{s} \exp\left[\frac{r_D - R_D w}{2}\right] \left[\frac{Ai(Y)}{Ai(Y_0)}\right] \qquad (3.73)$$

where:

L_D = Laplace transform of dimensionless concentration.

s = Laplace transform parameter.

$Y = s^{-2/3}(sr_D + 1/4)$

$Y_0 = s^{-2/3}(sr_{Dw} + 1/4)$

The general form of the Airy function can be found in Abramowitz and Stegun (1964). An asymptotic expansion yields:

$$Ai(z) \cong \frac{1}{2} \sqrt{\pi}\, z^{-1/4}\, e^{-\xi} \sum_{k=0}^{\infty} (-1)^k\, c_k\, \xi^{-k} \qquad (3.74)$$

for $\arg |z| < \pi$,

where:

$$c_k = \frac{(2k+1)(2k+3)\ldots(6k-1)}{216^k\, k!}$$

$c_0 = 1$

$\xi = \frac{2}{3} z^{3/2}$

The computer code LTIRD calculates the dimensionless concentration of a solute injected into an aquifer. It has been adapted for single rotary distributors in the Advisory System, but should not be used for multiple distributors.

3.10 SEMI-ANALYTICAL MODEL BASED ON COMPLEX VELOCITY POTENTIAL, RESSQ

Semi-analytical methods are more powerful than analytic methods in terms of representation of the flow regime, and simpler than most of the complete numerical techniques. These methods apply a well-known concept of fluid mechanics: the complex velocity potential. A major limitation is that they apply only to steady-state two-dimensional fluid flow through homogeneous media. The computer program RESSQ calculates two-dimensional contaminant transport by advection and adsorption (no dispersion or diffusion) in a homogeneous, isotropic confined aquifer of uniform thickness when regional flow, sources and sinks create a steady-state flow field (Javandel et al., 1984).

The velocity potential is generally defined as:

$$\phi = Kh + c \tag{3.75}$$

Therefore, a component of the specific discharge or Darcy velocity vector in any arbitrary direction x is:

$$q_x = -\frac{\delta\phi}{\delta x} = -K\frac{\delta h}{\delta x} \tag{3.76}$$

The stream function can be obtained with a known velocity potential by using the Cauchy-Riemann equations:

$$\frac{\delta\phi}{\delta x} = \frac{\delta\psi}{\delta y}$$

$$\frac{\delta\phi}{\delta y} = -\frac{\delta\psi}{\delta x} \tag{3.77}$$

It is important to note that both the stream function and velocity potential are harmonic functions in that they satisfy the Laplace equation: therefore, their application is restricted to steady-state planar flow fields.

The complex velocity potential of a uniform flow with Darcy velocity U, in a direction making an angle α with the positive x axis, is:

$$W = -UZe^{-i\alpha} + c \tag{3.78}$$

Substituting for complex numbers Z and $e^{-i\alpha}$, the velocity potential and the stream function for such a flow system are obtained:

$$W = \phi + i\psi = -U(x + iy)(\cos\alpha - i\sin\alpha) + c \tag{3.79}$$

$$\phi = -U(x\cos\alpha + y\sin\alpha) = \text{constant} \tag{3.80}$$

$$\psi = U(x\sin\alpha - y\cos\alpha) = \text{constant} \tag{3.81}$$

The latter two equations represent equipotentials and streamlines, respectively. Components of specific discharge are:

$$q_x = -\frac{\delta\phi}{\delta x} = U\cos\alpha \tag{3.82}$$

$$q_y = -\frac{\delta\phi}{\delta y} = U\sin\alpha \tag{3.83}$$

The complex velocity potential of a source with strength m located at the point Z_0 is:

$$W = m \ln(Z-Z_0) + c \tag{3.84}$$

If the source represents a well which is being recharged at rate Q into an aquifer of thickness b, then the strength m of the source is simply:

$$m = - \frac{Q}{2\pi b} \tag{3.85}$$

Substituting for complex numbers Z and Z_0 in equation (3.84), the velocity potential and stream function are:

$$W = \frac{-Q}{2\pi b} \ln\left[(x-x_0)^2 + (y-y_0)^2 \right]^{1/2} - i \frac{Q}{2\pi b} \tan^{-1} \left[\frac{y-y_0}{x-x_0} \right] + c \tag{3.86}$$

$$\phi = \frac{-Q}{4\pi b} \ln\left[(x-x_0)^2 + (y-y_0)^2 \right] + c_1 \tag{3.87}$$

$$\psi = \frac{-Q}{2\pi b} \tan^{-1} \left[\frac{y-y_0}{x-x_0} \right] + c_2 \tag{3.88}$$

where x_0 and y_0 are the coordinates of the source and x and y are the coordinates of a point where the velocity potential and stream function are calculated. Components of specific discharge based on the above definitions are:

$$q_x = - \frac{\delta\phi}{\delta x} = \frac{Q}{2\pi b} \frac{(x-x_0)}{(x-x_0)^2 + (y-y_0)^2} \tag{3.89}$$

$$q_y = - \frac{\delta\phi}{\delta y} = \frac{Q}{2\pi b} \frac{(y-y_0)}{(x-x_0)^2 + (y-y_0)^2} \tag{3.90}$$

The complex velocity potential for a positive doublet is:

$$W = \frac{\Omega \bar{Z}}{|Z|^2} + c \tag{3.91}$$

where $\bar{Z}$ and $|Z|$ are the conjugate and modulus of complex number Z, respectively.

Substituting for these two values, the velocity potential and stream function for a positive doublet located at the origin are:

$$W = \phi + i\psi = \frac{\Omega(x - iy)}{x^2 + y^2} \tag{3.92}$$

$$\phi = \frac{\Omega x}{x^2 + y^2} = \text{constant} \tag{3.93}$$

$$\psi = \frac{-\Omega y}{x^2 + y^2} = \text{constant} \tag{3.94}$$

Equations (3.93) and (3.94) can be rearranged to give:

$$\left[x - \frac{\Omega}{2c}\right]^2 + y^2 = \left[\frac{\Omega}{2c}\right]^2 \tag{3.95}$$

$$x^2 + \left[y + \frac{\Omega}{2c}\right]^2 = \left[\frac{\Omega}{2c}\right]^2 \tag{3.96}$$

Equation (3.95) represents equipotentials and describes circles with centers along the x axis. Similarly, equation (3.96) represents a group of circles with centers on the y axis and tangent to the x axis. These circles are the streamlines for such a doublet.

Since the Laplace equation is a linear partial differential equation, the principle of superposition applies: as many flow components as needed can be superimposed to obtain the expression for the complex velocity potential of an entire system. For example, one or several point sources of contaminant recharge, together with some groundwater discharge wells, can be combined with a uniform regional groundwater flow regime. The overall complex velocity potential may be written as:

$$W = -UZ^{-ia} + \sum_{j=1}^{N} \frac{Q_j}{2\pi b} \ln(Z - Z_j) - \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \ln(Z - Z_k) + c \tag{3.97}$$

where:

W = overall complex velocity potential of the system.
U = Darcy velocity of uniform regional flow.
a = angle between the direction of regional flow and the positive x axis.
b = aquifer thickness.
Q_j = rate of discharge from well j.
Q_k = rate of discharge from well k.

The velocity potential of the above system, the real part of W, is (Javandel et al., 1984):

$$\phi = -U(x\cos\alpha + y\sin\alpha) + \sum_{j=1}^{N}\frac{Q_j}{4\pi b}\ln\left[(x-x_j)^2 + (y-y_j)^2\right]$$

$$- \sum_{k=1}^{M}\frac{Q_k}{4\pi b}\ln\left[(x-x_k)^2 + (y-y_k)^2\right] + c_1 \qquad (3.98)$$

and the expression for the stream function, the imaginary part of W, becomes:

$$\psi = U(x\sin\alpha - y\cos\alpha) + \sum_{j=1}^{N}\frac{Q_j}{2\pi b}\tan^{-1}\left[\frac{y - y_j}{x - x_j}\right]$$

$$- \sum_{k=1}^{M}\frac{Q_k}{2\pi b}\tan^{-1}\left[\frac{y - y_k}{x - x_k}\right] + c_2 \qquad (3.99)$$

At any given point with coordinate (x,y), components of the specific discharge for the overall system may be written as:

$$q_x = -\frac{\delta\phi}{\delta x} = U\cos\alpha - \sum_{j=1}^{N}\frac{Q_j}{2\pi b}\frac{(x-x_j)}{(x-x_j)^2 + (y-y_j)^2}$$

$$+ \sum_{k=1}^{M}\frac{Q_k}{2\pi b}\frac{(x-x_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (3.100)$$

$$q_y = -\frac{\delta\phi}{\delta y} = U\sin\alpha - \sum_{j=1}^{N}\frac{Q_j}{2\pi b}\frac{(y-y_j)}{(x-x_j)^2 + (y-y_j)^2}$$

$$+ \sum_{k=1}^{M}\frac{Q_k}{2\pi b}\frac{(y-y_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (3.101)$$

Components of the average pore water velocity for an individual fluid particle moving through the overall flow system are, introducing a retardation factor, R:

$$v_{cx} = q_x/nR \qquad v_{cy} = q_y/nR \qquad (3.102)$$

The path line traveled by a contaminant particle can be divided into increments dl, traversed in time intervals dt. The projections of dl on the x and y axes are given by dx and dy, respectively:

$$dx = v_{cx}dt = q_x dt/nR \tag{3.103}$$

$$dy = v_{cy}dt = q_y dt/nR \tag{3.104}$$

$$dl = \sqrt{(dx^2 + dy^2)} = \sqrt{(q_x^2 + q_y^2)}\ dt/nR \tag{3.105}$$

Numerical integration of equation (3.105) yields travel time between any two points of a given streamline. If a contaminant particle is at a point (x_j, y_j) at time t, its new position at time t + Dt on the same streamline can be calculated by using:

$$x_{j+1} = x_j + \Delta x = x_j + q_x \Delta t/nR \tag{3.106}$$

$$y_{j+1} = y_j + \Delta y = y_j + q_y \Delta t/nR \tag{3.107}$$

According to Javandel et al. (1984), the combination of a uniform flow in the positive x direction with a positive doublet and a point source (both centered at the origin) represents outflow from a completely penetrating cylindrical pond in the presence of a uniform flow in the positive x direction. The complex velocity potential, then, is:

$$W = -UZ + \frac{\Omega \bar{Z}}{|Z|^2} - \frac{Q_p}{2\pi b} \ln Z + c \tag{3.108}$$

and the velocity potential and stream function are:

$$\phi = -Ux + \frac{\Omega x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln(x^2 + y^2) + c_1 \tag{3.109}$$

$$\psi = -Uy - \frac{\Omega y}{x^2 + y^2} - \frac{Q_p}{2\pi b} \tan^{-1}\left(\frac{y}{x}\right) + c_2 \tag{3.110}$$

where:

U = Darcy velocity of uniform flow in the positive x direction.

Q_p = rate of outflow from the pond.

b = thickness of the aquifer.

Ω = constant of the doublet.

The value of the constants in equation (3.109) can be determined such that the velocity potential satisfies the appropriate boundary conditions. Holding ϕ constant and equal H_0 at $r = r_0$,

$$\phi = H_0 - Ux + \frac{Ur_0^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln\left[\frac{x^2 + y^2}{r_0^2}\right] \qquad (3.111)$$

Incorporating the velocity potential of sources and sinks, the result is:

$$\begin{aligned}\phi = {} & H_0 - Ux + \frac{Ur_0^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln\left[\frac{x^2 + y^2}{r_0^2}\right] \\ & + \sum_{j=1}^{N} \frac{Q_j}{4\pi b} \ln\left[\frac{(x-x_j)^2 + (y-y_j)^2}{x_j^2 + y_j^2}\right] \\ & - \sum_{k=1}^{M} \frac{Q_k}{4\pi b} \ln\left[\frac{(x-x_k)^2 + (y-y_k)^2}{x_k^2 + y_k^2}\right] \end{aligned} \qquad (3.112)$$

where Q_j and Q_k are the rates of discharge and recharge of sinks and sources, respectively. Components of the average pore water velocity at any point (x,y) within the overall flow regime where the velocity potential is defined may be written as:

$$v_x = -\frac{1}{n}\frac{\delta\phi}{\delta x} = \frac{U}{n} + \frac{Ur_0^2}{n}\left[\frac{x^2 - y^2}{(x^2 + y^2)^2}\right] + \frac{Q_p}{2\pi nb}\frac{x}{x^2 + y^2}$$

$$- \sum_{j=1}^{N} \frac{Q_j}{2\pi nb} \frac{(x-x_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi nb} \frac{(x-x_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (3.113)$$

$$v_y = -\frac{1}{n}\frac{\delta\phi}{\delta y} = \frac{Ur_0^2}{n}\left[\frac{2xy}{(x^2 + y^2)^2}\right] + \frac{Q_p}{2\pi nb}\frac{y}{x^2 + y^2}$$

$$- \sum_{j=1}^{N} \frac{Q_j}{2\pi nb} \frac{(y-y_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi nb} \frac{(y-y_k)}{(x-x_k)^2 + (y-y_k)^2} \qquad (3.114)$$

3.11 Method of Characteristics Two-Dimensional Solute Transport Model, MOC

Theoretical Background and Governing Equations

This model can be applied to a wide variety of one- and two-dimensional problems involving steady-state or transient flow. It computes changes in concentration due to the following processes (Konikow and Bredehoeft, 1978 ; Konikow, 1985, 1986) :

(1) convective transport by which dissolved chemicals move with the flowing groundwater;

(2) hydrodynamic dispersion, by which molecular and ionic diffusion and small-scale variations in the velocity of flow through the porous media cause the path of dissolved molecules or ions to spread from the average direction of groundwater flow;

(3) fluid sources, causing mixing or dilution;

(4) reactions, by which the concentration of chemical is modified by its interaction with other species present in the groundwater solution or the solid aquifer materials.

The model assumes that the gradients of fluid density, viscosity and temperature do not affect the velocity distribution. The solute can be reactive or conservative, and the aquifer can be heterogeneous and/or anisotropic. The computer program first solves the governing equation that describes the transient two-dimensional areal flow of a homogeneous compressible fluid through a nonhomogeneous anisotropic aquifer :

$$\frac{\delta}{\delta x_i} \left(T_{ij} \frac{\delta h}{\delta x_j}\right) = S \frac{\delta h}{\delta t} + W \qquad (3.115)$$

where T_{ij} = transmissivity tensor (L^2/T) = $K_{ij}b$

K_{ij} = hydraulic conductivity tensor (L/T)

S = storage coefficient

W = source or sink term

x_i = cartesian coordinates (L)

h = hydraulic head (L)

b = aquifer thickness (L)

The source or sink term, W, is the volume flux per unit area. When only the following terms are considered: a) direct withdrawal or pumpage (well pumpage, evapotranspiration or well injection); b) steady leakage into or out of the aquifer through a confining layer, then the term W may be expressed as

$$W(x,y,t) = Q(x,y,t) - \frac{K_z}{m}(H_s - h) \qquad (3.116)$$

where Q = rate of withdrawal (positive sign) or recharge (negative sign), (L/T);
K_z = vertical hydraulic conductivity of the confining layer, (L/T);
m = thickness of the confining layer, (L);
H_s = hydraulic head in the source, (L).

Darcy's Law provides a basis to calculate the average seepage velocity of groundwater:

$$V_i = - \frac{K_{ij}}{\epsilon} \frac{\delta h}{\delta x_j} \qquad (3.117)$$

where V_i = seepage velocity in the direction of x_i (L/T);
ϵ = effective porosity of the aquifer.

The mass transport equation is :

$$\frac{\delta C}{\delta t} = \frac{\delta}{\delta x_i}\left(D_{ij}\frac{\delta C}{\delta x_j}\right) - \frac{\delta}{\delta x_i}\left(CV_i\right) - \frac{C_0 W}{\epsilon b} + \sum_{k=1}^{m} R_k \qquad (3.118)$$

where C = concentration of solute (M/L^3);
D_{ij} = coefficient of dispersion (L^2/T);
C_{ij}^o = solute concentration in source or sink fluid (M/L^3);
R_k = rate of addition or removal of solute by physical or chemical reactions (M/L^3T);
b = saturated thickness of the aquifer (L).

The first term on the right hand side of equation (3.118) describes the hydrodynamic dispersion, the second term represents the convective transport, and the third and fourth term describe, respectively, fluid sources or sinks and changes in concentration due to chemical or physical reactions occurring in the groundwater solution. The first step in solving equation (3.118) is to estimate the value of D_{ij}. According to Scheidegger (1961), the dispersion coefficient can be computed as a function of the velocity of

groundwater flow and the nature of the aquifer. Assuming that the molecular diffusion is negligible,

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} \tag{3.119}$$

where α_{ijmn} =dispersivity of the aquifer (L);

V_m, V_n =components of velocity in the m and n directions, respectively (L/T);

$|V|$ =magnitude of the velocity (L/T)=$(V_x^2 + V_y^2)^{1/2}$

For an isotropic medium, the dispersivity tensor may be defined in terms of the longitudinal and transverse dispersivities of the aquifer (α_L and α_T, respectively). The components of the dispersion coefficient may be described as

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} \tag{3.120}$$

$$D_{yy} = \alpha_L \frac{V_y^2}{|V|} + \alpha_T \frac{V_x^2}{|V|} \tag{3.121}$$

$$D_{xy} = D_{yx} = (D_L - D_T) \frac{V_x V_y}{|V|^2} \tag{3.122}$$

where $D_L = \alpha_L|V|$ and $D_T = \alpha_T|V|$ are the longitudinal and transverse dispersion coefficients.

The sequence of steps involved in solving these equations is to determine the velocity distribution from equation (3.115) and Darcy's Law. Next, and given the values of α_L and α_T, equation (3.117) is solved subject to certain boundary and initial conditions. Flow and mass transport equations are treated as uncoupled equations in that concentration changes do not affect the flow field; this applies where density differences are negligible, which is the case in most contaminant problems, and one of the assumptions in the MOC model. There are two situations where solutions to the previous equations may be applied: 1) to assess the impact of proposed subsurface waste disposal sites that have not yet been contaminated; 2) to assess the impact of already contaminated sites, predict plume migration and recommend remedial actions.

Numerical Solution

Exact analytical solutions to the partial differential equations of flow , equation (3.115), and solute transport, equation (3.118) cannot be obtained directly due to variable properties of aquifers and complex boundary conditions. The solutions must be approximated by a numerical scheme. The basic method is to break up continuous space into cells, approximate the governing partial differential equations by differences between the values of the parameters over the network and then compute the discrete parcel. MOC utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid -- in which nodes are defined at the centers of the rectangular cells.

The numerical solution technique first solves the equation describing the transient two-dimensional flow of a homogeneous fluid through a nonhomogeneous anisotropic aquifer (equation 3.115), with the following implicit finite-difference approximation :

$$T_{xx[i-1/2,j]} \frac{h_{i-1,j,k}-h_{i,j,k}}{(\Delta x)^2} + T_{xx[i+1/2,j]} \frac{h_{i+1,j,k}-h_{i,j,k}}{(\Delta x)^2}$$

$$+ T_{yy[i,j-1/2]} \frac{h_{i,j-1,k}-h_{i,j,k}}{(\Delta y)^2} + T_{yy[i,j+1/2]} \frac{h_{i,j+1,k}-h_{i,j,k}}{(\Delta y)^2}$$

$$= S \frac{h_{i,j,k}-h_{i,j,k-1}}{(\Delta t)} + \frac{q_{w(i,j)}}{\Delta x \Delta y} \frac{K_z}{m} (H_{s(i,j)}-h_{i,j,k}) \qquad (3.123)$$

where i,j,k = indices in the x,y and time dimensions, respectively;

Δx, Δy, Δt = increments in the x,y and time dimensions, respectively;

q_w = volumetric rate of withdrawal or recharge at the (i,j) node (L^3/T).

This equation is solved numerically for each node in the grid using an iterative alternating-direction-implicit (ADI) procedure (Pinder and Bredehoeft, 1968; Prickett and Lonnquist, 1971; Trescott, Pinder and Larson, 1976). After the head distribution is computed, the velocity of the groundwater flow is computed for each node using an explicit finite-difference form of Darcy's equation:

$$V_{x(i,j)} = \frac{K_{xx(i,j,k)}}{\epsilon} \frac{h_{i-1,j,k} - h_{i+1,j,k}}{2\Delta x} \qquad (3.124)$$

Next, the solute transport equation is solved. This equation describes the two-dimensional areal transport and dispersion of a

given reactive dissolved chemical species in flowing groundwater. This equation is solved using the method of characteristics, through a three step procedure. If saturated thickness is considered as a variable and the convective transport term is expanded, equation (3.118) may be rewritten as

$$\frac{\delta C}{\delta t} = \frac{1}{b}\frac{\delta}{\delta x_i}\left[bD_{ij}\frac{\delta C}{\delta x_j}\right] - V_x\frac{\delta C}{\delta x_i} - V_y\frac{\delta C}{\delta x_j} + \frac{W\ (C-C')}{\epsilon\ b} + \sum_{k=1}^{m} R_k \quad (3.125)$$

which is in the form solved by the computer program.

Changes with time in properties of the fluid (e.g., concentration) may be described either for fixed points within a stationary coordinate system as succesive particles pass the reference points, or for reference fluid particles as they move along their respective paths past fixed points in space. $\delta C/\delta t$ is the rate of change of concentration as observed from a fixed point, whereas dC/dt is the rate of change as observed when moving with the fluid particle (material derivative).

- **Particle tracking.** This first step solved for the change in concentration over distance. It consists of placing a number of traceable particles in each cell of the finite-difference grid, to form a set of points that are distributed in a geometrically uniform pattern throughout the area of interest. The location of each particle is specified by its x and y coordinates. The initial concentration assigned to each point is the initial concentration at the node of the cell containing the particle. For each time step every point is moved a distance proportional to the length of the time increment and the velocity at the location of the point. The new position of the particle is then computed and, after all points have been moved, the concentration at each node is temporarily assigned the average of the concentrations of all points located within the area of that cell.

Finite Difference Approximations

A two-step explicit finite-difference approximation is now used to calculate the new nodal concentrations at the end of the time period. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence in velocity, changes in saturated thickness, adsorption or chemical reaction are calculated using an explicit finite-difference approximation. This change in concentration can be considered as the sum of two separate terms:

$$\Delta C_{i,j,k} = (\Delta C_{i,j,k})_I + (\Delta C_{i,j,k})_I I \quad (3.126)$$

where the subscript I represents the change in concentration caused by hydrodynamic dispersion, and the subscript II is the change caused by an external fluid source, changes in saturated thickness, adsorption or chemical reaction:

$$(\Delta C_{i,j,k})_I = \frac{\Delta t}{b}\left[\frac{\delta}{\delta x_i}\left(bD_{ij}\frac{\delta C}{\delta x_j}\right)\right] \qquad (3.127)$$

$$(\Delta C_{i,j,k})_{II} = \frac{\Delta W_{i,j,k}}{\epsilon\, b_{i,j,k}}\left[C_{i,j,k-1} - C_{i,j,k}\right] \qquad (3.128)$$

Recent modifications (Konikow; 1985, 1986) include first-order radioactive decay (lamda) and a retardation factor, R_f:

$$\lambda = \frac{\ln 2}{t_{1/2}} \qquad (3.129)$$

where $t_{1/2}$ is the half life of the solute, (T). The decay is applied directly to the tracer particles (rather than at the nodes of the finite difference grid):

$$C_p^k = C_p^{k-1} \exp(-\lambda \Delta t) \qquad (3.130)$$

where c_p = solute concentration of the tracer particle, and

k = time dimension index.

This exponential formulation has no numerical stability restrictions, but some numerical accuracy is lost if the half-life is much smaller than the time step for solving the transport equation. The expression for retardation has been defined earlier in this report for other models (e.g., section 3.7).

- **Stability criteria.** The explicit numerical solution of the solute-transport equation has some stability criteria associated with it, which may require that the time step used to solve the flow equation is subdivided into a number of smaller time increments to accurately solve the solute-transport equation. The stability criteria may be stated as follows:

$$\Delta t \leq \underset{\text{(over grid)}}{\text{Min}} \left[\frac{0.5}{\frac{D_{xx}}{(\Delta x)^2} + \frac{D_{yy}}{(\Delta y)^2}} \right] \tag{3.131}$$

$$\Delta t \leq \underset{\text{(over grid)}}{\text{Min}} \left[\frac{\epsilon \, b_{i,j,k}}{W_{i,j,k}} \right] \tag{3.132}$$

$$\Delta t \leq \frac{\gamma \, \Delta x}{(V_x)_{max}} \tag{3.133}$$

$$\Delta t \leq \frac{\gamma \, \Delta y}{(V_y)_{max}} \tag{3.134}$$

where γ is the fraction of the grid dimensions that particles are allowed to move at each time step ($0 \leq \gamma \leq 1$).

If the time step used to solve the flow equation exceeds the smallest of the time limits determined by the above equations, then the time step will be subdivided into the appropriate number of smaller time increments required for solving the solute-transport equation.

-Boundary and initial conditions. Several different types of boundary conditions can be incorporated into the solute-transport model. Two general types have been used in this model: constant flux and constant-head conditions. A constant head boundary can be used to represent aquifer underflow, well withdrawals or well injection. A finite flux is defined by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant flux boundary. The numerical procedure requires that the area of interest be surrounded by a no-flow boundary. No-flow boundaries can also be located elsewhere in the grid to represent natural barriers to groundwater flow. No-flow boundaries are designated by setting to zero the transmissivity at appropriate nodes.

A constant-head boundary represents parts of the aquifer such as recharge boundaries or areas beyond the influence of hydraulic stress. Constant-head boundaries are represented by adjusting the leakage term at appropriate nodes. If a constant-flux or constant-head represents a fluid source, then the chemical concentration in the source fluid must also be specified. The initial conditions can be determined from field data and from previous simulations. The head and concentration in the aquifer at the start of the simulation must be specified, because solute transport depends directly upon hydraulic and concentration gradients.

Monte Carlo Simulation

The MOC model as described in the preceding sections involves a large degree of uncertainty originated by the combination of model error, natural and parameter uncertainties. As an alternative to the deterministic approach in which detailed data are required for the simulation, the Monte Carlo technique enables a prediction which incorporates the uncertainty associated to the inputs and parameters of the model. This is achieved by a random generation of the most sensitive inputs to the model, followed by a large number of computations to yield a well defined distribution of outputs.

An analysis of the sensitivity of model predictions of contaminant concentrations to sources of uncertainty in the inputs and parameters of the model was carried out. Up to five sources of uncertainty were considered. Two of them concerned the variance in time to failure of a landfill and release concentration, while the other three concerned natural and parameter uncertainty and spatial clumping in the hydraulic conductivity field. These are the sources of uncertainty most likely to be of interest in model evaluation. The effects were measured in terms of the effect on the probability distribution of the contaminant concentration for a twenty year target at five different positions along the main flow axis. For each point, the mean and variance of the contaminant concentration and the probability of exceeding the background and an arbitrary standard were calculated. The sensitivity analysis suggested the need to incorporate in the Monte Carlo simulation the effects of release concentration and hydraulic conductivity uncertainty (see results of this type of simulation in Chapter II).

The Monte Carlo process proceeds as follows:

1. The release concentration and hydraulic conductivity (as ln k, natural logarithm of the hydraulic conductivity) are generated at random.

2. The model is run with a set of predetermined inputs and parameters and the random-generated parameters obtained from step 1.

3. The parameter generation and computation steps are repeated a large number of times to produce a well-defined output distribution.

4. The output values are analyzed for presentation as a distribution.

3.12 ANALYSIS OF LEACHING FROM A LANDFILL: HELP

The Hydrologic Evaluation of Landfill Performance (HELP) program was developed to facilitate rapid, economical estimation of the amounts of surface runoff, subsurface drainage, and leachate that may be expected to result from the operation of a wide variety of possible landfill designs (Schroeder et al., 1984). These phenomena arise from the interaction of a large number of complex hydrologic processes, including precipitation, surface storage, runoff, infiltration, percolation, evapotranspiration, soil moisture storage and lateral drainage. HELP takes what is essentially a water-balance approach to the problem, within a quasi-two dimensional process. The model uses climatologic, soil, and design data to produce estimates of water movement across, into, through, and out of landfills. To accomplish this, daily precipitation is partitioned into surface storage (snow), runoff, infiltration, surface evaporation, evapotranspiration, percolation, stored soil moisture, and subsurface lateral drainage to maintain a water budget. Calculations may be performed for up to nine layers of a landfill design. These layers may include a vegetative layer, other types of vertical percolation layers, lateral drainage layers, barrier soil layers and waste layers.

Surface Runoff

Surface runoff is computed by the SCS curve number technique (USDA, 1972). This method was chosen because it is well established, easy to use, and the required input data is generally available. Generally, the curve number for a watershed is determined for average moisture conditions in the SCS method (CN_{II}). The curve number for the lowest antecedent moisture conditions, CN_I, is related to CN_{II} by a polynomial developed for the CREAMS model (Knisel, 1980):

$$CN_I = -16.91 + 1.348CN_{II} - 0.01379CN_{II}^2 + 0.0001177CN_{II}^3 \quad (3.135)$$

The maximum retention factor for a soil, S_{mx} is then determined from:

$$S_{mx} = \frac{1000}{CN_I} - 10 \quad (3.136)$$

From this information we can calculate the daily depth weighted retention factor, S_i, and the daily runoff, Q_i, using the method documented by Knisel (1980). The soil profile of the vegetative or evaporative depth was divided into seven segments. The thickness of the top segment was set equal to 1/36 of the thickness of this depth, while the thickness of the second segment was 5/36 of this depth. Each of the remaining 5 segments was defined as 1/6 of the thickness of the vegetative or evaporative depth. We may then state:

$$S_i = \left\{1 - \sum_{j=1}^{7} W_j \left(\frac{SM_j - WP_j}{UL_j - WP_j}\right)\right\} \quad (3.137)$$

where:

SM_j = soil water content of segment j, inches
UL_j = saturated capacity of segment j, inches
WP_j = wilting point of segment j, inches

and

$$W_j = 1.0159 \left\{\exp\left(-4.16 \frac{D_j - 1}{VD}\right) - \exp\left(-4.16 \frac{D_j}{VD}\right)\right\} \quad (3.138)$$

where:

D_j = depth to bottom of segment j, inches
VD = vegetative or evaporative depth, inches.

and

$$Q = \frac{(P - 0.2S)^2}{(P + 0.8S)} \quad (3.139)$$

where:

P = actual rainfall
S = maximum retention including the initial abstraction

Infiltration

Infiltration is equal to the difference between the daily precipitation, the sum of the change in the surface storage of precipitation (snow), the daily runoff, and the surface evaporation. Thus the net daily infiltration, IN_i, is given by:

$$IN_i = P_i - Q_i - ESS_i \quad (3.140)$$

where

ESS_i = surface water evaporation on day i, inches.
Q_i = daily runoff, inches.
P_i = net rainfall, given by:

$$p_i = PRE_i + SNO_{i-1} - SNO_i \quad (3.141)$$

where:

PRE_i = actual precipitation on day i, in inches.
SNO_i = amount of snowwater at end of day i, inches.

Evapotranspiration

The potential evapotranspiration calculation is also adapted from Knisel (1980), and is computed using a modified Penman method developed by Ritchie (1972). The potential evapotranspiration on day i, E_{oi}, is given by:

$$E_{o_i} = \frac{1.28\ A_i H_i}{(A_i+G)\ 25.4} \tag{3.142}$$

where:

H_i = net solar radiation on day i, langleys.

G = psychrometric constant which equals 0.68

A_i = slope of saturation vapor pressure curve on day i, computed from:

$$A_i = \frac{5304}{T_i^2}\ e^{(21.255-5304/T_i)} \tag{3.143}$$

where:

T_i = mean temperature in °K on day i.

The daily potential evapotranspiration demand is applied first on water available on the surface. Any demand in excess of the surface water is exerted on the soil column in the forms of soil evaporation and plant transpiration. The potential soil evaporation, ES_{oi}, is given by:

$$ES_{o_i} = E_{o_i}\ e^{-0.4\ LAI_i} \tag{3.144}$$

where LAI_i is the leaf area index on day i, or the winter cover factor in non-growing seasons. Soil evaporation proceeds at this rate when evaporation is not limited by transmission of water to the surface. Again following Knisel (1980), this limit is given by:

$$U = \left(9\ (a_s-3)^{0.42}\right)/25.4 \tag{3.145}$$

where a_s = soil transmissivity parameter for evaporation, $(mm/day)^{0.5}$.

After reaching this limit, soil evaporation proceeds at a stage-two rate, $ES2_i$, given by:

$$ES2_i = \left(\sqrt{t_i} - \sqrt{(t_i-1)}\right)/25.4 \tag{3.146}$$

where t_i = days since stage one evaporation ended.

The potential plant transpiration, EP_{oi}, is computed from:

$$EP_{o_i} = \frac{E_{o_i} \; LAI_i}{3} \qquad (3.147)$$

Actual plant transpiration depends on soil moisture and plant transpiration demand, where the plant transpiration demand, EPD_i, is equal to the potential plant transpiration except when limited by low soil moisture or when the daily total of the surface evaporation, soil evaporation and plant transpiration exceeds the daily potential evapotranspiration. The actual plant transpiration, EP_i is then given by:

$$EP_i = EPD_i \left[1.20 - (4 \; EPD_i) + \frac{SM_i - WP}{FC - WP} \right] \qquad (3.148)$$

in which:

SM_i = depth weighted soil moisture on day i,
WP^i = depth weighted wilting point,
FC = depth weighted field capacity.

Full details of the weighting procedure are given in Schroeder et al. (1984).

Soil Moisture Storage

The HELP model uses a daily time interval to evaluate the components of the water balance equation. Soil moisture storage is then given in general terms as:

$$SM_i = SM_{i-1} + \frac{1}{2}\left(IN_i - PE_i - ET_i + IN_{i-1} - PE_{i-1} - ET_{i-1} \right) \qquad (3.149)$$

where:

SM_i = soil moisture storage at midday i
IN_i^i = infiltration on day i
PE_i^i = percolation and drainage from landfill on day i
ET_i^i = evapotranspiration on day i

In application in the model the vegetative or evaporative zone is divided into seven segments. Soil water is then distributed among these segments and all underlying layers, with the equations connected by vertical drainage terms. The model assumes that barrier layers always remain at saturation. After distributing the water among the layers the model checks to see that the soil moisture storage does not exceed the saturated capacity. Any excess above this amount is added to the soil moisture storage of the layer above, or, if an excess in the topmost segment, added to the surface runoff.

Vertical Flow

The model assumes that the soil profile consists of discrete segments that are homogeneous with respect to hydraulic conductivity, total porosity and field capacity. The rate of downward flow is assumed to follow Darcy's law. However, it is further assumed that free outflow occurs from each segment above the barrier soil layer, in which case the rate of flow equals the hydraulic conductivity, k. This assumption is valid as long as the hydraulic conductivities of the segments above the barrier soil layer are similar, or increase with increasing depths of the segments. The effective hydraulic conductivity, k_v, is a function of the saturated hydraulic conductivity, k_s, and the soil moisture content, defined through:

$$k_v = K_s \ (SM_i - MDC)/(UL - MDC) \qquad (3.150)$$

where MDC is the minimum soil water content for drainage to occur.

The routing of moisture from segment to segment is done using a routing procedure computed at the mid-point of the time interval, proceeding sequentially from the top segment to the bottom segment. The model then solves simultaneously for drainage rate and soil moisture. If the moisture content of a segment is greater than its total porosity the excess is backed up into the segment above it.

After convergence is obtained for the segments above a barrier layer, the hydraulic head may be computed on the barrier. Flow through the barrier layer is then also computed using Darcy's Law, as:

$$q = k_s \frac{TH + TS(n+1)}{TS(n+1)} \qquad (3.151)$$

where:

k_s = saturated hydraulic conductivity of the barrier layer
TH = total head on the barrier layer
TS(n+1) = thickness of the barrier soil layer

Lateral Flow

The lateral drainage procedure is based on the Boussinesq equation, which is unsteady and non linear:

$$f \frac{\delta h}{\delta t} = K \frac{\delta}{\delta x}\left[(h - x\alpha)\frac{\delta h}{\delta x}\right] + R \qquad (3.152)$$

where:

f = dimensionless drainable porosity

t = time in days

h = gravitational head in inches

K = effective saturated lateral hydraulic conductivity, inches/day

x = lateral position in the direction of drainage

α = dimensionless slope

R = recharge flux in inches/day perpendicular to the direction of flow

With the selection of a small time step, the steady state assumption is made, $\delta h/\delta t = 0$. The equation is then linearized following the form given by Skaggs (1982), but incorporating an additional correction factor developed by Schroeder et al. (1984). This yields the approximate relationship for lateral drainage, QLAT, as:

$$QLAT = \frac{2\ (0.510 + 0.00205\alpha L)\ Ky\left[y(y/L)^{0.16} + \alpha L\right]}{L^2} \qquad (3.153)$$

where:

L = lateral distance from the crest to the drain, inches

y = average thickness of water profile above barrier soil layer between x=0 and x=L, inches

The vertical and lateral flow routines are then linked under two assumptions:

- Steady-state conditions hold such that change in head is not a function of time.

- The drainage rate estimated at the mid-point of the time interval is effective throughout the time interval.

These assumptions are valid only if the computational time interval is sufficiently small so that there is little change in head. The model is set to use a time step appropriate for most common conditions. The authors contend that four equal time steps per day yields acceptable accuracy for heads less than 30 inches.

Finally, the model must perform a convergence to insure that the drainage rate from the bottom of the profile is equal to the sum of lateral flow and vertical percolation. The results are converged to the 5% level by an iterative scheme commencing with an a priori estimate of drainage rate from the bottom profile segment. This estimate is updated until convergence within the 5% level is obtained.

CHAPTER IV

GROUNDWATER ADVISORY SYSTEM USER'S MANUAL

This chapter provides a detailed guide to the use of the Advisory System, as presently implemented. The intended audience is a user who is familiar with the general theory of contaminant transport in porous media, but who may not have experience with a given transport model.

As noted in Chapter II, the present implementation consists of only a subset of the total proposed Advisory System. The section which has been implemented focuses on the problem of risk analysis for proposed sites (site permitting). Therefore, the user's manual is arranged with this application in mind.

The general structure of this chapter is as follows. First, A "generic" guide is provided to the use of the system, which will be generally applicable regardless of the particular contaminant transport model chosen (section 4.1, "System User's Manual"). The prospective user should thoroughly familiarize himself with this section before proceeding further. Included in this section are complete details of the pathways available for model selection, including the CHOICE algorithm. Details of loading the System are in Chapter V.

In the next section of this chapter (section 4.2) detailed notes are provided on the use of the specific models included within the system. For each model, discussion will be organized under three headings. These are "Applications", providing notes on the applicability of a given model; "Limitations", discussing the inherent limitations of a particular modeling approach; and "Data Input", providing specific notes on data preparation for the model. The user may wish to refer to Chapter II for discussion of the derivation of the solutions employed in assessing the applicability of a specific model to a given problem.

In the final section of this chapter (section 4.3) we provide five partial examples of use of the System. Because the System has considerable breadth, with many transport models available, these examples can represent only a small part of the potential applications of the System. However, they should be useful in providing a feel for the use of the System.

4.1 SYSTEM USER'S MANUAL

The following section provides the generalized concepts of operting the advisory system. Details of use of specific models will be

provided in the next section.

Starting the System

It is assumed that the system has been properly installed on a fixed disk drive on a properly configured PC (see Technical Notes for installation instructions). The system is then started by typing 'GW'. This will result in presentation of a brief memorandum on current updates to the system, followed by the introductory screen:

*

State of North Carolina

*

Advisory System

for

Groundwater Quality Permitting and Monitoring

*

Version 2.0 : June, 1987

*

Developed by : Jonathan B. Butcher
Dr. Miguel A. Medina
Duke University
School of Civil & Environmental Engineering
Dr. Carlos M. Marin
Duke University
School of Forestry & Environmental Studies,
Durham, N.C.

File Management

The first task of the system is identifying the site studied and setting up the needed disk files. On entering the system you will be presented with the following menu:

LEVEL 0 OPTIONS:

1. Continue analysis of the most recently analyzed site. Allows continuation of an interrupted analysis.
2. Analyze a previously analyzed site, not necessarily the subject of the last analysis. Includes compliance monitoring.
3. New site analysis. Can also be used when it is desired to reanalyze a site with a completely new data set.
4. QUIT

***

5. Quick reentry to Level 1, using most recent data files. Skip check and updating of files.

Option 5 is provided so that those experienced in the operation of the system can avoid having to update file headers on reentry. The other entries determine whether a site has been previously analyzed, and so should have existing data files. The user is then prompted for the site name and site ID. The latter should consist of a letter followed by 5 digits and/or letters. This ID will be used to identify files associated with the site, and so should be formulated to some regular scheme.

On forming the file names the appropriate files must be located. The user may define the drive on which these files are to be located. The most frequently used options will be to specify data storage on floppy disk (A), or on an assigned partition previously set up on the hard drive (e.g., D). Note that if output files are maintained on floppy disks you must beware of using up the disk space. Encountering a full data disk will generally not result in a fatal error, but will typically cause the last model results not to be recorded in the output file. (These will however be present as temporary files on the default drive, and can be recovered). Because the output files grow continuously, an option is provided for printing and then deleting the contents of these files to clear disk space.

The file names selected will be echoed to the screen. If the site indicated is a previously analyzed site the system will attempt to locate these files. On the other hand, if the site is a new site the system will check to make sure that files with these names do not already exist. Appropriate options will be presented if these conditions are found to be violated.

Preliminary file maintenance is completed by entering a header, identifying the analyst, date, and title of the project. The system then proceeds to Level 1.

Level 1, Master Menu

After setting up the files, the system proceeds to Level 1, which provides control pathways to the whole system. Upon accessing Level 1 a selection menu will be displayed. This is shown on the following page.

MENU FOR LEVEL 1

MODELS |	A: LeGrand method for preliminary analysis.
	B: Impact scenario definition. Provides user selection for more sophisticated models.
	C: Scheduled compliance monitoring of site.
	R: Algorithm for regulatory model choice, guides model selection (for impact on groundwater only).
FILE |	D: Display directory of site and output files.
UTILS |	N: Restart, analyze new site.
	P: Dump current output file to printer and delete.
	Q: Print current output file.
	S: Scroll output file to screen.
	Z: Abandon analysis, exit to system.

The options presented here are divided into two categories: "Models" and Utilities". The utilities are self explanatory, but the list may be augmented on similar screens as you proceed further into the system.

Preliminary Analysis

In many cases it may appear to the analyst that a proposed site is so poorly situated that it can be rejected without detailed modeling. Conversely, some sites may seem so innocuous that a permit can be granted without detailed modeling. To formalize this subjective process we have provided for preliminary analysis using the LeGrand method. In most cases, the first stage of analysis should thus be to apply this model (option A). Full details of utilizing the LeGrand method will be set forth below.

Access to Models: Scenario Definition

Access to contaminant transport models is provided by two routes, the Scenario Definition pathway and the Choice pathway. The Scenario Definition pathway adopts a fully generalized approach to potential risk resulting from groundwater contamination, following the methodology set forth by the U.S.E.P.A. (1986).

For regulatory purposes contaminants may be monitored either for environmental standards or for human exposure standards (CADI). Further, the impact of contaminants may be in the groundwater itself, or in "downstream" surface waters that are impacted by the contaminated groundwater. This leads to the definition of five scenarios of impacts which may result from a proposed site. These are briefly identified as follows:

Scenario 1A: Violation of an environmental standard for contaminant concentrations in groundwater at some specified distance from a site.

Scenario 1B: Exposure of humans through drinking water drawn from wells contaminated by leachate.

Scenario 2A: Violation of an environmental standard in surface water contaminated by leachate. This scenario involves failure of the waste container, followed by transport in groundwater and mixing with uncontaminated stream water.

Scenario 2B: Exposure of humans through drinking water coming from surface water contaminated by leachate. This continues the previous scenario with downstream transport, intake by water treatment plant, and exposure of humans via drinking water.

Scenario 3: Exposure of humans through consumption of fish from surface waters contaminated by leachate carried through groundwater. This proceeds as in Scenario 2A, followed by uptake of contaminant by fish (bioconcentration and/or biomagnification), and human exposure via fish consumption.

Choice of an input scenario will depend on both the regulatory concerns regarding a given contaminant, and the particular aspects of a given site. In many instances a site will need to be evaluated under several different scenarios, as well as for different contaminants, although an unacceptable degree of risk under any scenario may be sufficient for permit rejection. The rationale of the scenario definition pathway is first to determine the impact scenario involved, then present the array of applicable models for selection. One of these models will then be chosen for analysis of contaminant risk in the Monte Carlo mode. For instance, under Scenario 1A, you would be presented with the following initial selection menu:

SCENARIO 1: Exposure of humans through drinking water drawn from wells contaminated by leachate; or, violation of environmental standards in groundwater.

AVAILABLE MODELS	SUMMARY OF SITE DATA REQUIREMENTS
1. Return to scenario menu	----
2. EPAGW model	low - uses regional data for MC simulation in a detailed model, relatively fast.
3. (blank)	
4. Analytical solutions	low-moderate - simple site data; fast running but not very flexible.
5. MOC (Konikow & Bredehoeft)	high - detailed site data required; long run time for Monte Carlo analysis.
10. terminate analysis	

From this menu, selection of option 4 would lead to another menu

containing various analytical solutions.

In addition to these scenarios, the Scenario Definition procedure also provides an option for choosing a model to run in a deterministic mode. This is particularly useful for preparing maps of possible plume development. However, use of the deterministic mode will of course not reflect the effects of parameter uncertainty in the analysis of risk.

Once a model has been chosen by this method several additional queries will appear. These will ask for the name of the contaminant studied, the applicable standard level, and whether or not you wish to include a call to the HELP model to analyze leaching rates from a site. The program module will then write a batch file that will control the next stage of processing.

Access to Models: Choice Algorithm

The Scenario Definition pathway provides a flexible format for model selection, but depends on user choice in this process. An alternative access route to the models is provided by the Choice Algorithm, which attempts to interactively guide the choice of an appropriate model, and is thus a simple expert system.

Note that the applicability of this algorithm is limited to impacts in groundwater, i.e. Scenarios 1A and 1B in the previous section. The objective of the Choice Algorithm is to consider a wide range of real-world permitting situations, and, in each case to determine whether there is an appropriate analytical solution available with which Monte Carlo analysis of the risk associated with the site can be analyzed. Where such a solution is not available in some instances semianalytical methods will be appropriate for preliminary analysis. Otherwise one may need to proceed to more complex numerical models for analysis of the site.

The Choice Algorithm also provides an option for direct user selection of a model in either a deterministic or Monte Carlo mode. The user will note that this is the most efficient way to gain access to a specific model.

The selection process implemented by the Choice Algorithm is detailed in Fig. (IV-1). The logic employed in this algorithm is given in detailed tabular form on the following page. The entry point for the table is at level 0. Each non-terminal branch indexes another subheading in the table, so that any pathway will eventually lead to the selection of a model, or the determination that no applicable analytical solution is available for use.

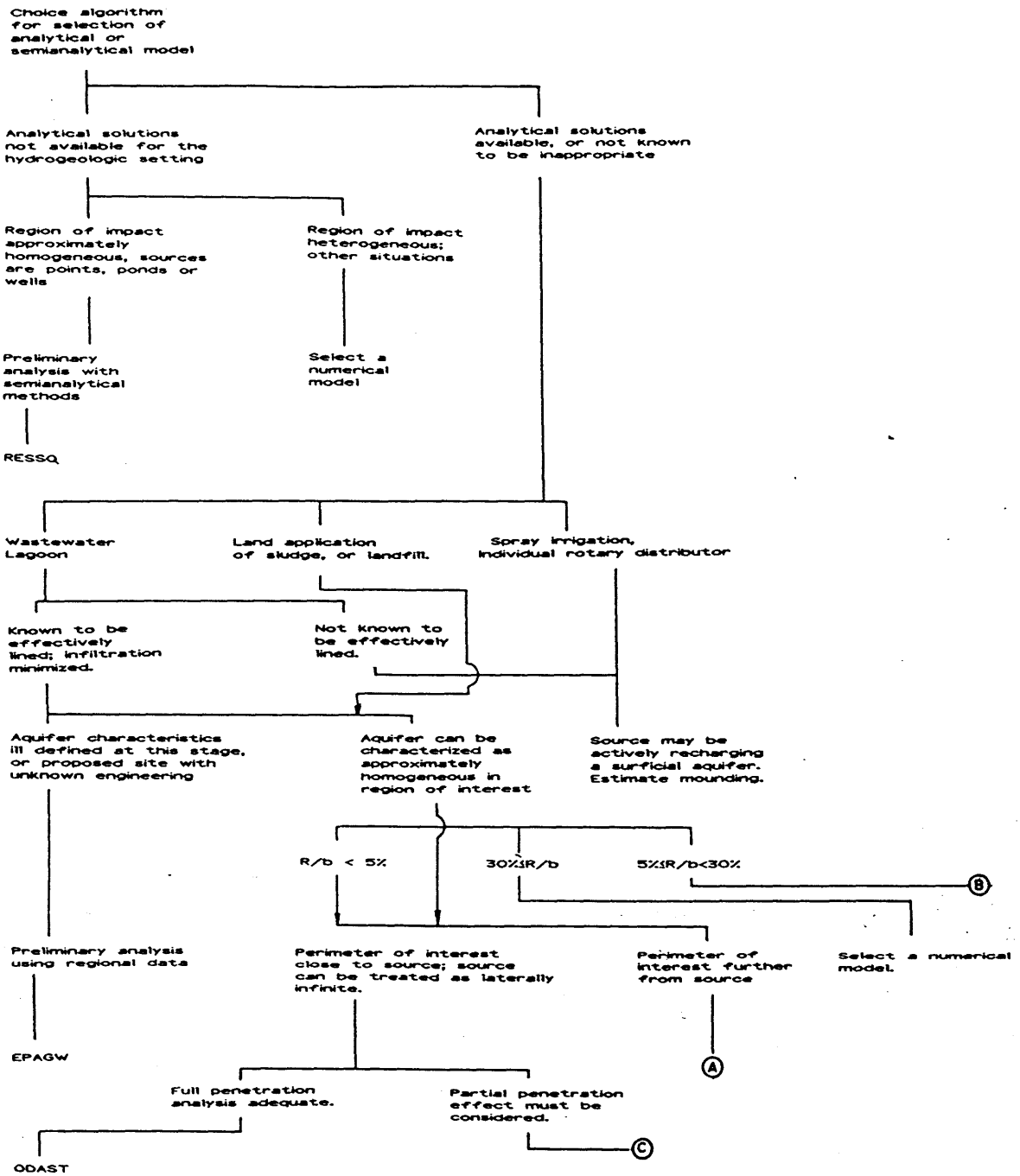

Figure IV-1. Sequence of Logical Steps in the Choice Algorithm

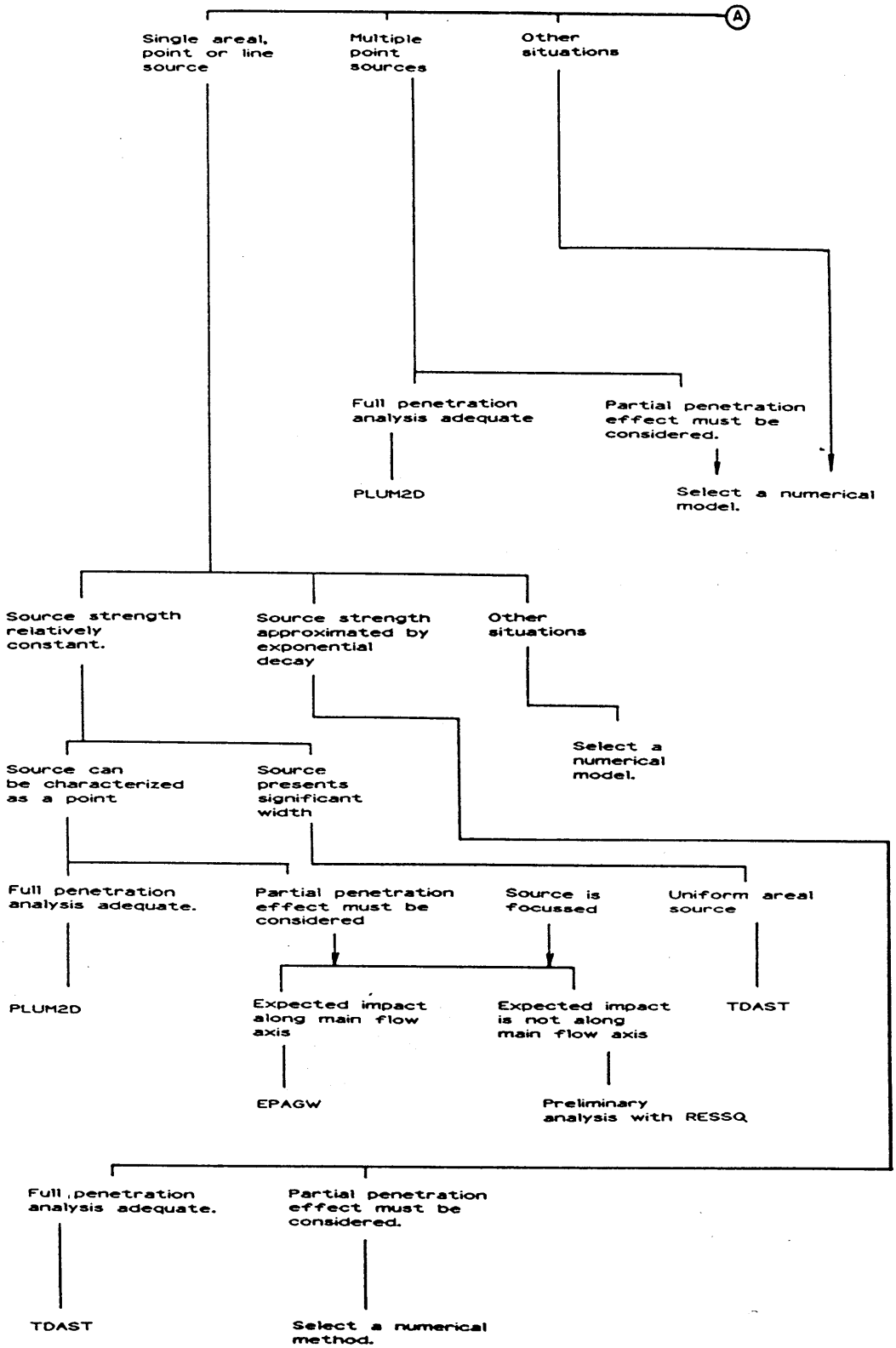

Figure IV-1. Sequence of Logical Steps in the Choice Algorithm

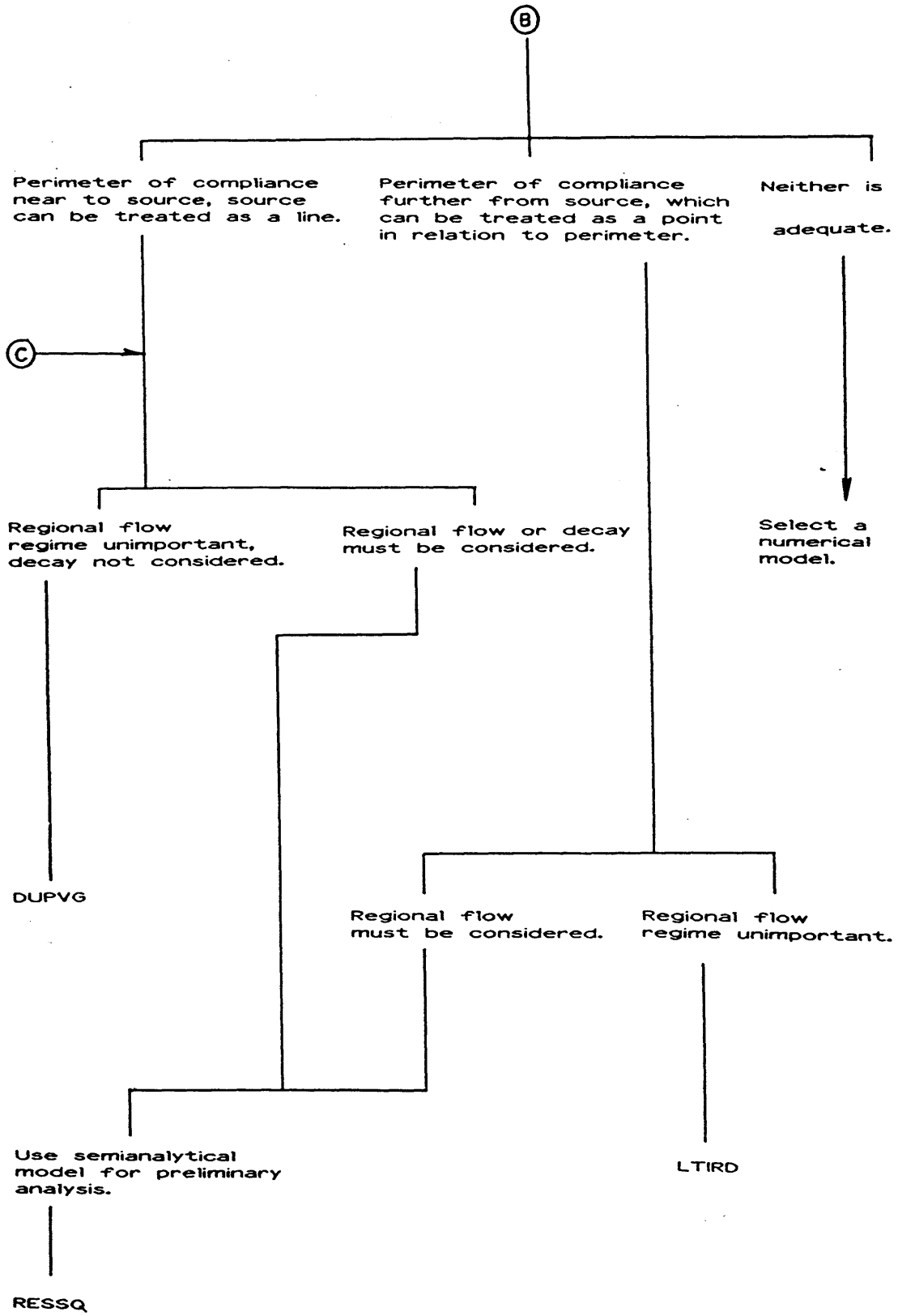

Figure IV-1. Sequence of Logical Steps in the Choice Algorithm

Choice Algorithm

0. Initial site analysis. If the site and aquifer are well-characterized, a numerical model can be used in a deterministic mode to identify risk. However, it may still be appropriate to first analyze the site using an analytical approximation. Commonly, the available data will be insufficient for application of a numerical model. In this case the objective will be to find an appropriate analytical solution, if such exists, which can be used in a Monte Carlo mode to approximate site risk. If such an analysis indicates an inappropriate degree of contamination risk further data may then be required so that a numerical solution can be used. Even where an appropriate analytical solution is not available, in many cases a semianalytical solution can be used for an initial definition of the problem. Such solutions do not consider diffusion, but will enable formation of the pattern of plume development, and can provide the basis for further analysis.

0.1 Quit this procedure.

0.2 Invoke direct user selection of model.

0.3 Continue. ->1

1. Choice algorithm for analytical and semianalytical models. First check that such solutions apply.

1.1. One or more of the following conditions apply: 2

a. The horizontal extent of the region of permit interest in the aquifer is KNOWN to be within 250 ft. of a distinct hydrogeologic boundary, such as an intersecting river, intersecting aquitard, or distinct inhomogeneity in the medium.

b. The regulatory perimeter is in an aquifer that is distinct from the aquifer directly affected by the site. For instance, a site may impact a shallow water table aquifer, while the regulatory perimeter is in an underlying system separated by an aquitard.

c. Contaminant of interest is a liquid that is immiscible in water or has a specific gravity significantly different from water.

d. Flow in region of site is suspected to be strongly affected by pumping wells.

e. Impacted aquifer is a fractured rock system.

f. Source input must be treated as slug injection.

1.2. None of the above apply. ->3

2. Analytical solutions are inappropriate. Check for utility of semianalytical solutions.

2.1. Aquifer can be characterized as not drastically inhomogeneous in the region of interest, but may be affected by constant head boundaries or pumping wells. Sources can be modeled as points, ponds or wells. ->5

2.2. Systems other than 1. ->6

3. Analytical solutions may be appropriate. Now determine type of site. Site can best be characterized as:

3.1. Wastewater Lagoon. ->3A

3.2. Spray irrigation of wastewater. ->7

3.3. Land application of sludge. ->4

3.4. Individual Rotary distributor. ->7

3.5. Landfill. ->4

3.6. Injection of waste into confined aquifer. ->9

3.7. septic tanks. ->7

3A. Subset of lagoon systems. Waste water lagoon, is:

3A.1. known to be effectively lined so that the effect of infiltration on regional flow is slight. ->4

3A.2. not known to be effectively lined, so that significant volume of infiltration may occur. ->7

4. Confined aquifer, or situation that can be approximately modeled by confined aquifer solutions, or characteristics unknown.

4.1. Aquifer characteristics are ill-defined at this stage of the analysis, or proposed site with unknown engineering. ->8

4.2. Aquifer can be characterized as approximately homogeneous and infinite in the region of interest. ->9

5. Aquifer not drastically inhomogeneous in region of interest. Semianalytical methods seem appropriate. ->RESSQ

6. Complex flow situations, analytical methods do not appear to be appropriate.->Select numerical method

7. This type of source may be actively recharging a surficial aquifer. We now estimate the long term head rise (R) due to recharge using the Hantush method to estimate the approximate degree of deformation of the regional flow. This returns the ratio of head rise to aquifer thickness (R/b). Alternatively this value may be directly input.

7.1. $R/b < 5\%$. The flow can be modeled as essentially non-radial and approximated by confined solution methods. ->9

7.2. $5\% \leq R/b < 30\%$. This implies that the Dupuit approximation is reasonably acceptable, particularly at distances not directly adjacent to the source. The cut-off criterion of 30% is rather subjective, and can be modified. ->10

7.3. $30\% \leq R/b$. Flow is strongly deformed by the recharge and the Dupuit approximation is not acceptable. ->6

8. Aquifer characteristics presently ill-defined, or proposed site with unknown engineering. Undertake preliminary analysis using regional data, with considerable uncertainty. ->EPAGW

9. Approximations of homogeneous, infinite aquifer with confined solutions acceptable.

9.1. Perimeter of interest is located close to the edge of the source, so that the source can be treated as approximately horizontally infinite. ->19

9.2. Perimeter of interest is far enough away so that effects of source lateral boundaries must be considered. ->12

10. Dupuit approximation methods for unconfined flow, with radial component induced by recharge. Applicable solutions depend on distance from source.

10.1. Perimeter of compliance is located near edge of the source, so that the source can be treated as infinite in the lateral direction in relation to the observation point of interest. ->14

10.2. Perimeter of compliance is located further from the source, so that the source can be approximated as a point. Distance is great enough so that full penetration is a reasonable approximation. ->15

10.3. Neither of the above is adequate. ->6

11. Radial flow in a surficial aquifer, Dupuit approximation not acceptable; or radial flow in a surficial aquifer with addition of a significant regional flow component. Try preliminary analysis with a semianalytical method. ->RESSQ

12. Confined aquifer solutions, source area cannot be treated as an infinite line source.

12.1. Single areal, finite line or point sources. ->13

12.2. Multiple point sources, of varying strength. ->17

12.3. Other situations. ->6

13. Single point, line or areal sources. Solution availability depends on whether source strength is constant.

13.1. Source strength is relatively constant. ->16

13.2. Source strength can be approximated by an exponential decay function. ->18

13.3. Other situations. ->6

14. Dupuit approximation, perimeter of compliance near enough to source so that the source can be treated as infinite in the y direction.

14.1 Regional flow regime thought to be unimportant in relation to recharge-induced radial flow. No consideration of decay or hydrolysis of contaminant. ->DUPVG

14.2. Regional flow regime is thought to be of importance in the transport of contaminant. ->11

14.3. Analysis requires consideration of decay. ->11

15. Dupuit approximation, perimeter of compliance far enough away that source can be treated as a point.

15.1. Regional flow regime thought to be unimportant in relation to recharge-induced radial flow. No consideration of decay or hydrolysis. ->20

15.2. Regional flow regime is thought to be of importance to the transport of contaminant. ->11

15.3. Analysis requires consideration of decay. ->11

16. Single point, line or areal source of constant strength.

16.1. Source can be characterized as a point. ->16A

16.2. Source presents significant width in relation to perimeter of interest. ->28

16A. Single point source in confined aquifer, or collection of point sources, source strength not decaying.

16A.1. Effects of partial penetration of contaminant into aquifer must be considered. ->21

16A.2. Full penetration analysis adequate. ->22

17. Multiple point sources in confined aquifer source strength not decaying.

17.1. Full penetration analysis adequate. ->23
17.2. Partial penetration effect thought important. Analytical solution is not available. ->6
18. Single source in confined aquifer, source strength may be decaying.
18.1. Full penetration analysis adequate. ->24
18.2. Partial penetration effect thought important. Analytical solution is not available, but first examine plume with semianalytical method. ->5
19. Semi-infinite line source in confined aquifer, source strength may be decaying.
19.1. Full penetration analysis adequate. ->25
19.2. Partial penetration effect thought important. See if DUPVG is appropriate. ->14
20. Dupuit assumption, radial flow, with regional flow unimportant to contaminant distribution. ->LTIRD
21. Areal source of non-decaying strength, partial penetration evaluation.
21.1. Expected maximum impact is along main flow axis. ->26
21.2. Expected impact not along main flow. Analytical solution not available. ->6
22. Point source of non-decaying strength, full penetration analysis is adequate. For initial analysis. ->PLUM2D
23. Multiple point sources, full penetration analysis is adequate, non-decaying source strength. ->PLUM2D
24. Finite line source in confined aquifer, full penetration, source strength may be decaying. ->TDAST
25. Semi-infinite line source in confined aquifer with full penetration, source strength may be decaying. ->ODAST
26. Areal (Gaussian) source, of non-decaying source strength, impact along main axis of flow. ->EPAGW
28. Source presents significant width along flow axis.
28.1. Source concentration is focussed in one area. ->21
28.2. Source is a large area of approximately equal source strength, as in land applications of waste. ->24

Generic Notes on Model Usage

Once a model has been selected by either of the above processes the system will proceed to run the appropriate model. Certain features will be found in common for all the available models. In general, the implementation will proceed as follows:

a). HELP Model. If requested, the HELP model will be called to analyze leaching rates. Note that if you wish to quit this procedure you may terminate out from the first screen of the HELP model and continue with the analysis without problem.

b). Preprocessor. After displaying an introductory message, the system will proceed to the appropriate model preprocessor. This is an I/O program designed to facilitate preparation of the necessary data. A typical preprocessor main menu will appear as follows:

```
PLUM2D  PREPROCESSOR MAIN MENU

          Data preparation options for Plume-2D
          -------------------------------------

          Prepare a new data set . . . . . 1
          Edit current data set  . . . . . 2
          Input data set from site file  . . 3
          Save data set for future use . . . . 4
          Show HELP screen . . . . . 5
          Exit preprocessor and run model. . . 6
                                               .
          Terminate session  . . . . . 7
                  ENTER SELECTION: _
```

If this particular site has been previously analyzed with this model one can select (3) and reload the data set. You should then check the data with the edit option. If no data set has been saved the option will return you to this menu. If the site has not been analyzed (1) will enable preparation of a new data set. Once data preparation has been completed you should save the data set (4) and then run the model (6). If you attempt to run the model without saving the data you will be reminded to save, but typing (6) again will override this option.

Once a data set has been loaded or created it may be edited. Option (2) will lead to an edit menu, such as the following:

```
PLUM2D                  EDIT SCREEN SELECTION
Select a screen you want to edit or review, and enter its number.
                    cards                        number
                    -----                        ------
          card 1. Title . . . . . .  1
          card 2. Control card 1. . . . . .  2
          card 3. Control card 2 (grid) . . .  3
          card 4. Hydrogeology card . . . . .  4
          card 5. Monte Carlo controls. . . .  5
       data set 1. Observation points. . . . .  6
       data set 2. Injection wells . . . . . .  7
                  All cards in sequence . . .  8

                  Selection (RETURN to exit):  _
```

The data is presented in the preprocessor as if it were stored in a card-image format, although this does not necessarily reflect

the actual storage mode used by the preprocessor. The user may here select a "card" or data set to edit, and the appropriate input screen will be presented. (Of course, card 5 in this example, the Monte Carlo controls, will not be accessible if the model is being run in a deterministic mode.) Choosing "all cards in sequence" will allow the user to view the entire data set without necessarily making any changes. It is always advisable to invoke this option when reloading a data set, as the specific application framework of the model may have changed from the previous call in which the data was stored.

Following selection of a choice from the above panel an input screen will be displayed, showing current values (if any) of the input variables. The screen may contain more variables than are needed by a particular configuration of the model, and these variables will be skipped over. Upon editing a screen the cursor will first be positioned at the end of the screen, with the option message:

SCREEN OPTION (RETURN:continue, 1:edit this screen, 2:help): _

Typing a carriage return at this stage will proceed back to the edit menu, or to the next data "card", as appropriate, while <2> will display a help screen for the set of variables displayed. Enter <1> if you wish to alter any of the displayed values. You will then be led through each of the active input positions on the screen. A carriage return will move you to the next position, and you must proceed through all active positions before you can exit the screen. For many variables the value that is input must be between certain specified bounds. One peculiarity of data entry should be noted here: In some cases the user will find it impossible to enter a zero value if a non-zero value is already in the slot. This is because the preprocessor interprets the zero as a request to move to the next input slot. This feature can be temporarily overridden by entering a character from the keyboard, followed by <CR>, 0, <CR>.

c) Transport Model. On exiting the preprocessor control will shift to the actual transport model. If in Monte Carlo mode you may be asked to input a random number seed at this stage. The model iterations will then be commenced, with an iteration counter displayed on the screen and a bell sounded when finished. Execution time is highly dependent on the particular model and data configuration. However, it is recommended that in all cases at least 500 Monte Carlo runs should be used in order to build up an accurate picture of the cumulative frequency of contamination risk.

Note that for all analytical models a standard layout of the axes is employed, such that the X axis represents the direction of regional flow (if any), and the Y axis is the direction normal to the regional flow. If used, the Z axis represents the vertical direction.

One option that is useful for consideration of multiple conservative constituent sources is to specify a generalized source concen-

tration of 1.0. The model output is then a dimensionless "dilution" factor, which may be applied to the actual input concentration of any particular constituent.

d) Model Output. Following the successful completion of a model application several things will happen: The data will be stored or displayed as appropriate, graphics will be displayed, and finally the user will be returned to the Level 1 menu, with an option to re-run the last applied model. Note that this option will query whether the user wishes to change the contaminant studied and concentration level.

Graphics display will depend on whether the model has been run in the deterministic or Monte Carlo mode. In either case, plots are provided only for the last time step modeled, although data from each time step specified will be incorporated in the output file. If in Monte Carlo mode, for each observation point the data will be sorted into ascending order and the probability of exceedance of the standard calculated. A cumulative frequency plot is then displayed. Note that this is an interactive plot, and new standard levels can be entered, with corresponding exceedance probabilities displayed. Entering -99. causes the exceedance probability legend to be removed from the screen. A return then exits the plot.

In deterministic mode for two dimensional analytical models a 3-dimensional perspective plot of the contaminant plume will be displayed. However, this option is valid only if the grid dimensions are at least 2 x 2. This plot is also interactive, and the user may display a standard level, and change color and fill design. Specifying a fill color of 0 results in a line drawing of the plot, which is usually best for obtaining a print on a single color printer. The user also has the option of recalculating the perspective plot after rotation, scaling or translation operations.

The semianalytical model RESSQ produces a special plot of the flow lines and pollutant fronts, followed by plots of concentration development at specified observation points. The flow line plot is currently performed by a BASIC program. We plan to replace this plot with a FORTRAN plotter in the future, for greater compatability with other graphics in the system.

If your system is properly configured and has the proper screen graphics drivers, all graphics screens can be printed through use of the control-printscreen key sequence. After printing a plot and returning to the menu, typing 'IP' will print the information file from the model to accompany the plot. Note that if there is an abnormal exit from the plot due to a run-time error the graphics card may not be properly reset. In this case it may be necessary for the user to re-boot the system to restore proper graphics control.

Recommendation

Permitting recommendations should be based on a series of Monte Carlo risk analyses of exceedance of the standard at points along the perimeter of interest. After model output has been sorted the user will be queried as to whether the exceedance probability calculated for this run should be saved as a criterion for permitting. The system then keeps track of the highest exceedance probability encountered. The recommendation option on the main menu will then base a decision on this highest exceedance probability. Currently, the system is currently set so that site acceptance is recommended if the highest exceedance probability is less than 0.025, while rejection is recommended if the exceedance probability is greater than 0.5. Values between 0.025 and 0.5 return an indeterminate recommendation.

Exit

On completing use of the system the user should select the 'Z' option to exit. As supplied, this cancels all invoked screen attributes and returns the form of the prompt to the standard. The user should alter the file Z.BAT to set the desired ending configuration, and also to return to any desired directory on your disk.

4.2 MODEL USER'S MANUAL

In this section we will provide details and suggestions on the use of each of the constituent models in the system. In each case we will address 1) applications of the particular model, 2) limitations of the model's approach, and 3) details of data input. The contaminant transport models will be discussed first, followed by several utility models.

4.2.1 LeGrand Model

Applications. Regulatory agencies typically lack the manpower to conduct detailed modeling analyses of permit applications of all sites that may have a potential effect on groundwater. In some instances a proposed site will have such a poor hydrogeologic setting that a permit can be rejected without any detailed modeling. Conversely, some cases will have such a low degree of contaminant severity and potential risk of contamination that a site could be passed without detailed modeling. Often such decisions are made subjectively. However, it is safer and more desirable to establish formal criteria for the bypassing of detailed modeling on a given site.

In the advisory system, criteria for this preliminary screening are formalized by use of the screening analysis developed by LeGrand (1983), which requires only readily available site-specific data. This approach is essentially a numerical rating system for evaluating the potential of ground water contamination from waste disposal sites. The system focuses on weighting four key geologic and hydrologic characteristics in the vicinity of contamination sources. The key parameters used are: 1) distance to a water supply or perimeter of compliance; 2) depth to water table; 3) hydraulic gradient; and 4) permeability-sorption, as indicated by the geologic setting. In a second stage attention is paid to the type and severity of the generalized contaminants likely to be associated with the use of the site. Weighting and integrating the site and contaminant characteristics then yields a numerical situation rating.

The LeGrand method may be used to evaluate hydrogeology alone, or extended to include consideration of the type of waste disposal site (PAR rating). When both analyses are undertaken these are combined to provide a combined situation rating. This combined situation rating can be used for the preliminary decision. Output of the model includes a shorthand summary of the analysis, as in the following example:

```
Description 21-3936ABWD+E
PAR          18     5
             +3    +1 =    +4E
```

The first line given here (Description) summarizes the analysis of site hydrogeology. Higher numbers here (on a scale of 0-9) indicate less favorable characteristics, so these may readily be identified from the description. In the analysis given above the entries in the Description line indicate the following:

21	Total rating (sum of next four digits)
-	
3	Distance from source to point of impact.
9	Depth to water table.
3	Water table gradient.
6	Permeability-sorption.
A	Letter identifier of permeability-sorption.
B	Degree of confidence in estimates.
W	Indicates measured in relation to a well.
D	Special identifier.
+	
E	Hydrogeologic grade.

In this case the hydrogeologic rating is in the poor range (E) because the total rating is >20. Analysis of the digits shows that the most important factor contributing to this poor rating is the depth to water table below the contamination source.

The second line (PAR rating) is obtained from a hazard potential matrix. In this case higher values indicate decreasing contaminant severity and/or decreasing aquifer sensitivity. The combined situation rating is then obtained by subtracting the PAR rating from the hydrogeologic rating.

LeGrand's method has been directly interpreted into an interactive program for inclusion into the system. Preliminary judgment is then based on the following criteria (which may be altered): For a combined situation rating of < -8 a site is judged probably acceptable, without further analysis, while for a situation rating > +4 a site is judged probably unacceptable. In the uncertain range from -8 to +4 further modeling is recommended.

The great advantage of the LeGrand method is thus in providing a standardized weighting system that is broadly applicable yet quick and easy to apply. Such analysis does not form the basis of a final recommendation, except in the extreme cases of very low contamination probability or very high contamination probability. The LeGrand method provides an effective means of identifying such cases. However, in all cases the user is free to proceed to more detailed analysis through actual modeling of contaminant transport. For instance, even where a very low probability of contamination is indicated by the LeGrand analysis the user may wish to proceed to more detailed modeling if the contaminant in question is particularly hazardous. In cases where the LeGrand analysis indicates that a site is highly unsuitable the burden of proof will generally be shifted to the applicant who must demonstrate, for instance, how proposed leach-

ing control or high degree of attenuation of the contaminant will reduce risk. In general a poor rating on the LeGrand analysis should be grounds to request detailed hydrogeologic and engineering data from the applicant, which can then be used as input for more detailed models.

Limitations. The LeGrand method is carefully designed to have a wide degree of applicability, and will be an effective tool for preliminary analysis in most situations. Its effectiveness is limited primarily by the fact that it is designed as a preliminary analysis tool, and, probably in the majority of cases, the model will not provide a definitive answer - as indeed is our intention. The user should of course realize that the method treats site hydrogeology in only a generalized manner. Where more specific details of the hydrogeology are known, the user should take these into account in analyzing the model results.

Data Input. Data input for the LeGrand method is interactive. The user may choose to rate site hydrogeology only (Stage 1) or continue analysis with consideration of the PAR rating (Stage 2). On completion the user has the option of reanalyzing the site. It will often be desirable to rate a site in regard to several different potential points of impact, and with consideration of varying degrees of engineering modifications.

In Stage 1 the following data is requested:

Step 1.
Choose distance on ground between site and nearest water supply (or specified boundary) from the following table.

	(feet)	(meters)
0	> 6200 ft.	> 2000 meters
1	3100-6200	1000-2000
2	1001-3100	300-999
3	501-1000	150-299
4	251-500	75-149
5	161-250	50-74
6	101-160	35-49
7	61-100	20-34
8	31-60	10-19
9	0-30	0-9

When the water table lies in permeable consolidated rocks, 6 points will be allotted on the distance scale; in poorly permeable rocks 4 points will be allowed.

Step 2.

Estimate the shallowest depth to the water table below base of contamination source more than 5% of the year from the following table:

	(feet)	(meters)
0	> 200 feet	> 60 meters
1	91-200	30-60
2	61-90	20-29
3	36-60	12-19
4	26-35	8-11
5	16-25	5-7
6	9-15	3-4
7	3-8	1.5-2.5
8	1-2	0.5-1
9	< 1	< 0.5

When the water table lies in permeable or moderately permeable consolidated rocks 6 points will be allotted - in poorly permeable rocks 4 points will be allotted.

Step 3.

Choose the most appropriate description of the general water table gradient from the following table:

0	Gradient away from all water supplies that are located closer than 1000 meters from the site.
1	Gradient is almost flat.
2	A gradient of less than 2% exists towards the water supply, but this is not anticipated direction of flow.
3	Gradient less than 2% towards the water supply, and this is the anticipated direction of flow.
4	Gradient greater than 2% towards the water supply, but this is not the anticipated direction of flow.
5	Gradient greater than 2% towards the water supply, and this is the anticipated direction of flow.

Step 4.

In step 4 a digit and letter identifier describing permeability-sorption for the site is chosen from table IV-1.

Step 5.

Indicate degree of confidence in accuracy of values:

A: Confidence in estimates of values for the parameters is high and estimated values are considered to be fairly accurate.

B: Confidence in estimates of values for the parameters is fair.

C: Confidence in estimates of values for the parameters is low and estimated values are not to be considered accurate.

Table IV-1. Selection of Permeability-Sorption Indicators for the LeGrand Model

unconsolidated material ----->	clay		clay with no more than 50% sand		sand with 15-30% clay		sand with less than 15% clay		clean fine sand		clean gravel or coarse sand	
category ----->	I	II	I	II	I	II	I	II	I	II	I	II
thickness of unconsolidated material overlying bedrock (in feet)	>95	0A	0A	2A	2A	4A	4A	6A	6A	8A	8A	9A	9A
	75-94	0B	1C	1D	2F	3E	4G	5F	6E	7F	8E	9G	9M
	60-74	0C	2C	1E	3D	4D	5E	5G	6F	7G	8F	9H	9N
	46-59	0D	3B	1F	4C	4E	6C	5H	7D	7H	8G	9I	9O
	28-45	0E	4B	2D	5B	4F	6D	5I	7E	7I	9D	9J	9P
	10-27	1B	6B	2E	7B	5C	7C	5J	8D	7J	9E	9K	9Q
	<10	2B	8B	3C	8C	5D	9B	5K	9C	7K	9F	9L	9R

For bedrock at land surface, use 5Z for category I, 9Z for category II.

Category I - unconsolidated material overlies shale or other poorly permeable rock.

Category II - unconsolidated material overlies permeable consoldiated rock (fractured or jointed igneous or metamorphic rocks, cavernous carabonate rocks and faults).

Step 6A.
Distance from contamination source is measured to:

W: a well.
S: a stream or perennial spring.
B: a property boundary or perimeter of compliance.

Step 6B.
Up to two additional letter identifiers may be selected from the following list:

C: SPECIAL CONDITIONS REQUIRE THAT A COMMENT OR EXPLANATION BE ADDED TO THE EVALUATION.
D: CONE OF PUMPING DEPRESSION NEAR A SOURCE OF CONTAMINATION. THIS MAY CAUSE DIVERSION TOWARD PUMPED WELL.
E: DISTANCE RECORDED IS THAT FROM A WATER SUPPLY (OR BOUNDARY) TO THE EDGE OF AN EXISTING PLUME RATHER THAN ORIGINAL CONTAMINANT SOURCE.
F: SOURCE IS LOCATED ON A GROUNDWATER DISCHARGE AREA, SUCH AS A FLOOD PLAIN, WHERE MINIMAL GROUNDWATER INTRUSION IS EXPECTED.
K: SITE LOCATED IN KARST TYPOGRAPHY, OR IS UNDERLAIN BY CAVERNOUS LIMESTONE.
M: MOUNDING OF THE WATER TABLE BENEATH A CONTAMINATION SITE - COMMON BENEATH WASTE SITES WITH LIQUID INPUT.
P: PERCOLATION MAY NOT BE ADEQUATE FOR SITE. THE PERMEABILITY-SORPTION DIGIT SUGGESTS THE DEGREE TO WHICH PERCOLATION MAY BE A PROBLEM, A DIGIT OF 3 OR LESS BEING A SPECIAL WARNING OF POOR PERCOLATION.
Q: DESIGNATES A "RECHARGE OR TRANSMISSION" PART OF AN EXTENSIVE AQUIFER THAT IS SENSITIVE TO CONTAMINATION. MAY BE SUGGESTED BY A HIGH VALUE ON THE PERMEABILITY-SORPTION SCALE.
R: RADIAL OR PARTIAL RADIAL FLOW FROM A HIGH WATER-TABLE POSITION. (TWO OR MORE SITE RATINGS MAY BE NEEDED.
T: INDICATES THAT THE WATER TABLE IS IN FRACTURED OR CAVERNOUS ROCK.
Y: ONE OR MORE CONFINED (ARTESIAN) AQUIFERS UNDERLIE THE WATER TABLE AQUIFER.

In Stage 2 of the LeGrand analysis the user must enter information relating to the contaminant severity and aquifer sensitivity. This information is best read from the PAR matrix diagram provided in LeGrand (1983). However, the option is also provided to estimate these values in response to a series of queries.

4.2.2 ODAST

Applications. The program ODAST evaluates the one dimensional analytical solute transport solution considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1984). The program has been modified to facilitate Monte Carlo analysis. The solution method can thus handle many types of transport conditions, and is also numerically stable and fast running.

The idealized situation from which the solution arises is as follows: The model considers an infinitely long column of a homogeneous isotropic porous medium with a steady state uniform flow of constant seepage velocity. A particular solute is injected from one end of the system for a period of time such that the input concentration may vary as an exponential function of time. The value of concentration may then be calculated at any time t and distance x from the injection boundary. In the field, such an idealized situation could be represented by an infinitely long ditch of contaminated waste water fully penetrating an infinitely long confined aquifer, with the ditch cutting the aquifer perpendicular to the direction of flow.

The idealized situation described obviously does not exist in the real world. However, the solution provides a valid approximation in many cases. As with most analytical solutions the assumption is made of isotropic, uniform, steady state regional flow. This will often be a reasonable approximation of actual flow conditions. Likewise, the assumption of a confined aquifer may provide a reasonable approximation for analysis of phreatic aquifers if the flow regime is not strongly altered by the rate of fluid input from the source, and the saturated thickness remains approximately constant. Even where the saturated thickness is to some extent variable over time use of the average saturated thickness will enable analysis of average contamination risk. This approximation will be particularly valid for analysis in the Monte Carlo mode. In the Monte Carlo mode the input concentration and regional flow velocity both become random variables, and the cumulative frequency estimated over these and other random parameters should provide a reasonable estimate of the average risk. If however the source itself contributes fluid that becomes an important factor of the flow regime, so that radial flow from the source is established, the confined aquifer assumption becomes inappropriate, and the phreatic surface will move in response to the source input. This condition is tested for in the CHOICE algorithm. Another model, DUPVG, may be appropriate under these conditions.

Obviously, real sources will not be of infinite length. However, the one dimensional solution provides a reasonable approximation for finite sources if the observation point is sufficiently near the finite width source so that the effect of the source edges will be minimal. For instance, if a source has a lateral extent of 200 feet and the perimeter of compliance is 50 feet from the source, the one

dimensional solution is likely to provide a reasonable (and conservative) approximation of contamination risk along the axis extending from the center of the source (but not near the source edges). The exact distance to which the one dimensional solution can be carried downstream from a finite source without introduction of unacceptable error will depend on the interaction of all the forces controlling the flow regime.

The method can also be extended to cover input configurations other than the ideal ditch perpendicular to flow. Many situations of interest will involve large areal surface applications of wastes. Modeling the actual distribution of contamination in such cases is a complex process. However, solutions such as ODAST may be appropriate given certain assumptions. The first step is to calculate the rate of mass loading at the water table surface, after any vadose zone attenuation. We must then make the assumption that the substance is more or less instantly vertically mixed in the aquifer. Such an approximation is of course more valid for relatively thin surficial aquifers. (Generally, when the degree of vertical penetration is a significant factor in determining plume development, a three-dimensional solution, such as EPAGW, must be employed.) This constant areal input must then be represented as a line source at the downflow edge of the area. To do this one can make the simplifying assumption that the whole aquifer volume beneath the landfill is thoroughly mixed by the time flow reaches the downstream edge of the source, and calculate an edge concentration based on the loading diluted by the regional flow. (The concentration at the edge of the aquifer will thus have a maximum possible value equal to the leaching concentration.) Such an approach is most applicable where the loading is approximately constant over the whole area. (An alternative is to model the areal source as a Gaussian source, maximum at the center and declining towards the edges. This option is provided by EPAGW.) Model input provides options for calculating concentration in this manner, or for direct input of the concentration at the source edge.

An example of the use of ODAST is provided in section 4.3.1.

Limitations. The nature of the solution, and the additional assumptions that may be needed to employ it, as indicated above, introduce a number of limitations in the applicability of the model. First, ODAST is clearly inapplicable when the source cannot be modeled as laterally approximately infinite in terms of the point of interest. As with all analytical solutions, the model will not be appropriate where there is a significant deviation from the conditions of uniform, steady-state regional flow. However, minor violations of these conditions will not have important effects on the general analysis of contamination risk, and the model will also be valuable for initial analysis when non-uniform flow is suspected, but not fully documented. The solution also assumes a semi-infinite flow regime, and thus cannot take into account aquifer interactions with

constant head boundaries, such as rivers. The CHOICE algorithm suggests avoiding use of this type of analytical solution when the perimeter of compliance or other point to be modeled is within 250 feet of a fixed head boundary.

Limitations that are more difficult to assess involve the assumptions that vertical concentration gradients can be ignored (full mixing), and that the source can be modeled as a uniform strength line. Clearly, the solution cannot be used for liquid contaminants that are not fully miscible and tend to float or sink within an aquifer. Further, ODAST may result in underestimation of contaminant risk at the aquifer surface if full mixing does not occur.

Data Input. The preprocessor developed for ODAST follows a standard format that is used for most of the models in the system. This consists of presentation of a number of screens, with input slots to be filled. However, ODAST shares a preprocessor with two other models, and thus not all the input slots on these screens are needed for this model. The data to be input for ODAST are as follows:

NUMX: Number of points modeled in the X direction, which establishes the 1-dimensional grid. From 1-25 points may be used. Grid size does not affect solution, and for Monte Carlo simulation you will normally wish to examine only one or two points at the perimeter of compliance in order to speed execution. The X direction is coincident with the regional flow vector.

NUMT: Number of time steps for calculation. In Monte Carlo applications only the last time step will be tabulated for cumulative frequencies. However, the output file will contain sample data from each time step. In deterministic mode full data will be provided for each time step.

MODE: In Monte Carlo applications two options are available for modeling uncertainty in hydraulic conductivities. MODE=(1) generates values of K from porosity and particle diameter distributions by use of the Karmen-Cozeny relationship, and is thus appropriate when actual values of K are poorly known. With option MODE=(2) K is generated as an independent log-normal process.

MODE4: This provides an option for the calculation of contaminant source strength from rate of leaching (MODE4=1) or for the direct input of concentrations in the aquifer at the source boundary (MODE4=2).

Q: leaching rate from source expressed as g/ft2-d. If the HELP model has been run for this site, the values obtained will be reported here. In ODAST the source is conceived as a trench of infinite horizontal extent and unit width. Another parameter (AEW) is then required to estimate the effective line concentration at the boundary

from the leaching rate. Leaching rate will not be required if the in-aquifer concentration at the source is directly input (MODE4=2).

POR: Total porosity of the medium, required for the calculation of concentration from leaching, and thus not used if MODE4=2.

B: Thickness of saturated layer (initial thickness). This is also used to calculate the input mixed concentration beneath the source and not required if MODE4=2.

MODE3: In Monte Carlo applications, distributions may be directly specified for dispersion coefficients (MODE3=2). If this information is not available, estimates of dispersion are formed from the scale (MODE3=1), using the technique of Mulkey and Brown (1985), as DL = 0.1·X·V, and DT = DL/3.

DL, DT: In deterministic mode, or in Monte Carlo mode if dispersion coefficients are not generated from scale you must input values here. For MC the coefficient of variation will be asked on the next card.

VO: Mean pore water velocity of the regional flow, required input for deterministic mode only. This can be estimated from the average observed flow velocity, v, as VO=v/P, where P is the porosity of the medium.

ALAM: The "radioactive" decay factor of the contaminant in the saturated medium.

$$ALAM = \frac{\ln 2}{HL} \qquad (4.1)$$

where HL is the half-life (days). Note that ALAM can be used to represent chemical hydrolysis by entering the generalized hydrolysis rate as ALAM. Specify ALAM=0. for no decay or hydrolysis. Hydrolysis rates typically vary with pH and can be estimated from acid, base and neutral rate constants (K_{hao}, K_{hbo} and K_{hno}). Table IV-2 gives representative values for some organic constituents. The generalized hydrolysis rate constant, K, can then be approximated by the relationship (Mulkey and Brown, 1985):

$$K = \frac{\left\{K_{hbo}[OH^-]\theta + (10K_{hao}[H^+]+K_{hno})\beta\rho_b\right.}{\theta + \beta\rho_b} \qquad (4.2)$$

for rates expressed in $days^{-1}$, in which $[H^+]$ is the hydrogen ion concentration, M, equivalent to exp(-pH); $[OH^-]$ is the hydroxyl ion concentration, where at equilibrium in water $[OH^-] = 1.0 \times 10^{-14}/[H^+]$; β is the soil-water distribution coefficient (see next section); θ is the volumetric water content of the soil (total porosity for

Table IV-2. Hydrolysis Rates for Organic Contaminants.

Hydrolysis values for some organic contaminants. Values vary with pH and can be specified for acid, base or neutral conditions. Calculation of a total effective decay constant (K) will depend both on the pH and the soil-water distribution coefficient (see equation 4. for details). The rates can be altered to additionally reflect biodegradation and volatilization where information is available. Total rates may also be directly estimated from an observed half life (HL) as K = ln2/HL. Rates are 1/days. (EPAGW model requires conversion to 1/years).

Compound	K_{hao} (acid)	K_{hbo} (base)	K_{hno} (neutral)
Acetone	0.	0.	0.
n-Butyl Alcohol	0.	0.	0.
Carbon Disulfide	0.	1.9E-3	0.
Carbon Tetrachloride	0.	2.6E-7	0.
Chlorobenzene	2.4E-4	0.	0.
Chloroform	0.	6.0E-7	0.
Cresols(p.m.o)	0.	0.	0.
Cyclohexane	0.	0.	0.
o-Dichlorobenzene	0.	2.4E-4	0.
Ethyl acetate	9.6	9504.0	0.
Ethyl benzene	0.	0.	0.
Ethyl ether	0.	0.	0.
Freon	0.	1.9E-4	0.
Isobutanol	0.	0.	0.
Methanol	0.	0.	0.
Methylene Chloride	0.	0.	2.6E-7
Methyl Ethyl Ketone	0.	0.	0.
Methyl Isobutyl Ketone	0.	0.	0.
Nitrobenzene	0.	0.	0.
Pentachlorophenol	0.	0.	0.
Pyridine	0.	0.	0.
Toluene	0.	0.	0.
1,1,1-trichloroethane	0.	2.6E-3	0.
Trichloroethylene	0.	0.	0.
Trichlorofluoromethane	0.	2.6E-7	0.
Xylene	0.	0.	0.

saturated media); and p_b is the soil bulk density as g/cm^3. In equation 4.2 the term $K_{hbO}[OH^-]$ represents the first-order hydrolysis rate for the dissolved constituent. Where K_{hbo} is not known this term may be replaced by $K_{hbo}[OH^-] = (K_{hao}[H^+] + K_{hno})$.

The rates can be altered to additionally reflect biodegradation and volatilization where information is available. Total rates may also be directly estimated from an observed half life (HL) as ALAM = ln2/HL. Rates are 1/days.

R: retardation coefficient, = v/vc, where v is the velocity of the regional flow and vc the apparent velocity of the contaminant. If we assume reversible linear adsorption, R can be estimated as:

$$R = 1 + \frac{\beta \rho_b}{\theta} \qquad (4.3)$$

where β is the soil-water distribution coefficient, p_b is the soil bulk density and θ is porosity. For this model, soil bulk densities are not explicitly considered, and the user must input a computed value for R. However, for the typically encountered ranges of porosities and soil bulk densities R, can be approximated as falling within a limited range (Freeze and Cherry, 1979):

$$(1 + 4\beta) \leq R \leq (1 + 10\beta) \qquad (4.4)$$

The value of β will also vary with the type of the medium, particularly the organic carbon fraction of the soil. Values of β are typically reported as K_{oc}, where K_{oc} is the distribution coefficient normalized to organic carbon. In the case where hydrophobic binding dominates the sorption process, the actual distribution coefficient can then be estimated by:

$$\beta = f_{oc} K_{oc} \qquad (4.5)$$

where f_{oc} is the fraction of organic carbon in the soil. Values of f_{oc} are not widely available, but are generally thought to lie in the range of 0.001 to 0.01 for most soils (Mulkey and Brown, 1985). Table IV-3 (in section 4.2.6) gives K_{oc} values for some organic constituents. For other binding mechanisms this relationship cannot be used (see Karickhoff, 1985).

ALFA: Similar to ALAM, but represents the rate of decay of the source strength. Specify ALFA=0. for constant source strength.

SST: Mean initial source strength, as ppm. Note that in cases of

surface disposal of liquid wastes, the strength of the waste should be diluted by the average rate of additional infiltration due to rainfall minus runoff and evapotranspiration. In many cases this calculation can be made using data from the HELP model.

ATTEN: Fraction of the solute remaining after vadose zone attenuation. If the HELP model has been run a conservative estimate of ATTEN can be calculated automatically.

Monte Carlo Controls: The following 8 parameters are required only for Monte Carlo simulation.

ITER: Number of Monte Carlo iterations to be run. 500 is recommended for good resolution of the cumulative frequencies. However, you may first wish to run a smaller number to test the model.

CVL: Specifies the variability in the source concentration through its coefficient of variation, where the coefficient of variation is equal to the standard deviation divided by the mean.

TH: 2 values express the bounds between which the MEAN particle size of the saturated medium will lie, following a log-10 uniform distribution.

GR: estimate of water table gradient, as ft/ft. This is expressed as a triangular distribution, and the user must input a most likely, maximum and minimum value (GR(1) - GR(3)).

CVD: coefficient of variation for dispersion coefficients. Used only if the dispersion coefficients are independently estimated.

CVLNQ: coefficient of variation for the leaching rate. If the HELP model has been run, the observed CV will be shown. Again, CV = Standard Deviation/Mean.

DKLN: If K is to be directly estimated, input mean LN K. Otherwise, K will be estimated from generated particle size, porosity and gradient, using the method documented for the model EPAGW.

DKLNV: Coefficient of variation of DKLN.

OBSERVATION POINTS: This screen identifies the grid set-up. Concentrations will be calculated at all combinations of X and T. However, for Monte Carlo applications cumulative frequency calculations will be made only for the last time step. For Monte Carlo you will therefore usually wish to specify only one time point, and 1 or 2 observation points. These numbers are set by NUMX and NUMT (above). The coordinate system is such that (X=0) is a point coincident with the source downstream edge. Regional flow is presumed to be coincident with the X axis. Note that all values of T should be > 0.

4.2.3 TDAST

Applications. The model TDAST evaluates the two-dimensional analytical solute transport solution, considering convection, dispersion, decay and adsorption in porous media (Javandel et al., 1985). The idealized conception of the model is related to that of ODAST, but covers another important class of cases. As with TDAST we assume conditions of steady-state, uniform flow in a confined aquifer. The source is again assumed to be fully penetrating, but in this case is of finite lateral extent (normal to flow), as in the case of a fully-penetrating ditch of finite length. Thus TDAST is applicable in conditions similar to those applicable for ODAST, except that here the observation point is far enough from the source boundary so that the effects of the source edge and transverse dispersion must be taken into account in the approximation. By using the same techniques as described above for ODAST, TDAST may be applied to constant areal waste sources. In such a case, ODAST would be accurate for analysis near to the center of the source edge, while TDAST could be used for such a location and also locations nearer to the source edge, and locations further away from the source boundary. In general, the numerical stability and speed of ODAST make that solution preferable where applicable. TDAST is also useful for analysis of contamination resulting from smaller sources.

Limitations. The same general limitations apply to TDAST as apply to ODAST, except that the effects of lateral source geometry and transverse diffusion are explicitly considered. That is, the approximations of full penetration (vertical mixing) and uniform, steady state flow must also be met here. TDAST also assumes that the source is aligned normal to the regional flow, although the solution could readily be altered to take into account other geometries.

An important practical limitation of the present version of TDAST arises from its use of a numerical technique to evaluate an integral. Presently TDAST uses a Gauss-Legendre polynomial method for this evaluation, making use of the same subroutine employed in the models EPASF and EPAGW. The number of terms in the polynomial evaluation may be set by the user, up to a certain limit. The solution routine begins with a lower number of terms and increments the number until the solutions converge (within 1%), or the limit is reached. Under certain conditions adequate convergence cannot be achieved within the limits available in the numerical integration scheme, which will result in the display of a warning message. In general, lack of convergence will be encountered when the ratio of Vt/X becomes much greater than 1 (where V is velocity, t is time and X is distance). This means that TDAST provides accurate calculation of the time period during which concentration increases at a given point, as the plume breakthrough occurs, but loses accuracy at a given point as time increases past breakthrough, resulting in underestimation of concentrations. However, this is merely an inconvenience for ana-

lysis, as the solution should approach a steady-state concentration before numerical instability overwhelms the solution. The user should thus fine-tune the application to avoid this problem. This can be done for the desired time step by eliminating those observation points that are well behind the breakthrough curve of the plume.

Data Input. TDAST shares a preprocessor with ODAST. The data input is thus essentially the same as that for TDAST, described above, with the addition of the following variables:

NUMY: Number of Y positions in the grid. Observations will be calculated at all combinations of NUMX, NUMY and NUMT.

NNS: This sets the accuracy of the numerical integration scheme used by TDAST, by choosing the degree of the polynomial for the Gauss-Legendre method. NNS selects the nth digit from (4, 5, 6, 10, 15, 20, 30, 40, 50, 60, 104, 256). Increasing NNS improves accuracy but decreases speed. NNS=8 seems to provide a good compromise value with which to start, but may be changed at will. If convergence warnings appear on screen during run time the user should try increasing the value of NNS.

DT: Transverse dispersion coefficient. As in ODAST, the dispersion coefficients must be input for deterministic modeling, but can be estimated from scale and velocity in Monte Carlo mode. In the latter case DT is estimated as 1/3 of DL.

A: Half-length of the source, being 1/2 of the lateral extent of the source normal to the direction of flow.

OBSERVATION POINTS: The observation points will now include points in Y. The coordinate system is such that (0,0) is a point at the center of the finite width source. As in ODAST, flow is considered to be coincident with the X direction. In Monte Carlo mode it will be desirable to use a limited number of observation points to speed execution. However, in deterministic mode you will wish to use a larger number to obtain good definition of the plume, and NUMX and NUMY must both be >= 2 in order to obtain a 3-D plot of the plume.

As noted above, because of convergence problems in the estimation of the integral, it is not practical to specify observation points very near the source as time increases. However, the user may always include points at X=0. At this point the concentration will simply be given as the calculated source concentration interpreted as a line source at the boundary.

4.2.4 PLUM2D

Applications. The model Plume 2D (van der Heijde, 1985), here

referred to as PLUM2D, is an analytical model for calculation of the tracer concentration distribution in a homogeneous, non-leaky confined aquifer with uniform regional flow. The solution method is based on the Hantush Well-function, in which the Well-function flow solution for a leaky confined aquifer is applied by analogy to account for transport and dispersion in a non-leaky confined aquifer. Source strengths are assumed constant, but the solute may be subject to adsorption and radioactive type decay in the porous medium.

An important advantage of this method is that it can readily treat multiple point sources, which sources may have been operational for differing amounts of time. This enables PLUM2D to treat certain situations that cannot be handled by other analytical methods.

The solution is based on an idealized situation, in which solute is introduced into a fully homogeneous confined aquifer through one or more fully penetrating wells in the presence of regional two-dimensional, horizontal ground water flow. The injection rate from these wells is considered to be sufficiently small that it does not alter the regional flow pattern. Thus the model is most applicable to the case of injection wells with relatively low injection rates. However, PLUM2D can provide a reasonable approximation for other situations as well. That is, surface sources can be modeled as fully penetrating sources if the assumption is made that the solute is fully mixed in the vertical direction soon after its introduction into the aquifer. Further, the solution method is approximately appropriate for use in a surficial aquifer, when the saturated thickness is relatively constant, and the leaching rate from the sources is of a small enough magnitude such that it does not affect the regional flow regime through mounding.

In incorporating the model into the system we have provided a complete preprocessor and equipped the model for Monte Carlo simulation. Generation of variables for Monte Carlo simulation is based on the techniques of Mulkey and Brown (1985), as incorporated in the model EPAGW. In order to account for the correlation of the various parameters controlling the regional flow regime these are generated from simpler, underlying variables (see discussion of EPAGW for more details). However, user option is also provided in the Monte Carlo mode for direct input of hydraulic conductivity and dispersion values.

A brief example of the use of PLUM2D is given in section 4.3.4.

Limitations. As with many of the other two-dimensional analytical models incorporated into the system, use of PLUM2D is limited to cases where it is reasonable to model the aquifer as if it were a confined aquifer with fully penetrating sources. These sources are treated as point sources, and thus the model is applicable to areal sources only where these can be treated as clusters of point sources.

The model further assumes that source strength is constant, once initiated, and cannot handle situations in which the strength of the source is decaying over time.

Data Input. As with most models in the system, we have provided a standard format preprocessor for PLUM2D. The user is provided with an option to specify input in either metric units [m, day] or English units [U.S. gallon, ft., day]. Data input is as follows:

UNITS: User option to select English or metric units.

TITLE: Title to be used for output.

NPTS: Number of solute injection wells specified, or other sources that can be approximated as injection wells. Up to 10 may be used in the present configuration of the model.

NOBS: Number of observation points for Monte Carlo simulation (up to 5). These are the points at which cumulative concentration frequencies will be calculated, and are in addition to the gridded calculation of concentration. For deterministic mode this variable is not needed.

NX: Grid dimension for calculation, number of nodes in x-direction. As this is an analytical solution, for Monte Carlo simulation a very sparse grid may be specified if interest is in only the frequency of concentrations at the observation points, rather than plume development. Specifying a sparse grid will greatly speed execution. The X axis is assumed to be coincident with the direction of regional flow. NX can range from 2 to 20.

NY: Grid dimension for calculation, number of nodes in y-direction. Range 2-20.

IRAD: User option to include radioactive decay (1=yes, 0=no). As in other models, decay processes such as hydrolysis can often be modeled as radioactive decay, if an effective "half-life" can be established (see table IV-2 above for hydrolysis rates for some common organic constituents and equation 4.2 for method of calculation). PLUM2D does not include the ability to model hydrolysis based on pH, with pH specified as a random variable.

MODE: User option for Monte Carlo simulation. Set Mode=1 to generate K from underlying variables of particle size and gradient, set Mode=2 to estimate K as a log-normal distribution independent of particle size.

XS: X-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

YS: Y-coordinate of origin of grid, in appropriate units. Range 0. to 5000.

DXOB: Grid spacing (interval) in the X direction. PLUM2D thus specifies an evenly spaced grid.

DYOB: Grid spacing in the Y direction, may differ from DXOB and is typically smaller than DXOB.

V: Average Darcy velocity of uniform regional flow, in the appropriate units, coincident with x axis. Required in deterministic mode only. In Monte Carlo mode V will be generated from underlying hydrogeologic variables, using the methods described by Mulkey and Brown (1985) and discussed in section 3.7.

M: Average aquifer saturated thickness, which is assumed constant.

P: Effective porosity (as a fraction). Required in deterministic mode only.

L: Longitudinal dispersivity, in units of length. Note that this model requires input of dispersivity, rather than dispersion coefficients.

T: Transverse dispersivity, in units of length.

RD: Retardation coefficient. RD= V/Vc, where V is the regional velocity and Vc the apparent velocity of the contaminant. Thus RD must be $\geq$ 1. Enter RD=1. for no retardation.

HL: If radioactive decay has been specified, enter half life, in years.

The next eight variables are required only in the Monte Carlo mode:

ITER: Number of iterations (runs) for Monte Carlo mode. ITER is recommended to be set to at least 500 to provide adequate definition of the frequency histogram. However, the user will usually wish to first test model performance by setting ITER to a smaller number.

CVL: Coefficient of variation of leachate (injection) concentrations, where the coefficient of variation is the standard deviation divided by the mean. The injection concentrations are modeled as a normal process.

TH(1), TH(2): The mean particle size is modeled as a log-10 uniform process, measured in centimeters. TH(1) is the maximum of the range of the mean, while TH(2) is the minimum. Thus TH(2) must be $\leq$ TH(1).

GR(1),GR(2),GR(3): The hydraulic gradient is modeled as a triangular distribution, in which GR(1) is the most likely value, GR(2) the minimum value and GR(3) the maximum value. The range of GR is restricted to 1.0E-5 to 0.1, expressed as length per length.

CVD: Coefficient of variation for dispersivities, applied to both L and T.

CVLNQ: Coefficient of variation of leaching (injection) rates. If the HELP model has been applied to this site the observed coefficient of variation from the HELP results will be reported.

DKLN: Required only if MODE is set to 2, and hydraulic conductivities are to be independently generated. DKLN is then the mean of the natural log of hydraulic conductivity, in cm/sec.

DKLNV: Standard deviation of mean LN hydraulic conductivity. Required only if MODE is set to 2.

DATA SET 1: OBSERVATION POINTS. Required only in Monte Carlo mode. For each observation point specified by NOBS the user must enter the x and y grid index (IXOBS and IYOBS).

DATA SET 2. INJECTION WELLS. For each injection well, or source modeled as an injection well, the user must enter the following values:

X: x grid coordinate of the source.

Y: y grid coordinate of the source.

Q: injection rate of the source, specified as gpd or m3/d, as chosen by UNITS.

C: solute concentration of injection, as mg/l or ppm.

TIME: time since start of injection (operation) of this source, in days.

4.2.5 DUPVG

Applications. The above two analytical models are limited in their use to situations in which the aquifer can be modeled as approximately equivalent to a confined aquifer. Serious problems with this assumption arise when leaching from a source is of sufficient volume relative to regional flow to create a significant radial flow component. The source then serves not only to introduce contamination, but also alters the flow regime, and the aquifer will possess a moving free surface. The significance of such effects is estimated in the CHOICE algorithm by a preliminary calculation of ground water mounding resulting from the source. Where significant movement of the

free surface is expected few analytical solutions are available. Model DUPVG provides a solution for a particular class of these problems (Volker and Guvanasen, 1987; Guvanasen and Volker, 1982).

DUPVG is a two-dimensional model in the X-Z plane, considering the longitudinal and vertical distribution of the contaminant. The geometry is thus an extension of the one-dimensional case. The source is represented as an infinitely long recharge basin of a fixed width which contributes a constant rate of recharge to the aquifer. The aquifer is assumed to be symmetrical in X about this source, and bounded by a constant head drain at a fixed distance, and there is assumed to be no pre-existing regional flow pattern. This enables the calculation of an approximate velocity distribution within the saturated zone, and thus contaminant distribution. The assumption of an infinitely long recharge basin implies that this model will be appropriate when the point of observation is sufficiently close to the source so that the effect of finite lateral extent of the source is unimportant, as in the application of ODAST. DUPVG is thus particularly important for estimation of plume development near to a large areal source which contributes significantly to the flow regime, such as surface irrigation systems.

It should be reemphasized that the only flow considered by DUPVG is that induced by the source. Thus dispersion is the only mechanism for dilution of the source concentration. As decay is not considered, this means that if DUPVG is run for a sufficiently long time it will eventually "flood out" the aquifer with water at the source concentration. It is thus not particularly useful to run the model for predictions at a given distance if the time involved is sufficient so that water at source concentration has fully occupied this point - for in this case the prediction is merely that the concentration is equal to the source concentration. A rough estimate of the occurrence of this phenomenon is when:

$$\frac{Q\ A\ t}{7.48\ s\ n\ R} \gg x \qquad (4.6)$$

where Q is the areal leaching rate in gallons per day per square foot, A is the half-width of the source along the direction of flow, in feet, t is time in days, s is the initial saturated thickness, in feet, n is porosity, R is retardation coefficient (v/v_c) and x is distance to the observation point in feet. Where this inequality holds the controlling criteria for concentration predictions will be the determination of Q, and any vadose zone attenuation of contaminant load. The analyst may also need to consider whether any processes of decay or dilution by regional flow, which cannot be considered by this model, may have a significant effect.

Limitations. In order to derive the analytical solution a number

of important simplifying assumptions were made, and the user should be aware of the implications of these assumptions. The solution method first assumes that the rise of the free surface is substantially less than the initial saturated thickness of the aquifer (tests of this condition are made in the CHOICE algorithm). Based on this premise it is assumed that:

- The unsteady free surface can be approximately described by a streamline, which implies that the flow pattern is equivalent to the confined case, but with an a priori unknown upper boundary.

- Near the source, streamline and equipotential functions change little with time, so that the transient velocity can be described by a steady state distribution modified by a simple time function.

- Further away from the source the velocity field is essentially horizontal and its spatial variation is negligible.

These conditions require that the slope of the free surface is relatively small, and that the distance to the constant head drain is sufficiently large so that equipotential lines at the downstream end are vertical. The final solution uses an approximation that is equivalent to the case where the distance to constant head goes to infinity, although the near source velocities are first computed using a finite value of this distance. In any case, the solution method will be accurate only when the constant head boundary is relatively far away from the source. Further, constant head boundaries must be assumed to be distributed symmetrically about the source axis.

The approximate solution employed for the transport equation (S1) is based on the assumption that the distance to constant head can be extended to infinity. However, the velocity distribution is first calculated without this approximation. Thus the solution method should provide an accurate estimation of the average position of the front. However, when the constant head boundary is closer to the source the vertical distribution of concentrations may not be accurate.

Other important limitations are obvious from the nature of the solution. The method cannot take into account any regional flow other than that induced by the source. Further, the method treats only conservative substances, which may be retarded but are not subject to decay.

Data Input. The preprocessor for DUPVG shares that of ODAST and TDAST, and information given in the discussion of ODAST is relevant to certain variables in common with DUPVG. The data to be input are as follows:

NUMX: Number of points modeled in the X direction, which

establishes the 1-dimensional grid. From 1-25 points may be used. Grid size does not affect solution, and for Monte Carlo simulation you will normally wish to examine only one or two points at the perimeter of compliance in order to speed execution.

NUMZ: Number of points modeled in the vertical, Z direction, counting downward from the top of the saturated zone.

NUMT: Number of time steps for calculation. In Monte Carlo applications only the last time step will be tabulated for cumulative frequencies. However, the output file will contain sample data from each time step. In deterministic mode full data will be provided for each time step.

NNS: The solution requires numerical integration of one simple time derivative. NNS sets the accuracy of the numerical integration scheme by choosing the degree of the polynomial for the Gauss-Legendre method. NNS selects the nth digit from (4, 5, 6, 10, 15, 20, 30, 40, 50, 60, 104, 256). Increasing NNS improves accuracy but decreases speed. NNS=8 seems to provide a good compromise value, but may be changed at will.

MODE: In Monte Carlo applications two options are available for modeling uncertainty in hydraulic conductivities. MODE=(1) generates values of K from porosity and particle diameter distributions by use of the Karmen-Cozeny relationship, and is thus appropriate when actual values of K are poorly known. With option MODE=(2) K is generated as an independent log-normal process.

MODE4: This provides an option for the calculation of source strength from leaching rates (MODE4=1) or the direct input of concentrations in the aquifer at the source boundary (MODE4=2).

Q: leaching rate from source expressed as gal./ft2-d. If the HELP model has been run for this site, the values obtained will be reported here. In DUPVG the source is conceived as a basin of infinite horizontal extent and finite width.

POR: Total porosity of the medium.

B: Thickness of saturated layer (initial thickness). This is used to calculate the initial mixed concentration beneath the source and is not required if MODE4=2.

MODE3: In Monte Carlo applications, distributions may be directly specified for dispersion coefficients (MODE3=2). If this information is not available, estimates of dispersion are formed from the scale (MODE3=1), using the technique of Mulkey and Brown (1985), as DL = 0.1•X•V and DT = DL/3.

DL, DT: In deterministic mode, or in Monte Carlo mode if dis-

persion coefficients are not generated from scale you must input values here. For Monte Carlo use the coefficient of variation will be asked on the next card.

A: For DUPVG, this measures the effective width of the "infinite" source along the X (flow) axis. This is properly the distance from the edge of the source to a flow divide. As the geometry is assumed symmetrical this is equivalent to half of the width of the source in X.

R: retardation coefficient, = v/vc, where v is the velocity of the regional flow and vc the apparent velocity of the contaminant.

SST: Mean initial source strength, as ppm.

FC: Field capacity (fraction). Porosity = P_e + FC, where P_e is the effective porosity.

PKW: In DUPVG, non-Monte Carlo mode, an initial estimate of K is required. In Monte Carlo mode K will be generated in the usual way.

AHW: Determination of the slope of the free surface requires specification of distance to a constant head boundary, assumed to be symmetrical about the source. Note that for the approximation method used in the solution accuracy decreases as the observation point becomes nearer to the constant head boundary.

ATTEN: Fraction of the solute remaining after vadose zone attenuation. If the HELP model has been run a conservative estimate of ATTEN can be calculated automatically. This calculation assumes that the substance proceeds downward through the unsaturated zone at pulses equal to the saturated hydraulic conductivity of that zone, subject to retardation, and thus provides a very conservative estimate of residence time. Specification of larger degrees of attenuation should normally require some justification on the part of the permit applicant.

Monte Carlo Controls. The following 8 parameters are required only for Monte Carlo simulation.

ITER: Number of Monte Carlo iterations to be run. 500 is recommended for good resolution of the cumulative frequencies. However, you may first wish to run a smaller number to test the model.

CVL: Coefficient of variation which specifies the variability in the source concentration, where the coefficient of variation = standard deviation/mean.

TH: 2 values express the bounds between which the MEAN particle size of the saturated medium will lie. This is modeled as a log-10 uniform process.

GR: estimate of water table gradient, as ft/ft. This is expressed as a triangular distribution, and the user must input a most likely, maximum and minimum value.

CVD: coefficient of variation for dispersion coefficients. Used only if the dispersion coefficients are independently estimated.

CVLNQ: coefficient of variation for the leaching rate. If the HELP model has been run, the observed CV will be shown.

DKLN: If K is to be directly estimated, input mean LN K. Otherwise, K will be estimated from generated particle size, porosity and gradient.

DKLNV: Coefficient of variation of DKLN.

OBSERVATION POINTS: This screen identifies the grid set-up. Concentrations will be calculated at all combinations of X, Z and T. However, for Monte Carlo applications cumulative frequency calculations will be made only for the last time step. For Monte Carlo you will therefore usually wish to specify only one time point, and 1 or 2 observation points. These numbers are set by NUMX, NUMZ and NUMT (above). The coordinate system is such that (0,0) is a point coincident with the source edge at the (free) surface of the aquifer. Values of Z then represent distance below the free surface.

4.2.6 EPAGW

Applications. The basic model employed here was developed by the EPA for analysis of restrictions on land based disposal, and is documented in Mulkey and Brown (1985) and U.S.E.P.A. (1986). The EPA approach is to model the transport of a given substance, subject to hydrolysis and retardation, determining a downflow dilution factor which is used to back-calculate an allowable concentration of the substance in a landfill, given a down-flow standard level. To do this, Monte Carlo simulation is undertaken over all the relevant hydrogeological variables, using a national data set, allowing the formation of generalized regulatory standards for allowable concentrations within the landfill. The method is carefully designed to account for the correlation among simulated parameter values. The transport model employed is Sudicky et al.'s (1983) 3-D steady-state solution, using Gaussian quadrature to solve the integral. We have modified this method in a number of ways. First, if we assume that the site characteristics are known, or can be specified by distributions, the method is readily inverted, so that the "dilution" factor is used to predict downstream concentrations from a specified source, using the same Monte Carlo analysis. Secondly, instead of using a national data base for the hydrogeologic parameters, one of several data bases can be selected that reflects the characteristics of a specific region within North Carolina. The selected data base

can then be modified in accordance with any available site-specific data. The method thus becomes appropriate for an analysis of contamination risk in a situation in which little is known about the specific hydrogeology of a site. The objective is then to simulate the expected risk over the range of hydrogeological conditions that are expected to apply for the specific region in which the site is located.

The source in the EPAGW model is assumed to be distributed as a Gaussian source. The source is thus areal, but concentrated towards a central point. This makes the model particularly applicable to landfills. However, it may be inappropriate for large scale areal sources, such as surface irrigation of wastes, in which contaminant input is relatively uniform across the source area.

EPAGW represents a complete and coherent Monte Carlo approach to contaminant risk analysis under uncertainty. It is thus the model of choice for preliminary analysis of risk in situations in which little site specific data is available on flow regime and hydrogeology, given that a Gaussian representation of source distribution is appropriate. The model development assumes that the direction of flow from the source is not accurately known. Analysis is thus made at a specified distance along the (unknown) main axis of flow. Equivalently the model may be applied to analysis along an explicitly known axis of flow.

EPAGW contains detailed routines for calculation of chemistry dependent hydrolysis of contaminants. It also considers the effects of vertical mixing. The model will thus also be useful for analysis in some situations where there is substantial knowledge regarding the flow regime, but the analysis requires consideration of partial penetration and/or complex hydrolysis reactions. This is especially useful for analysis of certain organic constituents with pH dependent hydrolysis rates.

An example of the use of EPAGW is given in section 4.3.2.

Limitations. EPAGW provides a highly flexible method for analysis. However, it can only be applied in the Monte Carlo mode. Further, solution is provided only at a point along the axis of flow at the surface of the aquifer. A steady-state concentration only is calculated, so that EPAGW cannot be used to calculate time history of contamination. From the nature of the solution the model will not be appropriate for large uniform areal sources, such as land applications. The usual assumptions of steady-state, uniform flow apply here, and the model will not be appropriate for sources that contribute a volume of fluid sufficient to significantly alter the flow regime.

Data Input. Data input for EPAGW consists of two phases. The

first phase concerns the parameters controlling site hydrogeology. To initiate this phase for a new site the user should first load a default regional data set from the list provided. Even where an appropriate regional data set is not available one should be loaded to guide input, then modified as needed.

Development of regional data sets is still in progress, but limited by available information. For regulatory analysis it will most commonly be the surficial aquifer that is of interest. These can be conveniently grouped according to the nature of the surface soil. It is our intention to develop data sets for each of the 16 general soil groups described in Soil Systems in North Carolina (Daniels et al. 1984). This readily available reference contains a color-coded map which enables ready identification of the soil group. The following data sets have presently been provided:

1. EPA national data base (Mulkey and Brown, 1985). This reflects generalized characteristics of surficial aquifers throughout the United States. It is thus not directly appropriate to use for North Carolina sites, but may be used as a template for data input for regions where a North Carolina data set has not yet been provided.
2. Surficial aquifer, N.C. soil system 1.
3. Surficial aquifer, N.C. soil system 4.
4. Piedmont N.C., generalized surficial aquifer. This provides an approximate generalized data set for systems 10, 11, 12 and 13.

The specification of the underlying hydrogeologic parameter distributions and their probability parameters is designed to allow a maximum of flexibility in selection. First, a regional data base with assumed distributions and metaparameters is selected. Where no additional site data or user knowledge is available, simulation may proceed with these unaltered distributions and values. This will provide an estimate of contamination risk based on the average characteristics of the area, and so should be modified to reflect any known differences of a specific site location from the average characteristics of the area. However, any parameter distribution may be altered in one or more of the following ways:

1. Respecify parameter distribution metaparameters.
2. Automatically update regional data by combination with site data.
3. Respecify parameter distribution type.

Where the user feels that a given parameter is known with considerable accuracy this may be indicated by specifying the distribution as a tightly restricted uniform or triangular distribution.

The types of distributions that may be specified for the various parameters are identified as follows:

0. No distribution has yet been specified. This must be replaced before running the model.

1. Triangular distribution. The user must specify most likely, minimum and maximum values for the distribution. The triangular distribution is an ad hoc, empirical distribution which takes a triangular shape. This can be used to readily approximate various peaked but skewed distributions.

2. Uniform distribution. The user must specify the minimum and maximum of the range.

3. Log10 Uniform distribution, in which the log values are uniformly distributed. The user must specify the UNTRANSFORMED minimum and maximum values of the range.

4. Normal distribution. The user must specify the mean and standard deviation.

5. Log-normal distribution, in which the log values are normally distributed. The user must specify the mean and standard deviation of the log transformed values.

6. Exponential distribution, in which the mean is equal to the standard deviation. The user must specify this single value.

7. Table-specified distribution. This is available in certain cases only.

Each of the pre-specified regional data sets will describe each of the parameter distributions by one of the above distributions. However, these may vary from data set to data set. For this phase of input, distributions must be specified on the following parameters:

DIAM: mean particle diameter (cm). Note that the specification is of the distribution of the mean, not the full range of particle diameters encountered.

GRAD: gradient of the water table (length per length).

FOC: organic carbon fraction of aquifer medium. This is an important factor in the chemical analysis of the fate of certain organic constituents.

PH: pH of groundwater.

T: groundwater temperature (Centigrade).

TH: thickness of the saturated zone (meters).

H: leachate initial penetration depth into the saturated zone (meters). This specifies vertical mixing beneath the site. Because of constraints in the solution method H must be equal to at least 2 meters.

QC: leaching rate distribution for engineered (lined) facilities.

QD: leaching rate distribution for non-engineered facilities (Default is table specified; for direct input use m/yr). If the HELP model has been applied to the site the leaching rates estimated from this model may be loaded to replace both the QC and QD values.

Phase one thus requires specification of the general characteristics of the aquifer. Phase two of data input requires information on the site engineering and the contaminant of interest. The following data is required:

CLM: mean leachate concentration, in mg/l (ppm).

CLS: standard deviation of leachate concentration mean.

DKA0: hydrolysis rate for the substance under acid conditions, 1/[molar*year]. EPAGW simulates the lumped degradation constant, K, based on pH, DKA0, DKB0 and DKN0, using equation 4.2. Values of hydrolysis rates for certain constituents are given in table IV-2 in $days^{-1}$. These values must be converted to $years^{-1}$ for input into EPAGW.

DKB0: base catalyzed hydrolysis rate, 1/[molar*year].

DKN0: neutral catalyzed hydrolysis rate, 1/year.

DKOW: $\log_{10}$ octanol/water partition coefficient for contaminant, describing the constituent's solubility. The actual value will be dependent on the organic carbon content and available surface area of the soil. Average values are given in table IV-3. If this value is not directly known it may be estimated from:

$$DKOW = 5.0 - 0.67 \log_{10}(Sw) \qquad (4.7)$$

where Sw=solubility in water. EPAGW also uses DKOW to estimate the adsorption coefficient of the constituent, using the approximate relationship:

$$\log_{10}K_{oc} = 1.029 \cdot \log_{10}K_{ow} - 0.18 \qquad (4.8)$$

Note that this relationship may not be valid for polar constituents.

ATTN: a factor which specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site a conservative value of ATTN may be calculated automatically from the HELP output. This is calculated in the same manner as for the model ODAST.

Table IV-3. Log Octanol-Water Partition Coefficients (LKOW) and Average Soil-Water Partition Coefficients (K_{oc}) for Various Organic Constituents.

Compound	LKOW	KOC
Acetone	-0.24	1
Benzene	1.56-2.15	97
n-Butyl alcohol	0.88	10
Carbon disulfide	2.16	63
Carbon tetrachloride	2.64-2.9	232
Chlorodifluoromethane		62
Chlorobenzene	2.80-2.87	318
Chloropentafluoroethane		708
m-Cresol	1.92-2.15	27
o-Cresol	1.92-2.15	17
p-Cresol	1.92-2.15	19
Cyclohexanone	0.81	10
o-Dichlorobenzene	3.58	898
Dichlorodifluoromethane		269
Dichlorofluoromethane		30
1,2-Dichlrotetrafluoroethane		437
Diethyl ether		9
Ethyl acetate	0.73	8
Ethyl benzene	3.15	622
Ethyl ether	0.77-0.83	
Isobutyl alcohol	0.65-0.83	8
Methanol	-0.75	0.6
Methylene chloride	1.26	25
Methyl ethyl ketone	0.26-0.30	4
Methyl isobutyl ketone	1.25-1.38	24
Naphthalene	3.36	
Nitrobenzene	1.85-1.90	67
Pentachlrophenol	5.06	
Pyridine	0.65-0.68	7
Tetrachloroethylene	2.60-3.03	303
Toluene	2.11-2.82	242
1,1,1-Trichloroethane	2.50	155
Trichloroethylene	2.28-2.37	152
Trichlorofluoromethane	2.52-3.10	479
m-Xylene	3.20	588
o-Xylene	2.77	363
p-Xylene	3.15	552

NPROB: number of Monte Carlo runs. A minimum of 500 is recommended for adequate definition of the cumulative frequency. However, the user will usually wish to test model performance by first trying a smaller number of runs. The value of NPROB is not saved with the data set, but defaults to 500, and thus may need to be respecified for each run.

AW: surface area of landfill, in square meters.

TR: reference temperature for the chemical rate constants, in degrees C (these are usually specified at 25° C).

XX: distance from the edge of the disposal area to the observation point, along the flow axis (meters). The exact value of XX is somewhat ambiguous for large areal sites.

Leaching Rate Distribution: Calculated from HELP model, or from table, where

C: table for engineered facilities
D: table for non-engineered landfills.

4.2.7 EPASF

Applications. The EPA surface water model (EPASF) was designed to assess impacts of waste disposal sites on surface waters (with hazard associated with human use of contaminated surface waters or consumption of fish from contaminated surface waters) in a manner analogous to the EPAGW model. Here, however, at least two stages must be considered: transport from the landfill via groundwater, and entry into and dilution in the stream. As with the EPAGW model, we have modified this model to provide risk assessment from a given landfill, and have likewise added a preprocessor. EPASF and EPAGW can share essentially the same input data set, with a few additions.

EPASF estimates groundwater contaminant transport to the stream using either a one dimensional or a three dimensional solution, and with or without consideration of dispersion. In the three dimensional case the transport solution is the same as that used in EPAGW. Note that lateral dispersion of the contaminant plume affects the concentration, but not the total mass loading to the stream. As EPASF provides only a very generalized approximation of the transport process analysis without dispersion will often be adequate for a first estimate.

Limitations. EPASF provides only a rough and preliminary estimate of impacts in surface waters. However, modelling the interaction of groundwater and surface water often presents formidable difficulties, so that one is forced, by default, to rely on a model such as EPASF for a preliminary estimate of risk. It should be remembered however that EPASF presents only a preliminary estimate. If contamination problems are suggested by application of EPASF the user may then need to attempt more sophisticated analysis.

Data Input. EPASF uses essentially the same data input format as EPAGW, and can share the same data sets. However, distributions for two additional parameters must be specified when characterizing the hydrogeology. These are:

FOCS: organic carbon fraction of suspended sediment in the stream.

FL: lipid fraction of fish biomass. This is needed only when using Scenario 3, in which human impact is assessed via consumption of fish from the stream. The lipid fraction is used to assess bioconcentration of certain lipophilic organic constituents.

Input of the site parameters is very similar to that for EPAGW, but possesses a few differences, including slight alterations in variable names. The site data input for EPASF are defined as follows (see descriptions in section 4.2.6 for further details):

DIMNSN: Dimension of problem; the groundwater transport phase may be run using a one dimensional or three dimensional solution. The

one dimensional solution of course results in much quicker execution of the model.

DSPRSN: Effects of dispersion may be included (1) or omitted (0).

X: distance from landfill edge to the stream, in meters.

CLM:leachate concentration, mg/L (ppm).

CLS: standard deviation of leachate concentration.

LKOW: log octanol/water partition coefficient for contaminant species.

KHA0: acid catalyzed hydrolysis rate, 1/[molar*year].

KHB0: base catalyzed hydrolysis rate, 1/[molar*year].

KHN0: neutral pathway hydrolysis rate, 1/year.

TREF: reference temperature for hydrolysis rates, degrees C (usually given at 25° C).

NUMRNS: number of Monte Carlo runs. At least 500 runs are recommended, and in most cases this model is moderately fast.

AW: area of waste site, square meters.

AS: area of watershed above point of impact, in square miles. This factor is used in the determination of in-stream dilution.

Leachate distribution: flux of leachate from landfill, in m/yr. Choices: subtitle C (engineered), subtitle D (non engineered). As in EPAGW these values may be replaced by rates calculated by the HELP model.

ATTN: factor specifies the fraction of solute remaining after passage through the unsaturated zone beneath the landfill. If the HELP model has been applied to this site a conservative value of ATTN may be calculated automatically from the HELP output.

4.2.8 LTIRD

Applications. LTIRD calculates the concentration of a particular solute in radial flow (Javandel et al., 1984), using a semianalytical solution originally written by Moench and Ogata (1981). This model is included for the explicit purpose of treating purely radial flow situations, in which regional flow is not present. The idealized situation treated by the model considers a confined aquifer of con-

stant thickness which is recharged through a fully penetrating well at a constant rate. The model considers steady-state plane radial flow only.

As with other solutions for confined aquifers, LTIRD is applicable as an approximation to unconfined aquifers in cases where mounding is sufficiently small so that the streamlines remain approximately parallel. LTIRD can also be used to treat surface inputs if the assumption can be made that the solute is vertically mixed in the aquifer soon after introduction.

LTIRD is presently available only in deterministic mode, although we intend to adapt it for Monte Carlo simulation as well.

Limitations. LTIRD has a rather limited range of applications in the advisory system. There is no consideration of regional flow, so this model should be used only when the radial flow from recharge dominates, but, in the case of a surficial unconfined aquifer, the rate of recharge is also sufficiently small so that the assumption of a confined aquifer is approximately valid. Use of the model is also limited by the fact that it does not include decay or retardation, and the fact that it assumes steady-state plane radial flow. The source is modeled as a well, so that the model is not appropriate to areal sources.

Data Input. Data input for LTIRD is quite simple. The following are required, in any consistent units:

NUMR: Number of radiuses at which to calculate concentrations.

NUMT: Number of time steps to calculate.

RDW: Radius of the well, or source approximated as a well.

R (1 to NUMR): Radial distances at which calculations are made.

T (1 to NUMT): Times for calculation.

ALPHA: Dispersivity.

Q: rate of recharge.

B: Saturated thickness of aquifer.

N: Porosity of aquifer.

CO: Concentration of solute in recharge.

4.2.9 RESSQ

Applications. RESSQ is a program for semianalytical calculation of contaminant transport (Javandel et al., 1985). The model calculates two-dimensional transport by advection and adsorption (no dispersion or diffusion) in a homogeneous, isotropic confined aquifer of uniform thickness when regional flow, sources, and sinks create a steady state flow field. Recharge wells and ponds act as sources and pumping wells act as sinks. The solution proceeds by calculating the streamline pattern in the aquifer and the location of contaminant fronts around sources at various times. RESSQ can thus be applied to a large variety of complex flow situations that can not be handled by analytical solutions.

Because the method is limited by neglecting dispersion, RESSQ, as other semianalytical methods, is most appropriate for preliminary analysis of the extent of probable contamination in a complex flow regime. If the semianalytical method does suggest a contamination problem at the perimeter of compliance the user may then need to apply a more complex numerical model. Because it is a preliminary analysis tool, RESSQ is provided only in a deterministic mode.

An example of the use of RESSQ is provided in section 4.3.3.

Limitations. The most obvious limitations of RESSQ are its neglect of dispersion and decay. Other limitations of the method are similar to those that apply to most two dimensional steady state analytical solutions. RESSQ requires that the medium is homogeneous and isotropic, with steady state uniform regional flow. Thus the method is not applicable when the medium is distinctly heterogeneous or anisotropic. Further, the method is not directly applicable to transient problems.

A more subtle limitation is due to the assumption made in the model that a steady state flow field exists. This implies that the sum of flow rates from all the injection wells should be equal to the sum of the flow rates from all the production wells. In practice, RESSQ can be applied to situations where these sums are not equal, if analysis is made at sufficiently large values of time so that quasi-steady flow prevails (see below). However, if attempts are made to apply the model to shorter time periods where the two sums are widely different bizarre results may occur. Note that this problem is avoided if a constant head boundary is specified through the use of image wells, in which case the two sums will be by definition equal.

The solution method used in the model is based on the assumptions of a uniform, confined aquifer. Application to a surficial aquifer is thus valid only when conditions in the surficial aquifer approximate those of a confined aquifer. For a preliminary analysis of contaminant risk this is appropriate when the surficial aquifer

does not show distinct seasonal variability, and the input from sources does not result in substantial mounding. The latter condition should be adequately met in situations for which the Dupuit approximations hold. In addition, and like most available two-dimensional analytical solutions, RESSQ assumes that sources fully penetrate the aquifer. This is equivalent to assuming that the contaminant loading from a source instantaneously displaces the pre-existing water throughout a vertical column of the aquifer. Note that RESSQ provides a sharp front approximation, and cannot account for mixing of the flow from a source with the water in the aquifer. Instead, the source flow displaces the water in the aquifer, without mixing. For a source that is not actually fully penetrating this approximation is obviously more valid for a thin saturated layer. However, an overly thin saturated layer is likely to result in violation of the confined aquifer approximation. The practical result is that RESSQ, when applied to a surficial aquifer with a non-penetrating source, is likely to provide inappropriate concentration results in the region close to the source, but more accurate results further away from the source.

Attempts to apply RESSQ to surficial sources which do not fully penetrate the aquifer are considerably complicated by the necessary assumption that no mixing occurs. This may result in overestimation of the concentration resulting from a source. This is a particular problem when the rate of regional flow is significantly large in relation to the rate of recharge from the source. In such cases the positions of contaminant fronts can still be calculated, but the concentration within these fronts cannot be interpreted as equal to the source concentration. In general, RESSQ is recommended for approximate application to surficial sources only in cases where the flow from such sources is of sufficient volume to overwhelm the regional flow in the neighborhood of the source and a radial flow pattern is established.

In sum, it should be emphasized that RESSQ is best thought of as a preliminary analysis tool. Despite the many limitations expressed above it provides a very powerful tool for preliminary analysis of complex flow situations.

Data Input. Appropriate use of RESSQ is somewhat of an art, and will require practice on the part of the user to obtain adequate results. This is because the model calculates concentration front positions on the basis of a finite number of streamlines. The results observed are thus to a degree sensitive to the number of streamlines modeled, and the starting angle of the first streamline leaving each source. The user may need to experiment with these values to obtain the desired results.

By proper formulation of the input data RESSQ can be used to model a wide variety of situations. The following suggestions for

data input are taken from Javandel et al. (1984):

1. If the total flow rate from all injection wells does not equal the total flow rate from all production wells, then, strictly speaking, a steady state flow field, as required by RESSQ, cannot be achieved. However, for large values of time one may assume that quasi-steady flow prevails, thus allowing RESSQ to be used. However, if the sum of the two rates are widely divergent, unexpected and inappropriate results may be found for shorter time periods.

2. In addition to modeling recharge or injection wells as point sources, RESSQ can model constant head ponds as finite radius sources. This is done by specifying the pond as a recharge well, with radius of the pond specified as the radius of the well. Such sources are however also considered to be fully penetrating.

3. RESSQ can include a linear no-flow or constant potential boundary using the method of images. A boundary is represented by adding an image well for each real well in the problem, with the boundary located on the perpendicular bisector of the line connecting each real well/image well pair. For a no-flow boundary the real and image wells have the same flow rate, that is, either both are injection or both are production wells. Since there is no flow through an impervious boundary, the only regional flow allowed in this case is parallel to the boundary. For a constant potential boundary the real well/image well pairs have flow rates equal in magnitude and opposite in sign. In this case the boundary must be an equipotential and the only regional flow allowed is perpendicular to the boundary.

4. The model requires that the number of injection wells specified must be greater than zero. This is because injection wells act as the starting points for streamlines, so without injection wells no streamline pattern can be draw. To allow greater flexibility in presenting streamline patterns. Zero-flow wells do not affect the velocity field, but provide starting points for streamlines whose paths may help explicate the velocity field created by regional flow and nonzero-flow rate sources and sinks present.

5. The techniques described in (4) allow the specification of a uniform regional flow by use of a row of zero-flow-rate wells. Streamlines describing regional flow can be drawn by placing a row of zero-flow rate wells perpendicular to the direction of regional flow at a distance relatively far from sources and sinks. The spacing between these wells must be determined as a function of the ratio of source flow rate to regional flow Darcy velocity. A routine (ZQWELL) is incorporated into the model preprocessor to provide for automatic calculation of the required line of zero-flow wells to describe the regional flow. However, the user may find it necessary to experiment with the input for this routine in order to establish a sufficiently small (or sufficiently large) number of such wells to describe the regional flow within the data input limitations of the code.

RESSQ, by neglecting dispersion, provides a sharp-front approximation of contaminant concentration. That is, water injected from a source undergoes no mixing with water already present in the aquifer, but displaces that water without dilution. Output of RESSQ includes plots of the time position of contaminant fronts around sources. Because these represent sharp fronts, the predicted concentration within the fronts is equal to the injection concentration, while the predicted concentration outside the fronts is equal to the ambient aquifer concentration. In actuality, the processes of dispersion and dilution should result in contamination extending beyond the position of the predicted fronts, but with a corresponding dilution of concentration. The user should pay careful attention to this phenomenon in interpreting the results.

If a production well is specified, the time evolution of concentration at the production well will be estimated (provided that at least two stream lines reach the production well during the simulation period). This time evolution is based solely on the number of stream lines from sources captured by the production well, and does not consider the effects of dispersion and dilution.

Input data for RESSQ requires the following information:

NWI: Number of injection wells (> 0), not including zero flow wells automatically specified in routine ZQWELL.

NWP: Number of production wells. May be zero, but see cautions regarding application of the model to non-steady state flow patterns.

C0: Ambient (preexisting) contaminant concentration in the aquifer.

CD: Default concentration of injection wells. This number can be overridden in the specifications for each well (below). However, it is necessary to specify C0 if the user wishes to observe the dimensionless concentration evolution at production wells. In general, the user should specify CD equal to the highest injection well concentration.

UNITC: Units of concentration. This is a character string used to label output. The default value is "Percent"

IZQ: Requests the use routine ZQWELL for automatic calculation of a line of zero flow wells to specify uniform flow (1: yes, 0: no). Generally the user will wish to enter 1 if regional flow is present.

ATTEN: (Default = 1.0). This option is provided for use with surficial sources. In such cases the strength of the contaminant may decrease significantly in the process of percolation through the unsaturated zone. The users may thus specify ATTEN to represent the fraction of the actual source concentration remaining when the flow

from the source enters the aquifer.

HEIGHT: Average saturated thickness of aquifer (in feet). This value is assumed to be constant throughout the region of study.

POR: Effective Porosity of the aquifer, expressed as percent (POR = Px100).

V0: Pore water velocity of uniform flow (ft/day).

ALPHA: Direction of regional flow, in degrees, measured counter-clockwise from the positive X axis.

ADSORB: Adsorption capacity of matrix, equals (1-1/R), where R is the retardation coefficient. The range of ADSORB is 0-1, as R = V/Vc, where V is the regional velocity and Vc the apparent velocity of the contaminant.

NFRNTS: Number of contaminant front positions to be calculated for each source (maximum 7).

DATE(1 to NFRNTS): Times at which fronts are to be calculated (in years).

TMAX: Period of study in years. This sets the maximum amount of time for calculating the trace of streamlines, and thus should be substantially greater than the time period of interest. TMAX should be set large enough so that streamlines can be fully drawn throughout the area mapped. The example problems given by Javandel et al. (1984) use TMAX=200. If you are specifying regional flow through use of zero-flow wells, TMAX should be long enough so that these flow lines can be drawn across the area to be mapped.

DL: The step-length or spatial increment used to trace out the streamlines, in feet. If left blank this defaults to (XMAX-XMIN)/200. Using a larger step-length will decrease run time, but will also decrease the resolution of the streamline plot.

NTL: Plot option, set NTL = -1 to suppress plot of streamlines.

NTF: Plot option, set NTF = -1 to suppress plot of pollutant fronts.

XMIN: Origin of area of study, X axis (in feet). It is often convenient, particularly when specifying regional flow, to set up the axes so that (X=0, Y=0) is the center of the area of study.

XMAX: Limit of area of study, X axis (in feet).

YMIN: Origin of area of study, Y axis (in feet).

YMAX: Limit of area of study, Y axis (in feet).

The next seven variables control the automatic calculation of a row of zero-flow wells to simulate uniform regional flow. They will be requested only when IZQ=1. The number of ZQWELLs calculated will be displayed after the data is input. If this number is too large you may modify the input and try again. In this case instructions for modification will be displayed.

XREF: X coordinate of arbitrary reference point near the sources and sinks (in feet).

YREF: Y coordinate of the arbitrary reference point.

DIST: Distance from reference point to row of zero flow wells, in feet. Ideally, DIST must be large enough so that near the zero-flow rate wells the streamlines are essentially parallel.

WIDTH: Width of the row of zero-flow wells (in feet). This determines the area that will be covered by the regional flow streamlines.

Q1: Flow rate of the first source (injection well) in gpd. This value will be carried to the source input screen as well.

NSL1: Number of streamlines calculated for the first source.

ITR1: Ratio of NSL1 to the number of streamlines plotted for the first source.

WELLS: The following data must be specified for each source and sink (injection well and source well). The injection wells (sources) must be specified first. Monitor source wells may be specified in order to observe contaminant concentration development.

NAMEW: Name of the well, source or sink (character).

XW: X coordinate of the well (feet).

YW: Y coordinate of the well.

QW: absolute value of flow from/to this well, gpd.

RADDW: radius of well (or pond), in feet. This value will default to 0.2461 ft.

C: concentration of an injecting well in units of UNITC. This will default to C0.

BETA1: angle (degrees) of the first streamline calculated for each injection well. This value can be modified to obtain better streamline definition. The angle is calculated counter-clockwise from the positive X axis.

NSL: number of streamlines calculated for an injection well. Default value is 40. Set NSL = -1 for no streamlines.

ITR: ratio of NSL to number of streamlines actually plotted. Determines the density of the plot. Set ITR = -1 to suppress plotting of streamlines from this well.

INDW: Plot option. Set INDW = -1 to suppress plot of fronts in the case of an injection well, or suppress study of concentration in the case of a production well.

4.2.10 MOC

Applications. The Method of Characteristics (MOC) model of Konikow and Bredehoeft (1978) is a well-tested and accepted, highly flexible numerical groundwater transport model. Unlike analytical models, this model can consider heterogeneity and anisotropy of the porous medium, and also offers great flexibility in specifying sources, sinks and boundary conditions. The version included in the advisory system includes several updates distributed since the publication of the 1979 manual that extend the method to allow consideration of retardation and radioactive-like decay in the model.

By using a numerical method, the characterization of the aquifer is not constrained by the availability of analytical solutions. The numerical method requires that the area of interest be subdivided by a grid into a number of smaller subareas. MOC utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid, in which nodes are defined at the centers of the rectangular cells. If sufficient information is available, the user may individually specify distinct values of controlling parameters at each of these nodes. The technique employed seeks numerical solutions first to the head distribution, then to the flow equation, and finally to the transport equation. The transport equation is solved using the Method of Characteristics, which avoids the problem of numerical dispersion often encountered in numerical models.

We have modified MOC for use in Monte Carlo simulation as well. However, only some of the many possible sources of uncertainty are considered in this procedure. These were selected on the basis of a sensitivity analysis, under the assumption that the hydraulic heads along the boundaries are exactly known. Thus the Monte Carlo method is not implemented in full generality here, but rather designed to be most applicable for the specific case of analysis of proposed hazardous waste landfills. The Monte Carlo procedure employed here is summarized in figure IV-2. Of particular interest in this method is the specification of a spatially covariant hydraulic conductivity random field, which is well adapted to the simulation of the natural uncertainty in this parameter, where it is expected that hydraulic conductivity values will tend to show a higher degree of similarity between nodes that are closer together in space. The Monte Carlo procedure also conceives of a situation at which contaminant input begins following the failure of a containment structure, prior to which there is essentially no input from the source. This conception is most applicable to the analysis of a proposed hazardous waste landfill, in which the analyst must consider the possibility of contamination resulting from failure of the landfill liner.

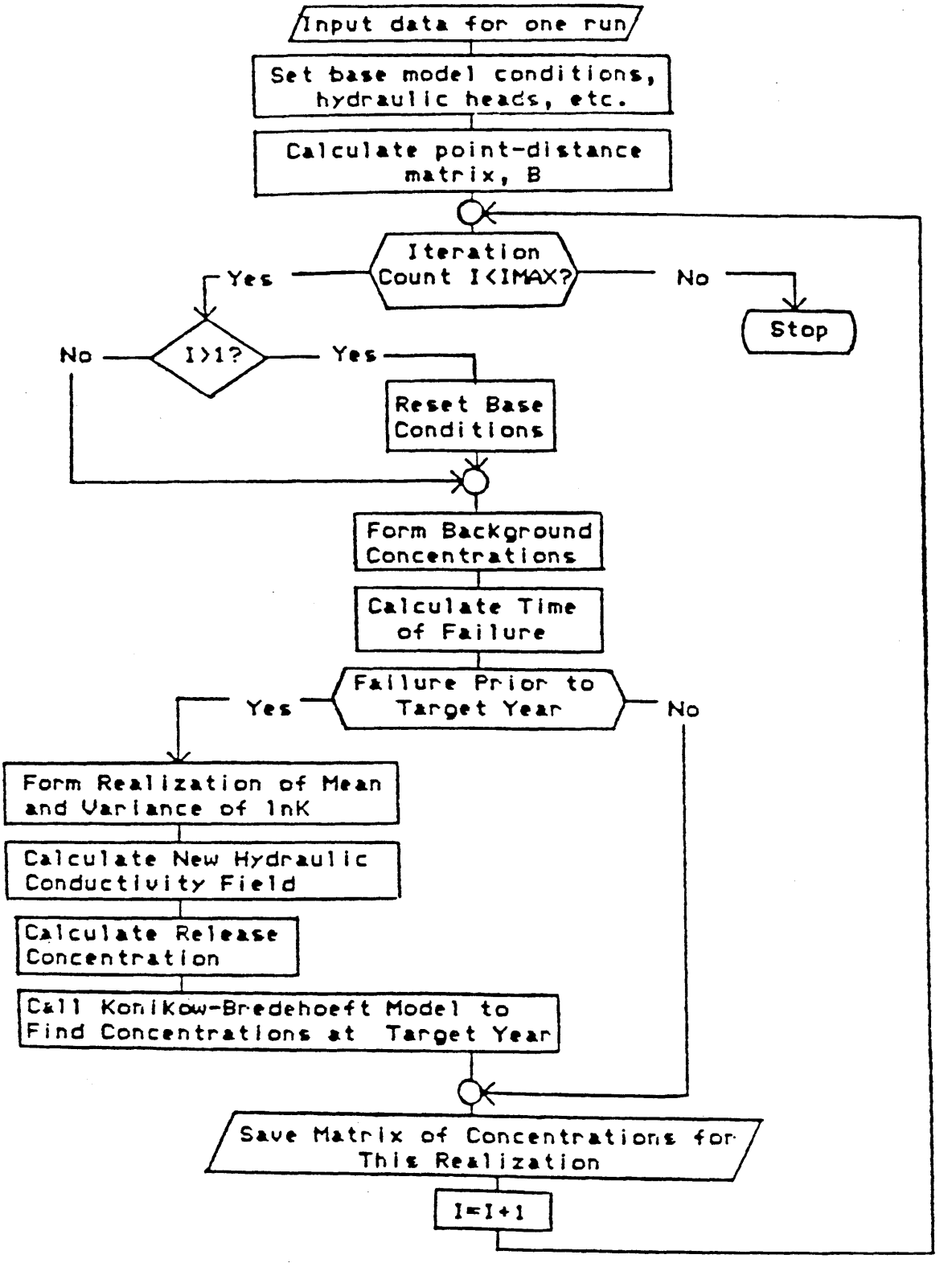

Figure IV-2. Monte Carlo Simulation Procedure For The Method Of Characteristics Model

The component models for the Monte Carlo simulation procedure with MOC were given as an example in Chapter II. We repeat these here for the purposes of guiding data input.

1. SITE RELIABILITY MODEL

Given that the probability that the landfill will fail in any year is p, then t_f, the year in which the landfill liner fails is geometrically distributed with parameter p:

$$\text{Prob}(t_f=t|p) = p(1-p)^{t-1} \tag{4.9}$$

It is very likely that the value of p can be estimated only with limited precision. To reflect this uncertainty, we assume that the parameter p is a priori beta distributed with parameters a and b:

$$p \sim \text{Beta}(a,b) \tag{4.10}$$

2. LEACHATE RELEASE CONCENTRATION

Given that a failure has occurred, the probability of the amount/ characteristics of the released point source contaminant, C_L, at time t_f is a priori normally distributed with mean u_c and variance v_c:

$$(C_L|t_f) \sim N\ (u_c, v_c) \tag{4.11}$$

As in most numerical models, areal sources will be assumed to be represented by a number of point sources.

3. HYDRAULIC CONDUCTIVITY RANDOM FIELD

It is well documented that the spatial variability of hydraulic conductivity can have a significant effect on the field-length dispersion of contaminant plumes and that hydraulic conductivity is lognormally distributed (Freeze, 1975; Smith and Schwartz, 1980, 1981). We assume a two level stochastic model to reflect both natural and parameter uncertainty in the hydraulic conductivity field distribution. For the case of m nodes, it is assumed that $\underline{K}=\ln(\underline{K}_0)$, the (mxl) vector of the natural logarithm of the hydraulic conductivity, follows an m-dimension normal multivariate distribution with mean $u_k\underline{b}$ and covariance $v_k B$:

$$\underline{K} \sim N\ (u_k \underline{b},\ v_k B) \qquad (4.12)$$

where $\underline{b}=(1,1,\ldots,1)^T$, is an mx1 vector of ones, B is an mxm matrix whose diagonal elements are equal to one, and whose ij-th off-diagonal elements are given by $\exp(-d_{ij}/d_0)$, where d_{ij} is the distance between the ith and jth point and d_0 is the correlation length. In addition, in order to reflect uncertainty about the parameters of the distribution, it is assumed that a priori u_k conditioned on v_k is normally distributed with mean M and variance v_k/τ:

$$(U_k|v_k) \sim N\ (M,\ v_k/\tau) \qquad (4.13)$$

and $(1/v_k)$ is gamma distributed with parameters c and d,

$$(1/v_k) \sim \text{Gamma}(c,d) \qquad (4.14)$$

In practice, v_k is generated from CO/(2X), where X is an inverse chi-square deviate.

4. BACKGROUND CONCENTRATION

The pre-existing concentration of solute in the aquifer, prior to landfill failure, C_B, is assumed to be uniform throughout the aquifer and specified by a log-normal distribution:

$$\ln\ (C_B) \sim N\ (u_B,\ v_B) \qquad (4.15)$$

Note that this requires that the background concentration cannot be exactly zero.

Limitations. MOC, particularly in the deterministic mode, provides a highly flexible tool for analysis of many contaminant transport situations. However, the user must also be aware of certain limitations. The development of the solution required a number of assumptions, and the degree to which field conditions deviate from these assumptions will affect the applicability and reliability of the model. These include the following:

- Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow. Low velocity flow under other conditions is not considered.

- Solute transport is dominated by convective transport, an assumption required for the method of characteristics solution of the flow equation.

- The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.

- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.

- No chemical reactions occur that affect the fluid properties or the aquifer properties.

- The only chemical reactions considered for the solute species are linear retardation of velocity and decay that can be described as similar to radioactive decay. No pH dependent hydrolysis of constituents is considered.

- Ionic and molecular diffusion are negligible contributors to the total dispersive flux.

- Vertical variations in head and concentration are negligible.

- The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

The model in general is applicable to both confined and unconfined aquifers. However, the validity of the present code is somewhat limited in application to unconfined aquifers. That is, the saturated thickness is presently specified independent of the water-table elevation, and does not change in response to changes in water-table elevation. This means that if recharge and/or pumping do result in substantial changes in water-table elevation the solution will lose accuracy in the unconfined situation. The user should be particularly careful in attempting to apply the model to transient flow problems in an unconfined aquifer.

Additional limitations apply to the use of this model in the Monte Carlo mode. The most important practical limitation is that run time may be very long when using this model on a Personal Computer. As noted above, the Monte Carlo formulation used here considers only certain specific sources of variability. If there are other sources of variability that have an important affect on predicted concentrations use of the Monte Carlo method provided here will not provide an accurate analysis of risk.

Finally, in both the deterministic and the Monte Carlo mode, the user must specify the head in the aquifer at the start of the simulation, as an initial condition. Obviously, in many cases complete data on head distribution will not be available; however, no pro-

visions have been made to account for uncertainty in initial heads. It is possible to determine initial heads from previous simulations. However, it is important to note that the simulation results may be sensitive to variations or errors in the initial conditions. In discussing computed heads, Trescott, Pinder and Larson (1976) state: "If initial conditions are specified so that transient flow is occurring in the system at the start of the simulation, it should be recognized that water levels will change during the simulation, not only in response to the new pumping stress, but also due to the initial conditions. This may or may not be the intent of the user."

Data Input. MOC is provided with a preprocessor for data input supplied by the International Ground Water Modeling Center and written by P. Srinivasan. We have used the format of this preprocessor as a model for the development of the other preprocessors in the system. The preprocessor supplied by IGWMC has been modified by us to allow input of the additional data required for Monte Carlo simulation. The preprocessor is equipped with detailed Help screens, which however relate primarily to the procedural details of entering data.

Considerable flexibility is available in the model through the specification of boundary conditions. Two general types are incorporated into the model, being constant-flux and constant-head boundaries. These can be used to represent the real boundaries of an aquifer as well as to represent artificial boundaries for the model which can be used to minimize the areal extent of the modeled part of the aquifer. The following descriptions of boundary conditions are taken directly from Konikow and Bredehoeft (1978):

A constant-flux boundary can be used to represent aquifer underflow, well withdrawals, or well injection. A finite flux is designated by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant-flux boundary. The numerical procedure used in the model requires that the area of interest be surrounded by a no-flow boundary. Thus the model will automatically specify the outer rows and columns of the finite-difference grid as no-flow boundaries. No-flow boundaries can also be located elsewhere in the grid to simulate natural limits or barriers to ground-water flow. No-flow boundaries are designated by setting the transmissivity equal to zero at appropriate nodes, thereby precluding the flow of water or dissolved chemicals across the boundaries of the cell containing that node.

A constant-head boundary in the model can represent parts of the aquifer where the head will not change with time, such as recharge boundaries or areas beyond the influence of hydraulic stresses. In this model constant-head boundaries are simulated by adjusting the leakage term at the appropriate nodes. This is accomplished by setting the leakance coefficient to a sufficiently high value (such

as $1.0s^{-1}$) to allow the head in the aquifer at a node to be implicitly computed as a value that is essentially equal to the value of H_s, which in this case would be specified as the desired constant-head altitude. The resulting rate of leakage into or out of the designated constant-head cell would equal the flux required to maintain the head in the aquifer at the specified constant-head altitude.

If a constant-flux or constant-head boundary represents a fluid source, then the chemical concentration in the source fluid must also be specified. If the boundary represents a fluid sink, then the concentration of the produced fluid will equal the concentration in the aquifer at the location of the sink.

The model allows the specification of a time-varying pumping schedule through the specification of a number of pumping periods. During each of these periods the pumping occurs at a constant rate. However, differing pumping configurations may be specified for subsequent pumping periods. For Monte Carlo simulation the model should be run in steady-state mode with only one pumping period specified.

The input data is organized by cards, as follows:

card 1. Title . . . . . .
card 1a. Monte Carlo card I . . . .
card 1b. Monte Carlo card II. . . .
card 2. Control card I. . . . . .
card 2a. Control card Ia (optional)
card 3. Control card II . . . . . .
card 3a.Control card IIa (optional)
data set 1. Observation points. . . . .
data set 2. Wells . . . . . .
data set 3. Transmissivity. . . . . .
data set 4. Aquifer thickness . . . . .
data set 5. Recharge/discharge. . . . .
data set 6. Node identification matrix.
data set 7. Instruction for node id's .
data set 8. Initial head. . . . . .
data set 9. Initial concentration . . .
data set 10. Additional pumping periods.

The two Monte Carlo control cards are, of course, required only when the model is used in Monte Carlo mode.

When the preprocessor for MOC is accessed and the site has not been previously analyzed using this model a default data set may be loaded to guide data input. If previous analysis has occurred the previously formulated data set will be reloaded.

Details for the input "cards" follow:

CARD 1. TITLE

TITLE: Title of the problem and contaminant studied (to 80 characters).

CARD 1A. MONTE CARLO CARD 1. Required only for Monte Carlo applications.

JTER: Number of Monte Carlo iterations to run. Ideally, JTER should be set to a relatively large number in order to yield good definition of the cumulative frequency histogram. However, MOC is quite slow when run in Monte Carlo mode on a PC. The user is advised to initially test the input data by running the model with JTER set to a small number. A complete run can later be undertaken at a time when the computer can be left to run overnight.

BACKM: Mean of the log background concentration of solute. As presently formulated, MOC in the Monte Carlo mode requires the specification of a non-zero background concentration. If there is not known to be any background concentration present this value may be set to the detection limit of the solute species.

SBACK: Standard deviation of BACKM. The background concentration throughout the grid is modeled as a log-normal process.

CARD 1b. Monte-Carlo data card II. Required only for Monte Carlo applications.

TARGY: Time horizon for simulations (years). This is the total time of simulation. Failure of the landfill liner may or may not occur within this time horizon.

UALPHA: MOC in the Monte Carlo mode presumes that contamination may commence at an unknown date within the scope of the simulation, as with the failure of the landfill liner. The probability of failure in a given year is described by a geometric distribution with parameter p, while p follows a Beta distribution. UALPHA describes the lower bound (a) of this distribution.

UBETA: Upper parameter (b) of the Beta distribution. To simulate a fixed time of failure, set TARGY to cover the time from known failure to the time of interest, and set UALPHA and UBETA to 1.

RELCM: Mean release concentration of solute (u_c), given failure, modeled as a normal process.

SRELC: Standard deviation of RELCM ($\sqrt{v_c}$).

The next five variables relate to the generation of the spatially covarying hydraulic conductivity field, which has covariance $v_k B$. The variable v_k is generated as CO/(2X), where X is an inverse chi-square deviate, where the conditional mean, u_k, is generated by a normal process with variance v_k/τ.

NOBS: Degrees of freedom for the inverse chi-square deviate. This may be interpreted as the equivalent number of observations for a prior distribution on the hydraulic conductivities.

KPRM: Transmissivity is modeled as a log-normal process, with spatial covariance throughout the grid. KPRM is the mean log transmissivity (M).

CO: May be interpreted as the sum of squares for the

transmissivity prior.

TAU: Divisor (τ), relating the variance of the mean hydraulic conductivity to the covariance of the hydraulic conductivity field. As stated above, $\underline{K} \sim N_m (u_K \underline{b}, v_K B)$, and $u_K | v_K \sim N(M, v_K/\tau)$.

DL: Integral scale (d_0): the correlation length (in feet) for the hydraulic conductivity covariance matrix B, the off-diagonal elements of which are given by $\exp(-d_{ij}/d_0)$. For information on this parameter the user may refer to Hoeksema and Kitanidis (1985).

CARD 2. CONTROL CARD I.

NTIM: Maximum number of time steps in a pumping period (limit 100).

NPMP: Number of pumping periods to be specified.

NX: Grid set-up, number of nodes in x-direction.

NY: Number of nodes in y-direction.

NPMAX: Maximum number of particles traced (limit 6400).

NPNT: Number of time steps between printouts. In the Monte Carlo mode a printout will be made after the first run. Subsequent printouts can be suppressed by specifying NPNT > NTIM.

NITP: Number of iteration parameters (usually between 4 and 7).

NUMOBS: Number of observation points to be specified in a following data set (maximum 5).

ITMAX: Maximum number of iterations to be used in the ADI (alternating direction implicit) solution procedure of the flow equation (usually between 100 & 200). A warning will be issued if this value is exceeded without convergence. The authors note that it may be difficult to obtain a solution using the iterative ADI procedure for cases of steady-state flow when internal nodes of the grid have zero transmissivity and for cases in which the transmissivity is highly anisotropic.

NREC: Number of pumping or injection wells to be specified. One such well is allowed per node.

NPTPND: Initial number of particles per node (allowable values 1,4,5,8,9, or 16). Increasing NPTPND decreases the mass balance error, but also substantially increases required CPU time for execution. The user can examine reported mass balance errors on the output. There will often be a trade-off between NPTPND and CELDIS in determining the accuracy, stability and time requirements of the solution, depending on whether or not CELDIS is the limiting stability criterion. The authors recommend specifying NPTPND as 4 or 5 for initial model calibration, then increasing NPTPND to 9 or 16 for final runs when maximum accuracy is desired. Higher values of NPTPND may not however be practical in Monte Carlo mode, due to length of execution time required.

NCODES: Number of node identification codes (maximum 10). These codes will be used to specify characteristics of identified nodes in a later data set.

NPNTMV: Particle movement interval (IMOV) for printing chemical data (in Monte Carlo mode enter 0 to suppress printing after

the first Monte Carlo run; 99 to print at the end of each run).

NPNTVL: Option for printing computed velocities (0: do not print, 1: print for first time step, 2: print for all time steps).

NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as for NPNTVL).

NPDELC: Should changes in concentration be printed (1:yes, 0:no).

NPNCHV: Option to write velocity data on unit 7 (0, 1 or 2).

NREACT: Should Retardation and Radioactive Decay be included?

CARD 2a. CONTROL CARD Ia (optional). This card allows the specification of a subgrid so that solute transport may be specified on a smaller grid than calculation of flow.

MX: X coordinate, within the primary grid, of the UPPER-LEFT node of the transport subgrid.

MY: Y coordinate, within the primary grid, of the UPPER-LEFT node of the transport subgrid.

MMX: X coordinate of LOWER-RIGHT node of transport subgrid.

MMY: Y coordinate of LOWER-RIGHT node of transport subgrid.

CARD 3. CONTROL CARD II.

PINT: Pumping period, in years. If more than one pumping period is specified data will be later requested for the subsequent periods.

TOL: Convergence criteria for the ADI iterative solution procedure (usually within 0.01).

POROS: Effective porosity of the medium, assumed constant throughout the aquifer.

BETA: Characteristic length (longitudinal dispersivity) in feet.

S: Storage coefficient (set 0 for steady flow problems).

TIMX: Time increment multiplier for transient flow problems. Ignored if S=0.

TINIT: Size of the initial time in seconds. This is required only for transient flow problems, and is ignored if S=0.

XDEL: Width of finite-difference cell in x-direction, in feet.

YDEL: Width of finite-difference cell in y-direction, in feet.

DLTRAT: Ratio of transverse to longitudinal dispersivity.

CELDIS: Maximum cell distance per particle move (between 0 and 1). Increasing CELDIS generally decreases CPU requirements. Effects on mass balance will be problem dependent, but will not affect the solution in problems for which CELDIS is not the limiting stability criterion. Further, if CELDIS is reduced to too small a level oscillations may be found in the initial time period of the solution, particularly if the initial distance that a particle can move is less than the spacing between particles (determined by NPTPND). The authors recommend setting CELDIS to 0.75 or 1.0 for initial calibration, then changing CELDIS to 0.50 for final runs.

ANFCTR: Anisotropy factor, ratio of T_{yy} to T_{xx}.

CARD 3a. CONTROL CARD IIa (optional). Required only when decay or adsorption are included.

DK: distribution coefficient of the solute.

RHOB: bulk density of the solid.

THALF: half-life of the solute (in seconds).

DATA SET 1. OBSERVATION POINTS. This data set specifies the location of observation wells at which detailed output will be provided. In Monte Carlo applications these will be the points at which cumulative concentration frequencies are calculated. For each observation point the user must enter:

IXOBS: grid index in x of the observation point.

IYOBS: grind index in y of the observation point.

DATA SET 2. WELLS. Specifies pumping and injection wells. For each well, the user must enter:

IX: grid index in x of the well.

IY: grid index in y of the well.

REC: pumping (>0) or injection (<0) rate of the well, in ft^3/sec.

CNRECH: solute concentration of injected water. Required only for injection wells.

DATA SET 3. TRANSMISSIVITY (deterministic mode only).
DATA SET 4. AQUIFER THICKNESS.
DATA SET 5. RECHARGE/DISCHARGE.
DATA SET 6. NODE IDENTIFICATION MATRIX.
DATA SET 8. INITIAL HEADS.
DATA SET 9. INITIAL CONCENTRATION (deterministic mode only).

For each of these data sets the user will first be queried for the following:

INPUT: The parameter is (0: constant, 1: varies in space).

FCTR: Constant value (or multiplication factor) for the parameter.

If INPUT=1 the user will then be queried for values throughout the grid. Note that the preprocessor allows block assignment of values to areas on the grid. This procedure is described in the on-screen Help available from the preprocessor.

DATA SET 7. INSTRUCTION FOR NODE ID'S. The NODE ID's identify special input for the appropriately coded nodes. For each of the codes the user is queried for the following:

ICODE: code number for this node ID. Code 2 cannot be used here, as this is reserved for generated releases in Monte Carlo applications.

FCTR1: leakance at the coded node.

FCTR2: concentration at the coded node.

FCTR3: recharge at the coded node.
OVERRD: Set OVERRD=0 to preserve values of RECH specified in Data Set 5.

DATA SET 10. ADDITIONAL PUMPING PERIODS. If more than one pumping period is specified, the following data must be entered for each additional pumping period. (See above, Card 2, for more detailed discussion of these variables).
ICHK: Should data be revised for this period(1:yes, 0:no).
NTIM: Maximum number of time steps in the pumping period (limit 100).
NPNT: Number of time steps between printouts.
NITP: Number of iteration parameters (usually between 4 & 7).
ITMAX: Number of iterations in ADIP (usually between 100 and 200).
NREC: Number of pumping or injection wells to be specified.
NPNTMV: Particle movement interval (IMOV) for printing chemical data (enter 0 for printing at the end of the simulation).
NPNTVL: Option for printing computed velocities(0: do not print, 1: print for first time step, 2: print for all time steps).
NPNTD: Option for printing computed dispersion coefficients (0, 1 or 2 - same as above).
NPDELC: Should changes in concentration be printed? (1:yes, 0:no).
NPNCHV: Option to write velocity data on unit 7 (0, 1 or 2)..
PINT: Length of pumping period in years.
TIMX: Time increment multiplier for transient flow problems.
TINIT: Size of initial time in seconds for transient flow problems.

4.2.11 HELP

Applications. In many permitting applications use of a contaminant transport model to analyze contamination risk will require estimation of the rate of leaching from a source, which is itself a complex phenomenon. To provide for calculation of leaching rates we have included in the system The Hydrologic Evaluation of Landfill Performance (HELP) Model (Schroeder et al., 1984). This program was developed to facilitate rapid, economical estimation of the amounts of surface runoff, subsurface drainage and leachate that may be expected to result from the operation of a wide variety of possible landfill designs. Thus the authors caution that the model "should not be expected to produce credible results from input unrepresentative of landfills." However, we feel that the method can also be extended to cover the general process of leaching in many types of sites other than standard landfills, although this contention has not been fully tested. Most models incorporated into the system thus include the

option of calling the HELP model to establish leaching rates. In addition, we have allowed for the addition of a fixed amount to rainfall rates, so that the model can provide a rough simulation of leaching resulting from spray irrigation. In these calculations the results can also be used to calculate a rough, conservative approximation of vadose zone attenuation, given knowledge on the half-life and distribution coefficient of the contaminant species.

An example of the use of HELP in a non-landfill situation is provided in section 4.3.1.

Limitations. An important limitation of the HELP model is its assumption that the layers in the design are horizontally uniform. This assumption may not be valid for some larger sites. Further, it should be repeated that the method has not been tested for types of sites other than hazardous waste landfills. When used in such situations the model output should be carefully examined and compared to estimates derived from other sources.

Other limitations are inherent in the simplifying assumptions used in the model development. These are primarily of importance in relation to calculation of daily and peak values (which are generally not of direct concern in the application of analytical ground water transport models). Infiltration through the surface is computed using the SCS runoff curve number technique. The actual rainfall intensity, duration and distribution are not considered. Factors such as slope and surface roughness, which would be important if individual rainfall or storm events were used, are considered only in the context of the land management factors used in the selection of the SCS runoff curve number.

In calculation of evapotranspiration, the model does not use actual daily temperature and solar radiation values. Instead, mean daily temperature and solar radiation data are used. Similarly, daily leaf area indices are interpolated from 13 values scattered throughout the year. As a result, calculated daily evapotranspiration values may be quite different from actual daily values. However, computed and actual monthly and annual totals of the daily evapotranspiration should be similar.

The model also assumes that the characteristics of the landfill do not change with age, and that the only effect of vegetation on the soil characteristics are those shown through the SCS runoff curve number. Barrier soil layers are assumed to remain saturated, and percolation through barrier layers is not restricted or aided by segments below the barrier soil. Finally, the model assumes that surface runon does not occur, and that the water table is below the landfill.

In sum, the HELP model represents a compromise to reduce the difficult question of hydrologic performance of a landfill to a

manageable scale. Other more accurate techniques are available, but will often be impractical to apply in the context of a site-permitting evaluation.

Data Input. Data input for the HELP model is interactive. When the program starts it first prints a header, and then asks the following:

```
1.1 DO YOU WANT TO ENTER OR CHECK DATA OR TO OBTAIN OUTPUT?
ENTER 1 FOR CLIMATOLOGIC INPUT,
      2 FOR SOIL OR DESIGN DATA INPUT,
      3 TO RUN THE SIMULATION AND OBTAIN DETAILED OUTPUT,
      4 TO STOP THE PROGRAM, AND
      5 TO RUN THE SIMULATION AND OBTAIN ONLY SUMMARY OUTPUT.
```

The program will return to this question each time it completes a portion of the program. For use in the advisory system the user will typically wish to enter soil or design input data (2), enter climatologic data (1), and then run the simulation to obtain only summary output (5). Choosing (4) will result in exiting from HELP, then proceeding to any other models requested in the currently operative batch file.

Climatologic data may be entered manually for a site, where this is available, or the user may select default climatologic data. We have currently specified default climatologic data for the following North Carolina stations:

1. Cape Hatteras
2. Charlotte
3. Elizabeth City
4. Fayetteville
5. Greensboro
6. Greenville
7. Lumberton
8. New Bern
9. Raleigh-Durham (airport)
10. Wilmington.

Twenty years of data are provided for most locations, including daily rainfall, average monthly temperature, monthly insolation, and tables of leaf area indices based on type of vegetative cover. This data will be loaded from disk on selection of a default climatologic data set. Note that the leaf area index data is provided only for grass and row-crop covers. The program is not designed to account for wooded cover, and if the user wishes to attempt to apply it to such cases the data must be entered manually.

Once the program has read the default climatologic data it requests the user to specify the type of vegetative cover if the vegetative type had not been previously specified during this run when entering default soil data. When default soil data are utilized the vegetation type is also used in selecting the SCS runoff curve

number for the site and to correct the hydraulic conductivity of the vegetative layer. If the value given in the default soil data input does not agree with the value specified here erroneous results may be obtained. Therefore the program warns:

2.8 IF YOU ARE USING DEFAULT SOIL DATA AND THIS VEGETATION TYPE IS NOT THE SAME AS USED IN THE DEFAULT SOIL DATA INPUT, YOU SHOULD ENTER THE SOIL DATA AGAIN OR CORRECT THE SCS RUNOFF CURVE NUMBER.

Design data must always be specified; however, for soil data the user may input all information manually, or choose to use default data. The details of manual input of soil data are largely self-explanatory, but the user may refer to Schroeder et al. (1984) for further details.

Specification of design data includes specification of the layer type, soil type and thickness of each layers. Four types of layers may be used:

1. Vertical percolation layer.
2. Lateral drainage layer, which may include an engineered leachate collection system.
3. Barrier layer.
4. Waste layer.

If the user attempts to use the model to simulate leaching from a non-engineered site, the design will typically include only vertical percolation and waste layers.

The specification of these layers is restricted by the following recommendations and rules:

1. Lateral drainage is not permitted from a vertical percolation layer.
2. Both vertical and lateral drainage are permitted from a lateral drainage layer.
3. A barrier soil layer should be designed to inhibit percolation.
4. An impermeable liner may be used on top of any barrier soil layer.
5. The waste layer should be designed to permit rapid drainage from the waste layer.
6. The top layer cannot be a barrier soil layer.
7. A barrier soil layer cannot be placed adjacent to another barrier soil layer.
8. Only a barrier soil layer or another lateral drainage layer may be placed directly below a lateral drainage layer.

Up to 9 layers may be specified in the design. These are numbered such that 1 is the top layer. For use in the context of estimating average leaching rates for use in the Advisory System, the bottom layer should be the soil layer directly above the average

water table position. The user will first be queried for the number of layers, and whether the top layer is an unvegetated sand or gravel layer. When using the default soil data, the user will be queried for each layer for thickness (in inches), layer type (from the above table) and soil type. The default soil types and their characteristics are given in table IV-4.

Once entry of the soil and design data is completed the program calculates the SCS runoff curve number based on the vegetation type and the soil texture of the top layer if one of the default soil textures was used for this layer and the top layer is not a waste layer. (If the top layer is a waste layer the SCS runoff curve number must be entered). The equation used to calculate the curve numbers was developed for a landfill with mild surface slopes (2 to 4 percent). The program provides the user with an opportunity to enter a curve number and override the default value if desired. Tables of SCS curve numbers may be obtained from many standard sources.

The model also provides complete facilities for checking and editing soil, design and climatologic data after input. Once the data entry is completed the user may run the program. The detailed output option allows the user to examine daily and monthly output. The summary output option will provide annual data and average monthly totals. This is usually sufficient for use of the model within the context of the Advisory System.

Upon selection of an output option, model execution will commence. The user will then be queried for the number of years of output desired (from 2 years to the maximum number of data years loaded, usually 20). For some designs, model execution may be rather slow. However, if the HELP output is later to be used as input to a transport model run in the Monte Carlo mode at least 5, and preferably the maximum available number of years should be used. This is because the model will attempt to calculate the variance of the rate of leaching from the bottom layer.

Table IV-4. Default Soil Types Used in the HELP Model.

Soil Texture Class HELP	USDA	USCS	MIR in/hr	Porosity vol/vol	Field Capacity vol/vol	Wilting Point vol/vol	Hydraulic Conductivity in/hr	CON mm/d **0.5
1	CoS	GS	0.500	0.351	0.174	0.107	11.95	3.3
2	CoSL	GP	0.450	0.376	0.218	0.131	7.090	3.3
3	S	SW	0.400	0.389	0.199	0.066	6.620	3.3
4	FS	SM	0.390	0.371	0.172	0.050	5.400	3.3
5	LS	SM	0.380	0.430	0.160	0.060	2.780	3.4
6	LFS	SM	0.340	0.401	0.129	0.075	1.000	3.3
7	LVFS	SM	0.320	0.421	0.176	0.090	0.910	3.4
8	SL	SM	0.300	0.422	0.256	0.133	0.670	3.8
9	FSL	SM	0.250	0.458	0.223	0.092	0.550	4.5
10	VFSL	MH	0.250	0.511	0.301	0.184	0.330	5.0
11	L	ML	0.200	0.521	0.377	0.221	0.210	4.5
12	SIL	ML	0.170	0.535	0.421	0.222	0.110	5.0
13	SCL	SC	0.110	0.453	0.319	0.200	0.084	4.7
14	CL	CL	0.090	0.582	0.452	0.325	0.065	3.9
15	SICL	CL	0.070	0.588	0.504	0.355	0.041	4.2
16	SC	CH	0.060	0.572	0.456	0.378	0.065	3.6
17	SIC	CH	0.020	0.592	0.501	0.378	0.033	3.8
18	C	CH	0.010	0.680	0.607	0.492	0.022	3.5
19	Waste		0.230	0.520	0.320	0.190	0.283	3.3
20	Barrier soil		0.002	0.520	0.450	0.360	0.000142	3.1
21	Barrier soil		0.001	0.520	0.480	0.400	0.0000142	3.1
22	User specified (program will query)							
23	User specified (program will query)							

Notes:

USDA: Soil classification system used by U.S. Dep. of Agriculture.
USCS: The Unified Soil Classification System.
MIR: Minimum infiltration rate.
CON: Evaporation coefficient (transmissivity).

Use of texture classes 22 and 23 allows the user to specify characteristics of some layers manually while using default soil data for other layers. Choice of manual input of soil data will require complete specification of all parameters for each layer.

4.2.12 MONITOR

Applications. The problem of compliance monitoring of existing sites is conceived as an important part of the Advisory System. However, it is also a topic that is largely separable from the task of risk evaluation for permitting. Therefore, detailed compliance monitoring routines have not yet been incorporated into the system. It is proposed that development of these routines should form the next phase of future development of the system.

When there is available detailed hydrogeologic information on a site, compliance monitoring will involve in large part the further calibration of models with monitoring observations. This may be done manually in the context of the present system, although no routines for automatic calibration are provided. Compliance monitoring must be addressed in a somewhat different manner when there is considerable uncertainty involved regarding the hydrogeology and the actual rate of contaminant introduction from the site. The program MONITOR has been provided to address some cases of compliance monitoring where there is considerable uncertainty, particularly regarding the rate of contaminant leaching into the aquifer from the site.

Under the guidelines presently being considered by the Division of Environmental Management, site permittees will be requested to place monitoring wells equidistant between the edge of the site and the perimeter of compliance. Evaluation of monitoring at this point may then be used to require additional monitoring, both at the perimeter of compliance and beneath the site. In the initial stages of monitoring, which this model addresses, the analyst will be required to draw conclusions regarding probability of standard violation at the perimeter of compliance, based on monitoring data, as well as to evaluate assumptions regarding the rate of leaching to the ground water from the site. Typically the monitoring data will be found to be quite noisy, without clear trend. This may result in part from unsteady (slug) input from the site and seasonal variations in flow patterns, but may also result from errors in analysis of samples.

MONITOR is designed to aid preliminary analysis of compliance monitoring for large areal sites. Many of the cases handled by the Groundwater Division involve such areal sites, which extend fairly near to the perimeter of compliance. In such cases the monitoring well is likely to be sufficiently near to the site that the site can be considered to be effectively infinite in the lateral direction, and a one-dimensional transport solution can be applied as a first estimate. We further assume that the time series of concentrations observed at the monitor well represents a noisy realization of an ideally uniform flow process, with unknown but constant injection rate. The objective of MONITOR is then to use the monitor well time series to generate a corresponding time series at the perimeter of compliance, with the actual source concentration presumed unknown.

This generated time series may then be analyzed to yield information on the probability of standard exceedance at the perimeter of compliance. Information is also yielded to test the assumptions employed in previous modeling regarding source concentration.

To do this, we first assume that solute movement can be described by a one-dimensional solution for movement of a radioactive tracer in a semi-infinite column, with constant flow and constant source concentration C_0, but subject to decay and adsorption (Bear, 1979). The solution at any point x and time t will then take the form $C(x,t) = C_0\ f(x,t,\theta)$, where θ represents the relevant hydrogeologic parameters. If the monitor well is located at point x_m and the perimeter of compliance is at point x_p, forming the ratio $C(x_p,t)/C(x_m,t)$ results in the cancellation of C_0. The unknown concentration at the perimeter of compliance can then be predicted from the monitoring observations, by:

$$C(x_p,t) = C(x_m,t)\ \frac{f(x_p,t,\theta)}{f(x_m,t,\theta)} \qquad (4.16)$$

This yields a generated time series at the perimeter of compliance which may then be analyzed. In addition, the observed concentration at the monitor well may be used to back calculate the implied source concentration, C_0, given the parameters, θ.

Limitations. MONITOR is intended only for preliminary analysis in cases where the actual source concentration is not well known. To be applicable a one-dimensional solution must be appropriate, which in general means that the site must be of a type such that the model ODAST would be applicable for initial permitting analysis (see above, sections 4.1 and 4.2.2). Use of MONITOR is also severely limited by the assumption that the flow parameters, including velocity and dispersivity, are known. The model is not yet implemented to run in Monte Carlo mode, to account for uncertainty in these parameters, but the user may wish to experiment with different values here.

Data Input. To run MONITOR the following data is required:

POR: total porosity of the medium.

Q: specific discharge (ft/day).

DH: Coefficient of hydrodynamic dispersion (ft2/day).

ALFLIF: Half-life of contaminant in the saturated zone (in days).

B: Linear adsorption coefficient.

Y: Distance from source to monitor well (ft).

X: Distance from source to perimeter of compliance (ft).

IOB: Number of observations in monitoring time series.

CYT(1 to IOB): Observed concentrations.

T(1 to IOB): Time of observation (days).

4.3 EXAMPLE APLICATIONS

In this section we provide several examples of the use of the system in the permitting process. These examples have been adapted from actual permit applications coming before the Groundwater Division and examined in the process of testing the system. However, names of actual sites are omitted as these may represent sites in the process of active review.

4.3.1 Example One: Spray Irrigation (HELP and ODAST)

Many cases coming before the Groundwater Division involve large-scale surface applications of waste water. Due to concerns over impact on groundwater this method has replaced the use of waste water lagoons in many instances. This approach offers at least the potential of vadose zone attenuation of waste loads. However, potential impact on groundwater must still be considered. Unfortunately, wide scale areal applications of liquid wastes present considerable difficulties in use of simple analytical models. This example therefore provides an example of the use of such models for a conservative, preliminary evaluation. Limitations of the technique employed are then discussed. This analysis may then shift the burden back to the permit applicant, who may need to demonstrate for instance that the vadose zone attenuation of the contaminant is sufficiently high to reduce the likelihood of violation of concentration standards at the perimeter of compliance.

In this case, wastewater is to be irrigated over a large area (3920400 sq. ft.) at an approximately constant and uniform rate of 0.005 gpd/ft^2. Surface runoff is minimized, and the unsaturated zone has an average thickness of 10 feet. Substantial degradation or attenuation of certain constituents is expected to occur in percolation through the unsaturated zone.

On entering the Advisory System we first employ the CHOICE algorithm. By using a circular recharge area approximation, this first estimates that the rate of head rise beneath the source is sufficiently small so that analytical methods based on confined aquifer assumptions may be employed. The area to be irrigated that is proposed in the application extends to within 50 ft. of the perimeter of compliance in the expected direction of flow. We may thus examine predicted impacts at the perimeter using a one-dimensional solution, given the assumption of vertical mixing. The CHOICE algorithm therefore recommends use of the model ODAST.

The wastewater to be irrigated contains a number of constituents of concern, and analysis may need to be undertaken for several of these. One of the constituents of concern is carbon tetrachloride, present in the irrigated waste water at a concentration of 10 ppm. This is a highly toxic substance of moderate mobility and known to

possess a small, but still significant rate of hydrolysis in groundwater.

The System first applies the HELP model, specifying only a single layer, to estimate the rate of percolation into the water table of the irrigated waste water plus precipitation. Default precipitation data is utilized from a station (Lumberton) about 25 miles distant, which is thought to provide a reasonable approximation of the (unmeasured) at-site precipitation. The source is to be maintained in a good grass cover to maximize evapotranspiration. The model ODAST is then applied in a Monte Carlo mode. Note that the input source concentration must be modified in ODAST to reflect the additional dilution of precipitation minus runoff and evapotranspiration.

In applying the model the hydrogeology is thought to be fairly well characterized (in terms of mean particle size and gradient) within certain bounds, and other hydrogeological parameters are generated from these distributions. The present analysis treats a two-year operating horizon only. The retardation coefficient has been rather arbitrarily set at 24.3 for the purposes of this example, and we do not intend to imply that this is necessarily a representative value for this constitutent. The in-aquifer decay constant is based on reported values of neutral hydrolysis of the constituent. This same value was used to automatically estimate a conservative rate of vadose zone attenuation, as no other documentation on this process was supplied. This results in estimation of essentially no vadose zone attenuation of the constituent, although the user should be aware that this results from complete disregard of processes of volatilization and biodegradation, and assumes that the constituent proceeds in pulses through the unsaturated zone at the maximum possible (saturated retarded) rate. We will return to consideration of these assumptions below.

Given these assumptions, the Monte Carlo application of ODAST suggests, as a preliminary estimate, that there is a probability of 89% of exceedance of a level of 0.1 ppm at the perimeter of compliance. The output of the system follows, with the cumulative probability plot shown as fig. IV-3.

```
[start of output file]
 State of North Carolina Groundwater Advisory System, Output File

 SITE NAME: Example One
 SITID = Exampl  FILES=  A:Exampl.OUT  A:Exampl.SIT
 COMMENT: Spray irrigation of waste, example.
 DATE ANALYSED: 7-11-1987
 ANALYST:  J. B. Butcher

Choice algorithm entered for model selection:
```

1. Wastewater Lagoon
2. Spray irrigation of wastewater
3. Land application of sludge
4. Individual Rotary distributor
5. Landfill

Option selected: 2

Source may be actively recharging a
surficial aquifer. We now estimate the long term head
rise (R) due to recharge using the Hantush method to
estimate the approximate degree of deformation of
the regional flow.

Estimation of mounding effect
assuming a circular recharge area
1.Recharge radius = 1117.1 ft
2.Rate of recharge = .50000E-02 gpd/sq ft
3.Hydraulic conductivity= .10000E-02 cm/sec
4.Storage coefficient = .20000
5.Initial saturated thickness = 50.000 ft
6.Time since start of recharge = 365.00 days
7.Initial depth to water table = 10.000 ft

Estimated head rise: 1.0739 ft (R/b= .021)

R/b < 5%. The flow can be modeled as
essentially non-radial and approximated by
confined solution methods.
2. Aquifer can be characterized as approximately
homogeneous and infinite in the region of
interest
1. Perimeter of interest is located close to the
edge of the source, so that the source can be treated
as approximately horizontally infinite.
1. Full penetration analysis adequate.
Model indicated:
ODAST

Entering HELP model

```
**********************************************************************
**********************************************************************
*                                                                    *
*      HYDROLOGIC EVALUATION OF LANDFILL PERFORMANCE                 *
*                        HELP VERSION 1                              *
*                                                                    *
*                          WRITTEN BY                                *
*                                                                    *
*                       PAUL R. SCHROEDER                            *
*                         AUGUST, 1983                               *
```

```
*                                                                     *
*                              OF THE                                 *
*                   WATER RESOURCES ENGINEERING GROUP                 *
*                       ENVIRONMENTAL LABORATORY                      *
*                   USAE WATERWAYS EXPERIMENT STATION                 *
*                            P.O. BOX 631                             *
*                          VICKSBURG, MS 39180                        *
*                                                                     *
***********************************************************************
*                                                                     *
*                   USER'S GUIDE AVAILABLE UPON REQUEST               *
*                   FOR CONSULTATION CONTACT AUTHORS AT               *
*                    (601) 634-3709 OR (601) 634-3710                 *
*                                                                     *
***********************************************************************
***********************************************************************
```

0.80210E-02 in/d added to precipitation to account for waste disposal.

Default data loaded: LUMB.HLP
Lumberton, N.C., 1963-82

****
****

Example One
Scotland Co., N.C.
7-11-1987

Design Data:

EXCELLENT GRASS

LAYER 1

VERTICAL PERCOLATION LAYER		
THICKNESS	=	120.00 INCHES
EVAPORATION COEFFICIENT	=	3.300 MM/DAY**0.5
POROSITY	=	.4010 VOL/VOL
FIELD CAPACITY	=	.1290 VOL/VOL
WILTING POINT	=	.0750 VOL/VOL
EFFECTIVE HYDRAULIC CONDUCTIVITY	=	5.00000000 INCHES/HR

GENERAL SIMULATION DATA

SCS RUNOFF CURVE NUMBER	=	25.00

TOTAL AREA OF COVER	=	3920400. SQ. FT
EVAPORATIVE ZONE DEPTH	=	18.00 INCHES
EFFECTIVE EVAPORATION COEFFICIENT	=	3.300 MM/DAY**0.5
UPPER LIMIT VEG. STORAGE	=	7.2180 INCHES
INITIAL VEG. STORAGE	=	1.8360 INCHES

MONTHLY MEAN TEMPERATURES, DEGREES FAHRENHEIT

JAN/JUL	FEB/AUG	MAR/SEP	APR/OCT	MAY/NOV	JUN/DEC
44.17	46.37	52.87	61.93	71.12	77.99
80.68	78.48	71.98	62.92	53.73	46.86

MONTHLY MEANS SOLAR RADIATION, LANGLEYS PER DAY

JAN/JUL	FEB/AUG	MAR/SEP	APR/OCT	MAY/NOV	JUN/DEC
222.37	283.95	374.71	470.33	545.19	579.23
563.33	501.75	410.99	315.37	240.51	206.47

LEAF AREA INDEX TABLE

DATE	LAI
1	.00
85	.00
108	1.84
130	3.00
153	3.00
175	3.00
198	3.00
220	3.00
243	2.70
265	1.96
288	.96
310	.50
366	.00

EXCELLENT GRASS

WINTER COVER FACTOR = 1.80

****

AVERAGE MONTHLY TOTALS FOR 1963 THROUGH 1982

	JAN/JUL	FEB/AUG	MAR/SEP	APR/OCT	MAY/NOV	JUN/DEC
PRECIPITATION	4.20	3.68	4.36	3.03	4.57	5.18
(INCHES)	5.61	5.75	4.08	3.58	2.62	3.48
RUNOFF	.000	.000	.000	.000	.000	.000
(INCHES)	.000	.000	.000	.000	.000	.000
EVAPOTRANSPIRATION	1.579	1.733	2.224	1.868	2.573	3.201
(INCHES)	3.319	3.202	1.980	1.557	1.282	1.400
PERCOLATION FROM BASE	2.5127	2.0831	2.2962	1.2026	2.0000	2.0287
BASE OF COVER (IN)	2.1787	2.5984	2.1322	1.8726	1.3973	1.9318
DRAINAGE FROM BASE OF	.000	.000	.000	.000	.000	.000
COVER (INCHES)	.000	.000	.000	.000	.000	.000

****

AVERAGE ANNUAL TOTALS FOR 1963 THROUGH 1982

	(INCHES)	(CU. FT.)	PERCENT
PRECIPITATION	50.15	16383800.	100.00
RUNOFF	.000	0.	.00
EVAPOTRANSPIRATION	25.917	8467093.	51.68
PERCOLATION FROM BASE OF COVER	24.23	7917351.	48.32
VAR. OF PERC. (IN/YR)	16.76	(FT3/YR) .1789E+13	
DRAINAGE FROM BASE OF COVER	.000	0.	.00

****
****

PEAK DAILY VALUES FOR 1963 THROUGH 1982

	(INCHES)	(CU. FT.)
PRECIPITATION	7.29	2381643.0

```
   RUNOFF                                .000              .0

   PERCOLATION FROM BASE OF COVER       4.3438       1419123.0

   DRAINAGE FROM BASE OF COVER           .000              .0

   HEAD ON BASE OF COVER                 .0

   SNOW WATER                            .00               .0

MAXIMUM VEG. SOIL WATER (VOL/VOL)        .1460

MINIMUM VEG. SOIL WATER (VOL/VOL)        .0750

**************************************************************************
**************************************************************************


 Calculation of conservative rate of attenuation
 of contaminant in vadose zone

 carbon tetrachloride
 DISPERSION COEFFICIENT ESTIMATED FROM VELOCITY

 HALF-LIFE:    .26660E+07 (days)
 LINEAR ADSORPTION COEF.:    23.300
 ATTENUATION ESTIMATED:    1.0000


 Application of analytical model ODAST


     Run #     1
     Monte Carlo application,    500 runs

     Time =    365.00      days
   MEAN SOURCE CONC.:    .29000      ppm (COEF. VAR.    .10000     )
   HALF LENGTH OF SOURCE:    609.60      (m)
   THICKNESS OF SATURATED ZONE:    15.240      (m)
   MEAN LEACHING RATE:    .12588E-01 (m/d ) (COEF. VAR.    .16900     )
   Dispersivities generated from velocity
   MEAN PARTICLE SIZE MAX:   .28000E-01
                      MIN:   .23000E-01 (cm - LOG 10 UNIFORM)
   GRADIENT: MOST LIKELY:    .50000E-02
             MINIMUM:    .40000E-02
             MAXIMUM:    .60000E-02
   SOURCE EFFECTIVE LENGTH:    603.50      (m)
   POROSITY:    .40100
   RETARDATION COEF:    24.300
   DECAY FACTOR OF SOURCE:    .00000      (1/day)
```

```
DECAY FACTOR OF SOLUTE:    .26000E-06 (1/day)
ATTENUATION FACTOR FOR VADOSE ZONE:    1.0000

  PARAMETER VALUES FOR THIS RUN
SOURCE CONC.:    .30377      (ppm)
LEACHING RATE:    .13092E-01 (m/d )
VELOCITY:    .67788      (m/day)
LONG. DISPERSIVITY:    1.0331      (m2/d)
TRANSV. DISPERSIVITY:    .34436      (m2/d)

  CONCENTRATION RESULTS

        Y AXIS (PERPENDICULAR TO FLOW)  (meters)
         .000
  X       ---------------------------------------
15.2    | .334E-01


  Time =    730.00      days
MEAN SOURCE CONC.:    .29000      ppm (COEF. VAR.    .10000     )
HALF LENGTH OF SOURCE:    609.60      (m)
THICKNESS OF SATURATED ZONE:    15.240      (m)
MEAN LEACHING RATE:    .12588E-01 (m/d ) (COEF. VAR.    .16900     )
Dispersivities generated from velocity
MEAN PARTICLE SIZE MAX:  .28000E-01
                   MIN:  .23000E-01 (cm - LOG 10 UNIFORM)
GRADIENT: MOST LIKELY:    .50000E-02
          MINIMUM:    .40000E-02
          MAXIMUM:    .60000E-02
SOURCE EFFECTIVE LENGTH:    603.50      (m)
POROSITY:    .40100
RETARDATION COEF:    24.300
DECAY FACTOR OF SOURCE:    .00000      (1/day)
DECAY FACTOR OF SOLUTE:    .26000E-06 (1/day)
ATTENUATION FACTOR FOR VADOSE ZONE:    1.0000

  PARAMETER VALUES FOR THIS RUN
SOURCE CONC.:    .30377      (ppm)
LEACHING RATE:    .13092E-01 (m/d )
VELOCITY:    .67788      (m/day)
LONG. DISPERSIVITY:    1.0331      (m2/d)
TRANSV. DISPERSIVITY:    .34436      (m2/d)

  CONCENTRATION RESULTS

        Y AXIS (PERPENDICULAR TO FLOW)  (meters)
         .000
  X       ---------------------------------------
15.2    | .149
```

```
  Run #  500
  Monte Carlo application,   500 runs

  Time =   365.00     days
MEAN SOURCE CONC.:   .29000     ppm (COEF. VAR.   .10000    )
HALF LENGTH OF SOURCE:   609.60     (m)
THICKNESS OF SATURATED ZONE:   15.240     (m)
MEAN LEACHING RATE:   .12588E-01 (m/d ) (COEF. VAR.   .16900    )
Dispersivities generated from velocity
MEAN PARTICLE SIZE MAX:  .28000E-01
                   MIN:  .23000E-01 (cm - LOG 10 UNIFORM)
GRADIENT: MOST LIKELY:   .50000E-02
          MINIMUM:   .40000E-02
          MAXIMUM:   .60000E-02
SOURCE EFFECTIVE LENGTH:   603.50     (m)
POROSITY:   .40100
RETARDATION COEF:   24.300
DECAY FACTOR OF SOURCE:   .00000     (1/day)
DECAY FACTOR OF SOLUTE:   .26000E-06 (1/day)
ATTENUATION FACTOR FOR VADOSE ZONE:   1.0000

  PARAMETER VALUES FOR THIS RUN
SOURCE CONC.:   .28613     (ppm)
LEACHING RATE:   .13765E-01 (m/d )
VELOCITY:   .61262     (m/day)
LONG. DISPERSIVITY:   .93364     (m2/d)
TRANSV. DISPERSIVITY:   .31121     (m2/d)

  CONCENTRATION RESULTS

        Y AXIS (PERPENDICULAR TO FLOW)  (meters)
         .000
  X       ---------------------------------------
15.2    | .225E-01



  Time =   730.00     days
MEAN SOURCE CONC.:   .29000     ppm (COEF. VAR.   .10000    )
HALF LENGTH OF SOURCE:   609.60     (m)
THICKNESS OF SATURATED ZONE:   15.240     (m)
MEAN LEACHING RATE:   .12588E-01 (m/d ) (COEF. VAR.   .16900    )
Dispersivities generated from velocity
MEAN PARTICLE SIZE MAX:  .28000E-01
                   MIN:  .23000E-01 (cm - LOG 10 UNIFORM)
GRADIENT: MOST LIKELY:   .50000E-02
          MINIMUM:   .40000E-02
          MAXIMUM:   .60000E-02
SOURCE EFFECTIVE LENGTH:   603.50     (m)
POROSITY:   .40100
RETARDATION COEF:   24.300
```

```
  DECAY FACTOR OF SOURCE:    .00000      (1/day)
  DECAY FACTOR OF SOLUTE:    .26000E-06 (1/day)
  ATTENUATION FACTOR FOR VADOSE ZONE:    1.0000

    PARAMETER VALUES FOR THIS RUN
  SOURCE CONC.:    .28613      (ppm)
  LEACHING RATE:    .13765E-01 (m/d )
  VELOCITY:    .61262      (m/day)
  LONG. DISPERSIVITY:    .93364      (m2/d)
  TRANSV. DISPERSIVITY:    .31121      (m2/d)

    CONCENTRATION RESULTS

          Y AXIS (PERPENDICULAR TO FLOW)  (meters)
           .000
    X       ---------------------------------------
 15.2     | .131


Example One

PROBLEM:          carbon tetrachloride

    STANDARD LEVEL:    .10000

 AT POINT  1 ESTIMATED PROB. EXCEEDANCE <=  .89134



PRELIMINARY REJECTION RECOMMENDED
PROBABILITY OF EXCEEDANCE OF STANDARD <=  .89134
FOR CONTAMINANT   carbon tetrachloride
[end of output file]
```

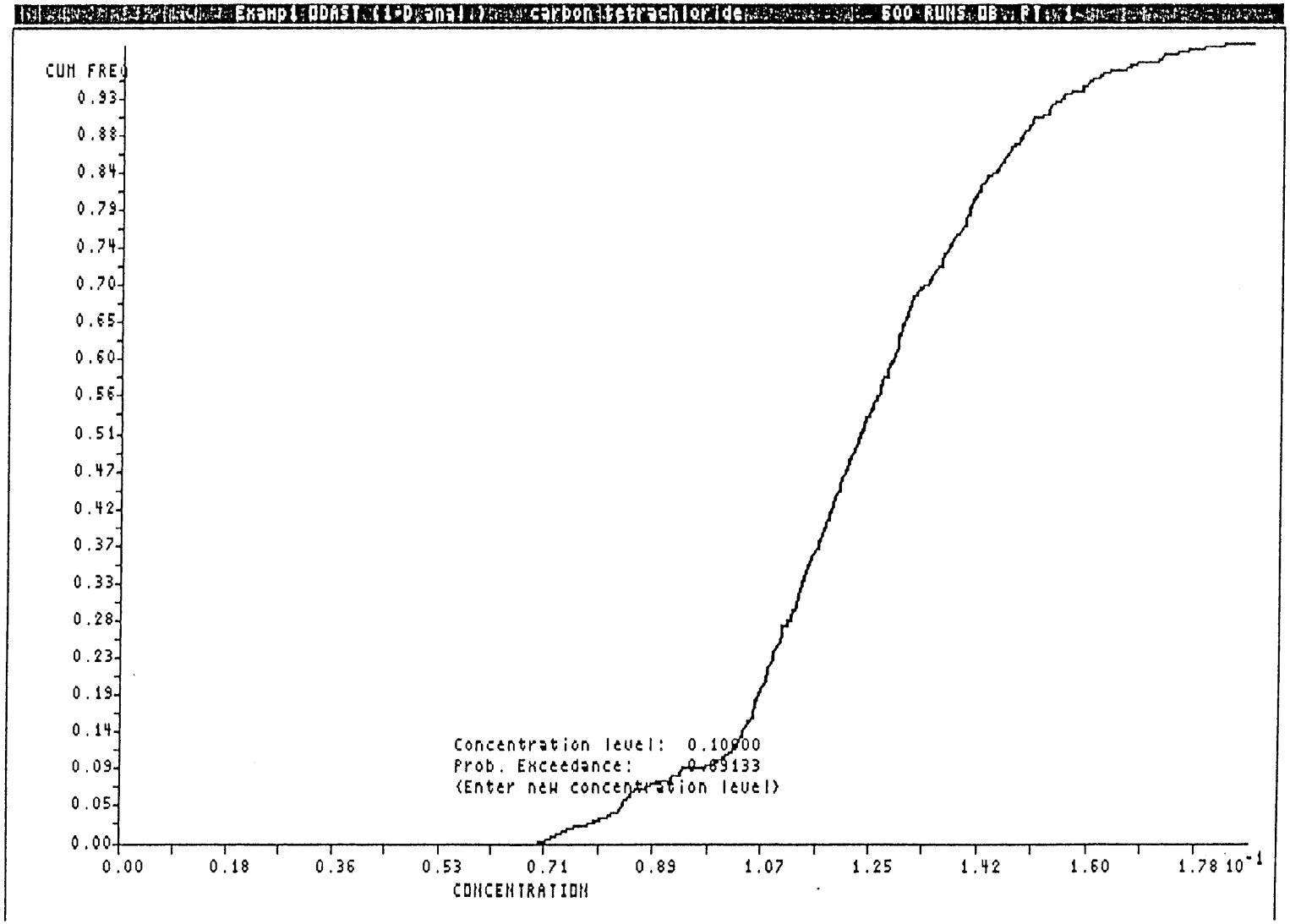

Figure IV-3. Cumulative Exceedance Probabilities For Example One

These preliminary results suggest that the site cannot be approved based on the presently available data, as there is a high predicted probability of exceedance of the standard. The simple-minded approach would be to recommend a greater setback from the perimeter of compliance, sufficient to result in a lower predicted probability of standard violation. However, the analyst should recognize the affects of certain conservative assumptions in the application of the model. He may then wish to notify the applicant that demonstrating that less conservative values are applicable in these areas may result in a reduction of the predicted probability of exceedance.

Leaving alone the question of the accuracy of the characterization of the hydrogeology, we note that a particularly important assumption in the analysis is the estimation of no vadose zone attenuation of the constituent. As emphasized previously, this is based on a very conservative estimate, which assumes that the flow proceeds through the unsaturated zone at saturated hydraulic conductivity, and that the only attenuation process available is the documented rate of hydrolysis. In actuality, the average residence time of the constituent in the unsaturated zone will be at least somewhat longer, and the constituent concentration may also be substantially attenuated by processes of volatilization and biodegradation, which have not been considered here. One approach would then be to shift responsibility to the applicant to provide justification as to why a higher degree of vadose zone attenuation may be applicable. This argument could be made on the basis of detailed modeling of unsaturated zone processes, or alternatively through empirical measurements of rate of attenuation of the constituent.

Another important conservative assumption is made in the way that ODAST attempts to calculate concentration at the edge of the source. Basically, ODAST, as implemented here, takes the total input load along a flow axis and dilutes this by the rate of regional flow to obtain a predicted concentration at the source edge. This assumption is conservative in that it does not allow for any degradation or attenuation of constituent loading traveling to the edge from areas upstream within the source. On the other hand, ODAST makes the non-conservative assumption that vertical mixing occurs. Thus in certain marginal circumstances full three-dimensional modeling of the source may be required.

4.3.2. Example Two: Hazardous Waste Landfill (EPAGW)

This example is designed to demonstrate application of the model EPAGW for preliminary analysis of a hazardous waste landfill in a situation in which there is little data available on hydrogeology surrounding the site. This proposed site is located in coastal North Carolina soil system 1 (Daniels et al., 1984). Applicant has provided detailed engineering information on the site, but little information

on the hydrogeology of the area, other than a topographic map. The site is not known to be near any distinct aquifer boundaries or discontinuities, and so the CHOICE algorithm recommends preliminary analysis with EPAGW. This model is specially designed for the assessment of contamination hazard risk under uncertainty.

To employ the model we first load the default parameter data set for soil system 1. Available topographic data enables us to modify this slightly, suggesting that the average hydraulic gradient is around 0.003. In addition, details provided with the engineering design suggest leaching from the landfill will proceed at a rate lying between 0.003 and 0.006 m/yr. The contaminant of interest is 1,1,1-trichloroethane. Concentration of this constituent in leachate is expected to be about 1000 ppm. However, this value is not very certain, so a standard deviation of 250 is applied to this value. A base hydrolysis rate of 0.964 year^{-1} and a log-10 octanol-water partition coefficient of 2.897 are assigned to the constituent based on data available in the tables. The landfill reaches a depth close to the water table, so no unsaturated zone attenuation is included. The output file then includes the following output from the model EPAGW (including fig. IV-4.):

```
[start of output file]
 State of North Carolina Groundwater Advisory System, Output File
     Analysis for:
 SITE NAME: Example Two
 SITID = EXAMP2  FILES=  C:EXAMP2.OUT  C:EXAMP2.SIT
 COMMENT: Hazardous waste landfill


 DATE ANALYSED: 7-12-1987
 ANALYST:  J. B. Butcher

 EPA MONTE CARLO GROUNDWATER MODEL

     PARAMETER DISTRIBUTIONS

  3. Diam.     Dist: 4; Params:   .36500E-01   .15000E-01
  4. Grad.     Dist: 6; Params:   .30000E-02
  5. FOC       Dist: 5; Params:  -5.7600       3.1700
  6. pH        Dist: 4; Params:   7.0000       1.2800
  7. GW temp   Dist: 2; Params:   15.000       22.000
  8. TH        Dist: 1; Params:   4.1150       .91400        30.480
  9. H         Dist: 2; Params:   2.0000       10.000
 10. QC        Dist: 2; Params:   .30000E-02   .60000E-02
 11. QD        Dist: 7; Params:
```

SITE/CHEMICAL PARAMETERS

```
 1 - CLM     (Value = 1000.0     )mean leach.con., mg/l
 2 - CLS     (Value = 250.00     ) std. dev. CLM
 3 - DKA0    (Value = .00000     ) acid hydrolysis
 4 - DKB0    (Value = .96400     ) base
 5 - DKN0    (Value = .00000     ) neutral
 6 - DKOW    (Value = 2.8970     )Log-10 octanol/water part
 7 - ATTN    (Value = 1.0000     )frac after atten
 8 - NPROB   (Value =         500)  # of MC runs
 9 - AW      (Value = 1000.0     ) landfill area m2
 10- T(ref)  (Value = 25.000     ) ref temp C
 11- XX      (Value = 200.00     ) distance, m
 12-         ( Subtitle C Used   )
          Leaching Rate Dist, C: engineered, D:unlined

  Pass =     1
ALFAL =  20.0000        ALFAT =  6.66667        ALFAZ =  1.93423
   AW =  1000.00        BAQFR =  8.62523          CD =  .671825E-05
 DKA0 =  .000000         DKB0 =  .964000        DKN0 =  .000000
  FOC =  .104237        HINIT =  8.49068      HSOURC =  4.31262
(-)PH = -7.39360         RHOB =  1.96302       SIGMA =  .100000E-02
    T =  293.684        THETA =  .259239          VW =  3214.29
   XX =  200.000        CLEACH = 970.683        CVERR =  .000000

  Pass =   500
ALFAL =  20.0000        ALFAT =  6.66667        ALFAZ =  .969141
   AW =  1000.00        BAQFR =  21.2357          CD =  .166519E-05
 DKA0 =  .000000         DKB0 =  .964000        DKN0 =  .000000
  FOC =  .202847E-02    HINIT =  2.22253      HSOURC =  2.22253
(-)PH = -4.40448         RHOB =  1.97232       SIGMA =  .100000E-02
    T =  291.231        THETA =  .255727          VW =  8608.97
   XX =  200.000        CLEACH = 1115.20        CVERR =  .000000

 EPA MCARLO GROUNDWATER MODEL

 PROBLEM:          trichloroethane

     STANDARD LEVEL:    .10000E-01

  AT POINT  1 ESTIMATED PROB. EXCEEDANCE <=  .17021E-01
[end of output file]
```

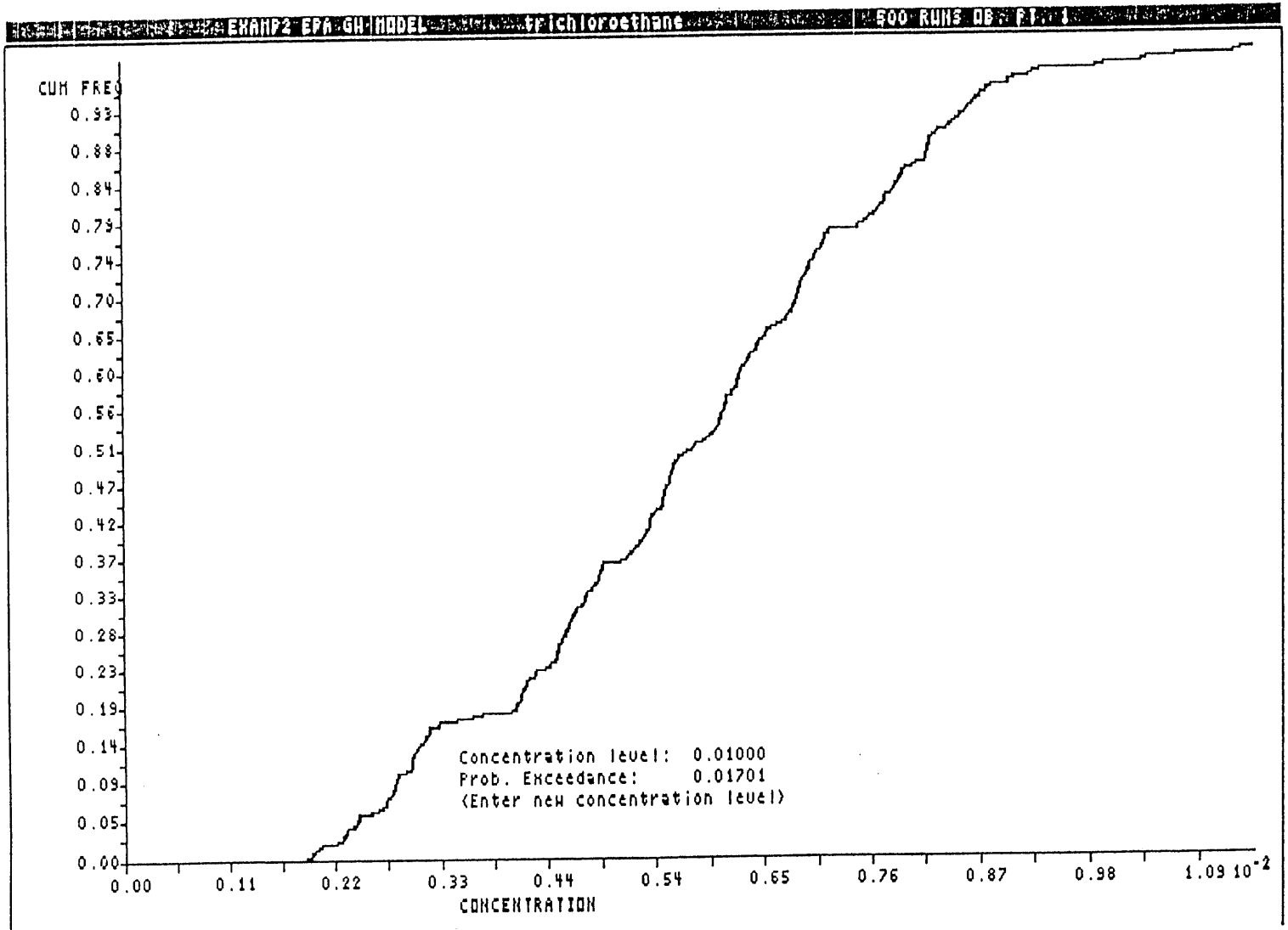

Figure IV-4. Cumulative Exceedance Probabilities For Example Two

Based on the preliminary analysis, the probability of exceedance of a standard of 0.01 ppm seems to be acceptably low (1.7%), but non-zero. However, use of the interactive facility of the plot shows that if the standard were lowered to 0.005 the probability of exceedance would be 63%.

The analyst should recall that this preliminary analysis is based on simulation over regional values, with little site-specific data. The results are thus representative of an average site location within soil system 1, but are not necessarily applicable to this specific site. That is, actual contamination at a specific site may differ from the average prediction if hydrogeologic conditions at that site are different from the average for soil system 1. Thus this preliminary analysis should not form a final basis for approval of a site if the contaminant is one of particular concern. Instead, the applicant should be requested to provide more data. At a minimum it would be desirable to have some site-specific data on mean particle size (which is used by EPAGW in the calculation of hydraulic conductivity distribution). This data would not be overly expensive to obtain, and should provide additional confidence in the predictions by EPAGW. Similarly, better information on water table gradient might be readily available from existing wells. Following receipt of this information, if reapplication of the model still provided an acceptably low estimate of probability of standard violation preliminary approval might be granted, with requirement of installation of a monitoring program. If, on the other hand, the probability of standard violation increased to a level at which a decision could not be safely made it would then be appropriate to request the permit applicant to provide sufficient data so that a detailed numerical model could be applied to the site.

4.3.3 Example Three: RESSQ Applied to a Wastewater Lagoon

This example demonstrates the use of the semianalytical model RESSQ for preliminary analysis of the probable effects of an unlined wastewater lagoon with a relatively high rate of recharge into the aquifer. There is a low rate of uniform regional flow, and the flow from the lagoon establishes a radial flow pattern in the aquifer. In addition, there are a number of relatively strong production wells in the region. The lagoon contains chlorides at a concentration of 1000 ppm. The objective of the study is to examine the potential impact on the production wells.

In this case no analytical solutions are available. However, the situation is well suited to the application of the semianalytical model RESSQ, which will enable us to establish the flow lines. Contaminant fronts are plotted through the lifetime of the lagoon, at 5, 10, 20 and 30 years. The output file follows, together with the flow-line plot (fig. IV-5).

[start of output file]
Model RESSQ

Contaminant studied: chlorides
Standard: 250.00

Example Three

PRACTICAL SYSTEM OF UNITS IS USED

REGIONAL FLOW, PORE VELOCITY	= 6.68	M/YR
ORIENTATION OF REGIONAL FLOW	= 40.00	DEGREES
THICKNESS OF THE AQUIFER	= 10.67	METERS
POROSITY	= 25.00	PERCENT
PERIOD STUDIED	= 250.00	YEARS
INITIAL AQUIFER CONCENTRATION	= 1.000E+01	ppm
DEFAULT INJECTION CONCENTRATION	= 1.000E+03	ppm
STREAMLINE STEP LENGTH	= 6.86	METERS
ADSORPTION CAPACITY OF ROCK	= .00	PERCENT

4 FRONTS ARE PLOTTED AT 5.000 YEARS 10.000 YEARS 20.000 YEARS 30.000 YEARS

20 INJECTION WELLS

WELL NAME	X METERS	Y METERS	FLOW-RATE M3/H	CONCENTRATION ppm	RADIUS METERS
ZQWELL- 1	-696.00	23.39	.00	1.00E+01	7.50E-02
ZQWELL- 2	-662.80	-16.22	.00	1.00E+01	7.50E-02
ZQWELL- 3	-629.60	-55.82	.00	1.00E+01	7.50E-02
ZQWELL- 4	-596.30	-95.43	.00	1.00E+01	7.50E-02
ZQWELL- 5	-563.10	-135.00	.00	1.00E+01	7.50E-02
ZQWELL- 6	-529.90	-174.60	.00	1.00E+01	7.50E-02
ZQWELL- 7	-496.60	-214.20	.00	1.00E+01	7.50E-02
ZQWELL- 8	-463.40	-253.90	.00	1.00E+01	7.50E-02
ZQWELL- 9	-430.20	-293.50	.00	1.00E+01	7.50E-02
ZQWELL-10	-396.90	-333.10	.00	1.00E+01	7.50E-02
ZQWELL-11	-363.70	-372.70	.00	1.00E+01	7.50E-02
ZQWELL-12	-330.50	-412.30	.00	1.00E+01	7.50E-02
ZQWELL-13	-297.20	-451.90	.00	1.00E+01	7.50E-02
ZQWELL-14	-264.00	-491.50	.00	1.00E+01	7.50E-02
ZQWELL-15	-230.80	-531.10	.00	1.00E+01	7.50E-02
ZQWELL-16	-197.50	-570.70	.00	1.00E+01	7.50E-02
ZQWELL-17	-164.30	-610.30	.00	1.00E+01	7.50E-02
ZQWELL-18	-131.10	-649.90	.00	1.00E+01	7.50E-02
ZQWELL-19	-97.83	-689.50	.00	1.00E+01	7.50E-02
Lagoon	-30.48	30.48	1.58	1.00E+03	4.57E+01

5 PRODUCTION WELLS

WELL NAME	X METERS	Y METERS	FLOW-RATE M3/H	RADIUS METERS	INDICATOR
prodwell1	243.80	457.20	.08	7.50E-02	0
prodwell2	365.80	-60.96	.16	7.50E-02	0
prodwell3	60.96	396.20	.32	7.50E-02	0
prodwell4	304.80	-91.44	.51	7.50E-02	0
prodwell5	762.00	.00	.51	7.50E-02	0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 1

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.2 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 2

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.1 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 3

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.3 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 4

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.9 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 5

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.0 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 6

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.4 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 7

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell3	131.9 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 8

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell3	136.4 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL- 9

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell4	134.2 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-10

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell4	111.0 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-11

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell4	101.1 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-12

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell4	95.7 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-13

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell4	93.8 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-14

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell2	102.0 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-15

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.3 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-16

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.6 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-17

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell5	146.3 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-18

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell5	141.0 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL ZQWELL-19

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	prodwell5	140.3 YEARS	.0

STREAMLINES DEPARTING FROM INJECTION WELL Lagoon

NUMBER OF STREAMLINE	WELL REACHED	TIME OF ARRIVAL	ANGLE BETA IN DEGREES
1	+++none+++	250.5 YEARS	42.0
2	+++none+++	250.2 YEARS	50.0
3	+++none+++	251.0 YEARS	58.0
4	+++none+++	250.8 YEARS	66.0
5	+++none+++	250.8 YEARS	74.0
6	+++none+++	250.9 YEARS	82.0
7	+++none+++	250.2 YEARS	90.0
8	prodwell1	45.8 YEARS	98.0
9	prodwell1	48.3 YEARS	106.0
10	+++none+++	251.0 YEARS	114.0
11	+++none+++	250.6 YEARS	122.0
12	+++none+++	250.4 YEARS	130.0
13	prodwell3	35.6 YEARS	138.0
14	prodwell3	35.9 YEARS	146.0
15	prodwell3	37.6 YEARS	154.0
16	prodwell3	40.2 YEARS	162.0
17	prodwell3	43.3 YEARS	170.0
18	prodwell3	47.0 YEARS	178.0
19	prodwell3	51.7 YEARS	186.0
20	prodwell3	57.9 YEARS	194.0
21	prodwell3	67.1 YEARS	202.0
22	prodwell3	90.4 YEARS	210.0
23	prodwell4	73.2 YEARS	218.0
24	prodwell4	63.6 YEARS	226.0

25	prodwell2	60.4	YEARS	234.0
26	prodwell2	53.6	YEARS	242.0
27	prodwell2	49.0	YEARS	250.0
28	prodwell2	45.7	YEARS	258.0
29	prodwell2	43.4	YEARS	266.0
30	prodwell2	43.4	YEARS	274.0
31	+++none+++	250.1	YEARS	282.0
32	+++none+++	250.1	YEARS	290.0
33	+++none+++	250.1	YEARS	298.0
34	+++none+++	250.6	YEARS	306.0
35	+++none+++	250.3	YEARS	314.0
36	+++none+++	250.1	YEARS	322.0
37	+++none+++	251.0	YEARS	330.0
38	+++none+++	250.0	YEARS	338.0
39	+++none+++	250.1	YEARS	346.0
40	+++none+++	250.2	YEARS	354.0
41	+++none+++	250.4	YEARS	2.0
42	+++none+++	250.7	YEARS	10.0
43	+++none+++	251.0	YEARS	18.0
44	+++none+++	250.4	YEARS	26.0
45	+++none+++	250.9	YEARS	34.0

EVOLUTION OF CONCENTRATION FOR PRODUCTION WELL prodwell1

TIME IN YEARS	CONCENTRATION IN ppm	(C-C0)/(CD-C0)
45.836	4.499E+02	.4444
48.342	8.899E+02	.8888

EVOLUTION OF CONCENTRATION FOR PRODUCTION WELL prodwell2

TIME IN YEARS	CONCENTRATION IN ppm	(C-C0)/(CD-C0)
43.413	4.500E+02	.4444
45.657	6.700E+02	.6667
49.046	8.900E+02	.8889
53.623	1.110E+03	1.1111
60.394	1.330E+03	1.3333
102.035	1.330E+03	1.3333

EVOLUTION OF CONCENTRATION FOR PRODUCTION WELL prodwell3

TIME IN YEARS	CONCENTRATION IN ppm	(C-C0)/(CD-C0)
35.584	1.200E+02	.1111
35.851	2.299E+02	.2222
37.649	3.399E+02	.3332
40.157	4.499E+02	.4443
43.287	5.598E+02	.5554
47.031	6.698E+02	.6665
51.697	7.798E+02	.7775

```
    57.861       8.897E+02          .8886
    67.121       9.997E+02          .9997
    90.442       1.110E+03         1.1108
   131.893       1.110E+03         1.1108
   136.368       1.110E+03         1.1108
EVOLUTION OF CONCENTRATION FOR PRODUCTION WELL prodwell4

   TIME IN     CONCENTRATION    (C-C0)/(CD-C0)
    YEARS       IN ppm

    63.598       7.768E+01          .0684
    73.173       1.454E+02          .1367
    93.838       1.454E+02          .1367
    95.737       1.454E+02          .1367
   101.128       1.454E+02          .1367
   110.994       1.454E+02          .1367
   134.196       1.454E+02          .1367
EVOLUTION OF CONCENTRATION FOR PRODUCTION WELL prodwell5

   TIME IN     CONCENTRATION    (C-C0)/(CD-C0)
    YEARS       IN ppm

   140.298       1.000E+01          .0000
   140.978       1.000E+01          .0000
   146.301       1.000E+01          .0000
[end of output file]
```

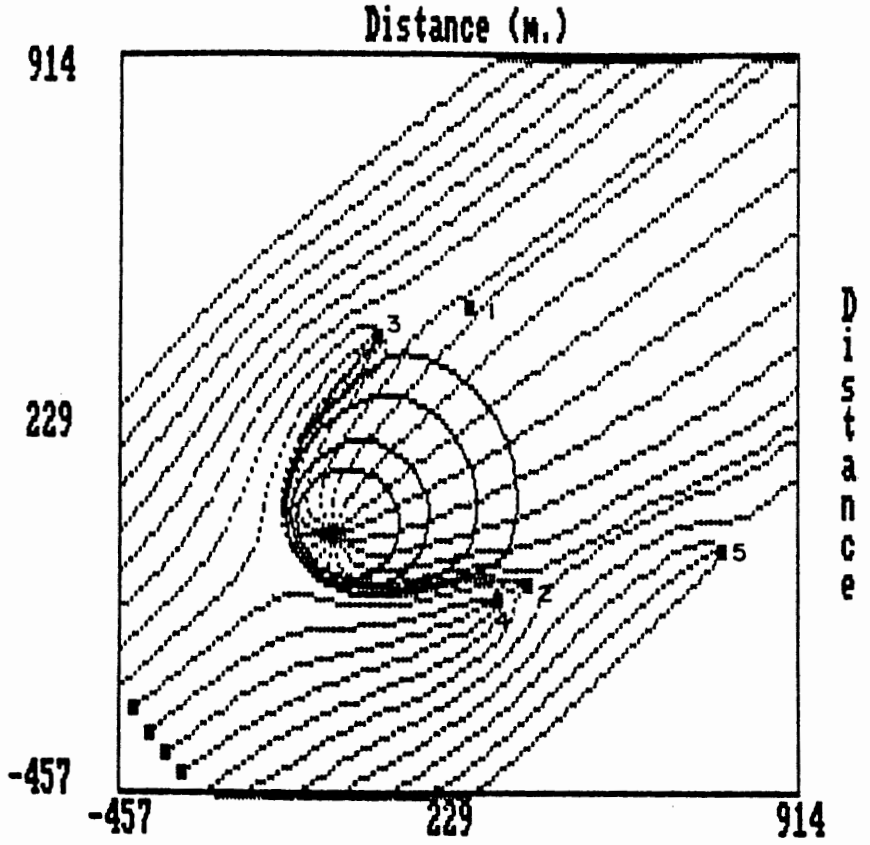

Figure IV-5. Streamline and Contaminant From Plot For Example Three

The analysis suggests that the advected contaminant will not begin to reach any of the production wells until 35 years from present. However, this does not mean that no concentration will be observed, as the model neglects the effects of dispersion.

The output also demonstrates one of the quirks of this model. Note that at production wells 1 and 2 the concentration is eventually predicted to exceed the input concentration. This is because concentration evolution is predicted on the basis of number of stream lines captured. This calculation can only be an approximation, because only a finite number of streamlines are plotted. Theoretically, the number of streamlines eventually captured by a production well with flow rate Q_p should be given by:

$$N_i \approx \frac{Q_p}{Q_i} \qquad (4.17)$$

where N_i is the number of streamlines from the production well and Q_i is the flow from the production well. However, this relationship can only hold exactly when Q_p/Q_i is an integer, which it is not in this case. Further, there are only a finite number of streamlines calculated, and there placement is somewhat arbitrary, which also has an effect on the prediction of capture. Results may be altered somewhat by respecification of BETA1, the angle at which the first streamline leaves the production well, and more accurate results should be obtained by specification of a larger number of streamlines.

4.3.4. Example Four: PLUM2D with Multiple Sources

This example demonstrates the use of the analytical model PLUM2D to handle multiple sources. In this case two extant sources are present in the area, being small solvent disposal pits which can be characterized as points and leach into the aquifer at a small enough rate so that distinct radial flow is not established. A third point source is to be added, and the objective is then to analyze the contamination probability given all three sources. PLUM2D can be used for this purpose, as it allows the specification of multiple point sources in operation for varying amounts of time.

For the analysis the model is first employed in a deterministic mode on a 20 by 10 grid, even though the hydrogeology is only moderately well characterized. This results in the 3-dimensional plot shown in fig. IV-6. Because there is uncertainty regarding the actual flow pattern this plot does not provide a final answer as to contamination risk. However, it does enable the analyst to identify the points on the perimeter of compliance where contamination appears likely. A full Monte Carlo analysis can then be employed to assess the risk of standard violation, given uncertain knowledge of the hydrogeology, at these points.

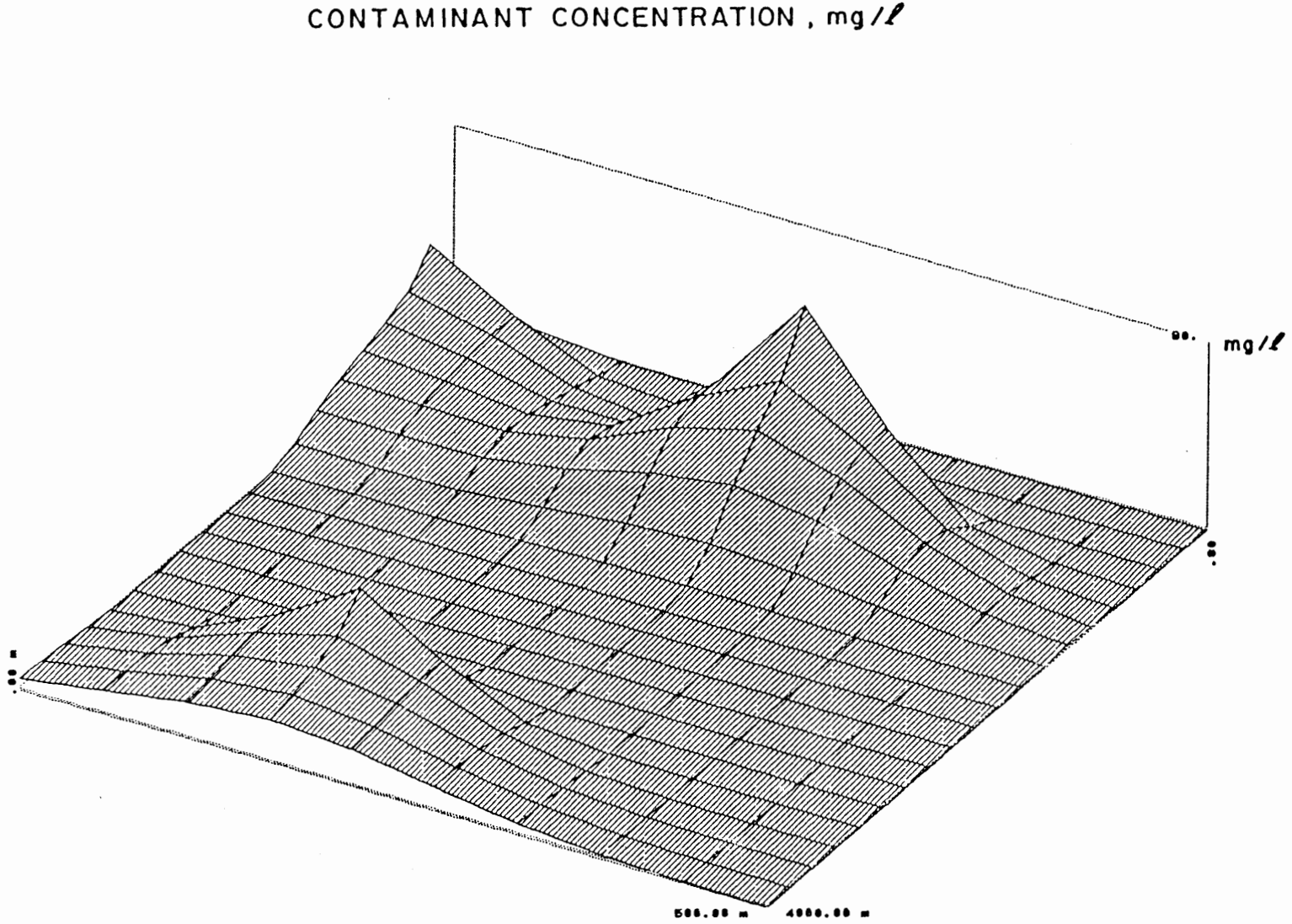

Figure IV-6. Three-dimensional Plot of Contaminant Plume For Example Four

CHAPTER V

TECHNICAL PROGRAMMING CONSIDERATIONS

5.1 DOS AND THE MICRO-COMPUTER ENVIRONMENT

This section (Chapter V) provides technical notes relative to the installation of the system and the method of programming. These notes are intended to be sufficiently detailed so that an experienced FORTRAN programmer would be able to readily extend or adapt the system.

Recent advances in the power and affordability of micro-computers have revolutionized the practice of groundwater pollution transport modeling. Now, all but the most complex groundwater models can be run on micro-computers (with expanded memory), freeing the user from reliance on mainframe computers. This increases the potential portability and availability of modeling systems, and the current system is designed with these goals in mind.

For maximum portability, the Advisory System is designed to run on micro-computers that emulate the IBM standard (IBM PCs and various clones). DOS (Disk Operating System) is the command system which controls operations of these types of computers. We have used MS-DOS Version 3 in the development of the system, but the system should be operational on any system that uses a DOS version 2.0 or higher. We have endeavored to develop the System, as far as possible, to run on any brand of micro-computer that operates under DOS, given sufficient available memory and the presence of a fixed disk drive.

Both DOS and availability of RAM memory limit the size of executable files to be used in the System. Because of this limitation, the System is designed in a modular fashion, and consists of many separate executable segments which are linked at the DOS command level through the use of batch files. The design of the Advisory System will be discussed in some detail below in section 5.3. First, however, we provide some notes on loading the Advisory System into your micro-computer.

5.2.LOADING THE ADVISORY SYSTEM

System Requirements

Operation of the Advisory System requires an IBM compatible micro-computer, operating under DOS, version 2.0 or higher. The system should be equipped with a fixed disk drive, onto which the system will be loaded, as well as a floppy disk drive. Because of the use of

several large text files it is not practical to run the system with floppy disk drives only. The system should ideally have 640 K RAM memory installed. It is possible to run most parts of the system with substantially less memory. However, certain component models, particularly HELP and MOC, will require the full 640 K. The version supplied also requires the presence of an 8087 math coprocessor. The capabilities of the 8087 are used to decrease execution CPU time. However, a version can also be supplied which does not require the 8087.

The system has been developed and tested using IBM PC-AT, IBM PC-XT and Zenith ZW-158 micro-computers, and utilizing various monitor and printer configurations. The system should also be usable on other systems compatible with the IBM Pc-AT or PC-XT.

In programming we have endeavored to provide flexibility in regard to screen monitor type. Standard implementation is an RGB color monitor with an IBM color graphics card. However, superior graphics are available if an EGA color monitor is used. The system is fully compatible with the EGA type monitor. However, the user may need to insure that an appropriate graphics printscreen utility is installed in order to be able to print graphics screens. The system may also be used with a high resolution monochrome monitor using a Hercules or compatible graphics card. This requires the installation of several alternate files, and an option for this installation is provided in the load procedure.

For use of the Advisory System, your micro-computer must be properly configured. The DOS file ANSI.SYS must be present in your root directory. Certain of the programs require a large number of concurrently open files. Therefore you should check to see that your root directory includes a file CONFIG.SYS, containing the following:

```
COUNTRY=001
buffers=17
FCBS=16,16
DEVICE=ANSI.SYS
FILES=16
```

The values for FCBS and FILES may be increased, but should not be decreased below 16.

Certain of the graphics files require the presence of the appropriate GSS Graphics Toolkit drivers. These will be installed in a special subdirectory called \DRIVERS\. An automatic installation routine is provided, which will also alter the CONFIG.SYS and AUTOEXEC.BAT files as needed. However, the GSS drivers are proprietary information, and the user should have a site license for their use. Therefore these drivers cannot be listed among the files which we distribute.

Loading the Advisory System

The advisory system is supplied as a collection of a large number of executable files, DOS batch files, data files and utility files. These currently occupy 10 double side, double density 5¼ inch floppy diskettes. The contents of these diskettes are intended to be loaded to a hard-disk drive. Loading is accomplished automatically by switching to the directory to be occupied by the advisory system, placing a load diskette in the A drive, and typing A:LOAD., then repeating for each of the seven diskettes. Certain options regarding your graphics hardware will be presented in the load process.

You will want to create a separate directory on the hard drive for the system. However, a PATH must be specified so that the system can access your DOS library. Entrance to the system is started by the file GW.BAT. Therefore you can readily create an access route to the advisory system from your main directory. For instance, if the system occupies a directory named \GWADV on drive D: you can create a batch file to initiate the system as follows:

```
D:
CD\GWADV
PATH=C:\dos;C:\;
GW
```

where for "C:\dos" you should substitute the name of the directory containing your DOS library, and "C:\" is the root directory.

Exit from the system is accomplished through the batch file Z.BAT, which also cancels the current screen attributes. You can modify this file to return control to your root directory or any other desired directory, and to configure the screen prompt as desired.

Catalogue of Executable and Data Files

The load disks should contain the following files (version 2.0):

Volume GWLOAD 1

GW	BAT	152	6-03-87	4:51p
B	BAT	175	2-16-87	5:10p
EPACM	BAT	349	5-18-87	10:58a
Z	BAT	28	2-16-87	10:35a
A	BAT	40	4-23-87	7:42p
M	BAT	62	6-16-86	1:17a
ERROR	MSG	568	8-19-85	12:12a
4X6	FON	285	2-25-85	3:50a
8X8	FON	2048	11-20-84	8:33p
GWEXP	EXE	54692	4-23-87	7:39p
LGRD	EXE	62374	4-23-87	8:19p
SCEN	EXE	52526	6-03-87	4:48p
MEN2	BOX	1987	9-24-86	5:31a
IP	BAT	71	6-03-87	4:38p

```
SFPLOT   COM    39390   7-08-86  12:34a
LOAD     BAT      620   6-01-87   2:39p
SFPLOTM  COM    39959   5-12-87  12:14a
Y        BAT      120   7-13-87  11:17a
MENU     BOX     1738   3-24-87   7:54p
MONO     BAT       31   6-01-87   2:39p
UPD      BAT     1023   4-08-87   9:00p
RESSQGR0 BAT      377   5-11-87  10:01p
RESSQGR  BAT      327   5-06-87   8:19a
R        BAT      177   3-22-87   7:07p
UPD      TXT     1031   7-09-87   9:00a

 Volume GWLOAD 2

EPAGW1   EXE   102790   7-13-87  12:56p
EPASF1   EXE   123420   7-13-87  10:12a
PREMOC3  EXE    86910   7-17-86   1:47a
EPASF2   DAT      891   3-31-87   9:31a
LOAD     BAT       17   6-01-87   2:40p
EPASF1   DAT      890   3-31-87   9:09a
EPASF3   DAT      886   3-31-87   9:31a
EPASF4   DAT      954   4-30-87  10:57a
GETNAM   EXE    25872   9-24-86   4:40a

 Volume GWLOAD 3

TRNCOV1  EXE    48014   6-18-86  12:11a
MOCMC    EXE   141336   7-17-86   2:36a
SCL2     EXE    21754   1-01-80  12:28a
SCL3     EXE    21770   1-01-80  12:29a
SCL4     EXE    23642   5-22-86   1:03a
LOAD     BAT       16   6-01-87   2:40p
PLUM2D   EXE    71754   6-08-87   6:39p

 Volume GWLOAD 4

EXAMPL   MOC     1019   6-29-94   1:00p
EXAMP2   MOC     1038   6-27-94   3:29p
PREMOCD  TXT   108240   7-21-86   2:25a
LOAD     BAT       16   6-01-87   2:41p
RECOM    EXE    44390   7-13-87  11:43a
CAN      EXE    24852   2-16-87  10:35a
GWEXP    TXT   119113   7-08-87  11:38a
SCROLL   EXE    27994   9-24-86   5:59a
P        BAT       89   9-24-86   4:42a
S        BAT       45   9-24-86   5:50a
D        BAT      319   9-25-86   3:28p
C        BAT       62   6-16-86   1:17a
SCL1     EXE    23642   5-21-86  12:06a
```

```
 Volume GWLOAD 5

HELP1     EXE   171450   5-29-87   9:32p
PSTHLP    EXE    44832   5-14-87   9:22p
TAPE8             2334   8-27-85   2:55a
TAPE12            1696   8-27-85   2:52a
LOAD      BAT       14   6-01-87   2:41p
ANAL      EXE   115144   7-13-87  10:09a
DEFCIT    HLP     1082   4-14-87   2:37p

 Volume GWLOAD 6

CHOICE    EXE    79374   7-13-87  12:00p
RESSQ     EXE    98508   5-04-87  12:47a
PRERES    EXE    68114   7-08-87  11:06a
RESSQGR   BAS     6332   7-09-87  10:39a
BASICA    COM    27520   3-07-85   1:43p
CNCPLTM   COM    39947   5-04-87  12:39a
LOAD      BAT       16   6-01-87   2:42p

 Volume GWLOAD 7

MONITOR   EXE    48332   5-28-87   8:39p
N         BAT       78   6-03-87   4:52p
REDO      BAT       47   5-18-87  11:00a
CUMFQ1    EXE    44564   7-13-87   1:46p
ANAL      HSC    12627   7-13-87   8:11p
GWP       BAT      123   4-23-87   7:13p
COMCHA    EXE    42228   5-18-87  11:24a
GETNAM2   EXE    27004   5-25-87   9:13p
Q         BAT       34   5-25-87   9:15p

 Volume GWLOAD 8

FXYPLT1   EXE   170418   6-22-87   4:57p
LOAD      BAT       16   6-01-87   2:38p
INSTALL   COM    53858   2-23-87  11:58a
INST      BAT      204   6-10-87   1:32a
AUTOEXEC  BAT      101   6-04-87   3:41p
AUTO2     BAT       55   6-04-87   3:41p
{ The GSS DRIVERS will also be required at this point.}

 Volume HELP DATA 1

ELIZ      HLP    52957   4-30-87  11:37a
FAYE      HLP    53698   4-30-87  11:38a
GREV      HLP    53695   4-30-87  11:44a
LUMB      HLP    53695   4-30-87  11:49a
HATT      HLP    53752   4-30-87  11:20a
CHAR      HLP    53695   4-30-87  11:57a
```

Volume HELP DATA 2

NEWB	HLP	53694	4-30-87	12:06p
RDUR	HLP	53763	4-14-87	3:01p
WILM	HLP	53750	4-14-87	3:04p
GREE	HLP	13792	4-14-87	2:07p
DEFCIT	HLP	1082	4-14-87	2:37p

5.3. MODULAR DESIGN OF THE ADVISORY SYSTEM

Concepts of Design

The total size of the files required in the system is now approaching 3 million bytes. For the System to be operational in a micro-computer environment only a small portion of the system can be loaded into memory at any one time. We have designed the Advisory System to overcome this limitation, while still preserving the appearance and "flow" of a single, integrated package. This is done through modular design. Only one executable module of the system is loaded at any one time. The current module is linked to the whole system through DOS batch files, while a special file structure is maintained for communication.

Batch Files

The individual executable files required in running the system are linked together at the DOS level. The linkage at this level requires maintenance of a special file system, which will be described below. Return through DOS level while the system is running will basically be invisible to the user, as the DOS prompt is masked as "Enter Selection ---->". At such points the user will be presented with a menu of options, distinguished by letters or brief names. Selection of one of these options results in the execution of a batch file (bearing the name of the option letter), which in turn will call the appropriate executable files in their proper sequence. However, the experienced user of the system may wish to recognize this disguised return to DOS command level, and can use it to his advantage if he wishes to issue other DOS commands or run utility programs at these points. In addition, certain DOS functions used with the system are hidden by temporarily setting screen color to black on black. The exit batch file, Z.BAT, restores the screen color and the prompt to their default values.

Because of this organization, additional branches are readily incorporated into the system. To do this, one need only add another item to the appropriate menu in the master text file, GWEXP.TXT, then write an appropriately named batch file to control the desired execution. In the execution of the early stages of the system, the menus are extracted from the file GWEXP.TXT and written as separate files

for later use. The batch file sequences should conclude with a TYPE command to redisplay the appropriate menu when command is returned to the (disguised) DOS level.

Access to most of the transport models is through one of two selection procedures, SCEN or CHOICE. In each of these procedures a file called MODEL.BAT is written by the procedure in accordance with the user's choices. Therefore, the batch files which have called either SCEN or CHOICE conclude by attempting to execute this newly created file, MODEL.BAT. If this file has not been created the menu is redisplayed.

Text Files

The system requires a large number of informational screens. Many, but not all of these, are maintained in separate direct access text files, which enables easy modification. These include:

GWEXP.TXT. This is the major text file for the system, and includes most of the menus and data-input screens for the various models. For ease of file maintenance this is maintained as two separate files, GWEXP1.TXT and GWEXP2.TXT, both of which are small enough to be edited using PC-WRITE or any other text editor with a 64 K limit. GWEXP.TXT can then be updated by using the command COPY GWEXP1.TXT+GWEXP2.TXT GWEXP.TXT.

PREMOCD.TXT. Input and help screens for the MOC model.

ANAL.HSC. Contains Help screens for the models ODAST, TDAST and DUPVG.

File Structure and Communications

As noted above, the system actually consists of a number of independent executable modules, linked at the DOS command level. To make these function as a whole communication is required between the various constituent models. This is accomplished through maintenance of a special file structure. In the course of a run of the system, analyzing a single site, three data files will be used, one specific to the run and two specific to the site. These are TEMP.DMP, {sitid}.SIT and {sitid}.OUT, where {sitid} is the code designation of the site. All three files will be created or located and updated upon entering the system, and must be present for the system to operate.

TEMP.DMP is a brief, direct access file (LRECL=80, FORM='FORMATTED') which keeps track of the current analysis, and informs the modules of the system of the site-specific names of the other two files. The first line of this file contains a number of status keys, which code various information relating to the analysis of the site.

These status keys are also stored in the {sitid}.SIT file. The file TEMP.DMP also allows the user to directly resume analysis of the last analyzed site.

{sitid}.OUT is an ordinary, sequential access file which records the results of all analyses of a site. Because this file can quickly grow to large size, an option is provided to dump this file to the printer and remove the current contents, in order to free disk space.

{sitid}.SIT is a direct access file (LRECL=80, FORM='FORMATTED') which primarily serves to preserve parameter values from each model run so that they can be reloaded for future applications on the same site. For some complex models, such as MOC, the parameter values are stored in a separate file which is however indexed by the SIT file. The status keys are also preserved here. The current allocation of space in the SIT file is as follows:

Line 1: Status keys (34I2).
Lines 2-4: Legrand model.
Lines 5-9: Chemical and site data for EPAGW1 and EPASF1.
Line 10: Reference to name of MOC data file.
Line 11: Rejection criteria: record of worst probability of standard exceedance noted for this site.
Line 12: Recommended next model choice.
Lines 13-19: Hydrogeological parameter set for EPAGW1 and EPASF1, together with distribution key (19).
Lines 21-28: Data for ANAL, which runs models ODAST, TDAST and DUPVG.
Line 29: Results of application of HELP model.
Lines 30-40: RESSQ data.
Lines 44-48: Data for ANAL, which runs models ODAST, TDAST and DUPVG.

The first line of both TEMP.DMP and {sitid}.SIT contain status keys, which record the process of the analysis. This consists of 34 integers, not all of which are presently in use. These have the following interpretations:

STAT(1): Type of previous analysis:
1. interrupted analysis.
2. reanalysis of previously analyzed site.
3. new analysis.

STAT(2): Type of current analysis:
1. interrupted analysis.
2. reanalysis of previously analyzed site.
3. new analysis.

STAT(3): Number of next screen to be displayed.

STAT(4): Initial level of previous analysis (level 0):
0. file creation only.
1. LeGrand, hydrogeology only.
2. LeGrand, full analysis.
3. proceeded to level 1.

STAT(5): General analysis result:
0. no result recorded.
1. accept.
2. indeterminate.
3. reject.

STAT(6): Last impact scenario choice:
1. Impact in groundwater, Monte Carlo risk analysis.
2. Impact in surface water, Monte Carlo risk analysis.
3. Impact through consumption of fish in contaminated surface water, Monte Carlo risk analysis.
4. Deterministic modeling.

STAT(7): Last model choice:
2. EPAGW1.
3. EPASF1.
4. PLUM2D.
5. MOC.
6. RESSQ.
7. TDAST.
8. ODAST.
9. DUPVG.
10. LTIRD.
11. PATH-S.

STAT(8): EPAGW1, site-chemical parameter set:
0. not applied.
1. analyzed, not saved.
2. analyzed, saved for future use.

STAT(9): EPASF1, site-chemical parameter set:
0. not analyzed.
1. analyzed, not saved.
2. analyzed, saved for future use.

STAT(10): last application of MOC model:
0. not applied.
1. deterministic mode.
2. Monte Carlo mode.

STAT(11): Sub-scenario choice:
0. Environmental standard.
1. Human exposure standard.

STAT(12): Last application of PLUM2d:
0. not applied.
1. deterministic mode.
2. Monte Carlo mode.

```
STAT(13): EPA models, hydrogeologic parameter set:
                0. not saved.
                1. saved.
STAT(14): PLUM2D parameter set:
                0. not saved.
                1. saved.
STAT(15): Use of HELP model:
                0. not used.
                1. Applied to this site.
STAT(16): Control for CHOICE model:
                0. Not used.
                1. Previously used, re-entry 1.
                2. Previously used, re-entry 2.
STAT(17): RESSQ data set:
                0. not saved.
                1. saved.
STAT(18): Site-type in CHOICE model:
                1. wastewater lagoon.
                2. spray irrigation.
                3. land application of sludge.
                4. rotary distributor.
                5. landfill.
                6. injection well.
                7. septic tank.
STAT(19): ANAL data set:
                0. not saved.
                1. saved.
STAT(20): LeGrand model data:
                0. not saved.
                1. saved.
STAT(21-33): Available for future use.
STAT(34): Temporarily used to turn on debug facility in certain
                models.
```

The general procedure upon entering one of the independent modules of the system is as follows:

1) Open file TEMP.DMP and read status keys and names of SIT and OUT file.
2) Open file {sitid}.SIT and temporary output file.
3) Open needed text files.
4) Determine sub-model choice, if needed, and whether application is in Monte Carlo or deterministic mode.
5) Determine sub-scenario choice STAT(11) and set factor to modify concentration calculations to CADI, if needed.
6) Determine if previous application has saved a data set which can be reloaded.
7) Input data as required.
8) Save data in {sitid}.SIT file if requested.
9) Run model. If in Monte Carlo mode output results to a file to be passed to the cumulative frequency plotter.

10) Copy temporary output file to end of {sitid}.OUT to form a sequential record of the analysis process. This temporary output file is also made available under the name MODEL.PRT for printing appropriate output data together with plots.

11) Proceed in accordance with instructions in controlling Batch file.

5.4 File Linkage Guide

In order to avoid limits on size of the executable file, the system is composed of a large number of smaller executable files. These in turn may be composed of a number of object files, each representing a source file. Modifications to the extant parts of the system may thus require modification of these source files, which must then be recompiled and linked. These are written in several programming languages.

FORTRAN files

The bulk of the system is programmed in Microsoft FORTRAN, version 3.3. Individual modules should be compiled with the $NOFLOATCALLS option specified at the beginning of the file. This enables the executable file to be compiled with or without use of the 8087 math coprocessor. In general, all executable files requiring extensive mathematical operations are presently compiled to take advantage of the increased speed of the 8087, but can readily be recompiled to function without the 8087. All files should be compiled using the /E switch to compress the size of the resulting executable file.

The FORTRAN executable files are linked as follows:

file name	linkage command	note
ANAL.EXE	LINK ANAL+ANAL2+EPASF4+RANS+ANSI+DUPVG+ATTN/E	1
CHOICE.EXE	LINK CHOICE+SCRNC/E	2
CUMFQ1.EXE	LINK CUMFQ1/E	1
EPASF1.EXE	LINK EPASF1+EPASF2+PARAM+EPASF3+EPASF4+SCRNC+ RAN+ATT/E	1
EPAGW1.EXE	LINK EPAGW1+PARAM+EPAGW2+RAN+SCRNC+ATT/E	1
FXYPLT1.EXE	LINK FXYPLT1+PLOT+MASK2,fxyplt1,fxyplt1, FORCGI.LIB+FORTRAN.LIB	4
GETNAM.EXE	LINK GETNAM/E	2
GETNAM2.EXE	LINK GETNAM2/E	2
GWEXP.EXE	LINK GWEXP+SCRNC/E	2
HELP1.EXE	LINK HELP1+HELP2+HELP3+HELP4+HELP5/E/SE:149	1,3
LGRD.EXE	LINK LGRD+SCRNC/E	2
MOCMC.EXE	LINK MOCMC+PARLOD3+SOLUTE+VELO3+MOVE3+CNCON3+RANS/E	1
PLUM2D.EXE	LINK PLUM2D+PLUM2D2+ANSI+RAN/E	1
PREMOC3.EXE	LINK PREMOC3+ANSI+IBMPCFIL/E	2

PRERES.EXE	LINK PRERES+ANS2/E	2
PSTHLP.EXE	LINK PSTHLP/E	1
RECOM.EXE	LINK RECOM/E	2
RESSQ.EXE	LINK RESSQ/E	1
SCEN.EXE	LINK SCEN+SCRNC/E	2
TRNCOV1.EXE	LINK TRNCOV1+RANS/E	1

Notes: 1). Recommended to link with 8087.LIB.
2). 8087.LIB not required.
3). The /SE:149 switch is required to increase available segments. The $LARGE option must be specified in the constituent FORTRAN files.
4) Must be linked with GSS FORCGI library first, which provides the graphics routines. To run, this program must have the proper graphics driver installed.

Other Executable Files:

Several files are currently written in Turbo PASCAL, and must be compiled using the Turbo PASCAL compiler, configured as appropriate to the graphics hardware present. For IBM graphics these are CNCPLT.PAS and SFPLOT.PAS, with corresponding mono graphics files CNCPLTM.PAS and SFPLOTM.PAS. Compiling these files requires the presence of the Turbo Graphix Toolbox system.

The file RESSQGR.BAS, supplied with the RESSQ package, is in uncompiled BASICA, and requires the presence of BASICA.COM, supplied on Load Disk 6. RESSQGR is currently not available for use on Hercules type monochrome graphics systems.

5.5 FUTURE DEVELOPMENT

It is our intent and hope that the Advisory System will continue to be improved and expanded. The modular design used in constructing the system should make this relatively easy to accomplish. It is of course to be expected that there will be minor bugs and cosmetic flaws in the presently implemented system (although we have endeavored to eliminate most of these), and future updates of the system should improve on what is already present. In addition, we intend to continue to incorporate additional transport models into the System, as needs and usefulness are identified.

We also conceive that there are several directions of major future development which should be pursued for the System. Most of these were outlined in the theoretical discussion given in Chapter 2. The user will note that the present Advisory System implements only a portion of the general algorithm given in Chapter 2. Other sections of this algorithm which remain to be implemented include:

- Detailed routines for compliance monitoring.

- Techniques of preposterior analysis for sampling recommendations.

- Development of a regional data base management system to operate in conjunction with the Advisory System.

We have pursued some development work in these areas, but the results are not yet ready for inclusion into the system.

A third important area for development includes the optimal methods of combining regional data based information with site-specific data in the analysis process, using techniques of Bayesian statistical analysis. Such methods are of great interest in the analysis of sites where there is considerable uncertainty concerning certain parameters at the site. They may be of particular importance in the ongoing analysis (compliance monitoring) of existing sites, where new data will be continually added.

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