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Quality Assurance and Quality Control in the Development and Application of Ground-Water Models

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QUALITY ASSURANCE AND QUALITY CONTROL IN THE DEVELOPMENT AND APPLICATION OF GROUND-WATER MODELS

by

Paul K.M. van der Heijde
International Ground Water Modeling Center
Institute for Ground-Water Research and Education
Colorado School of Mines
Golden, Colorado 80401

and

Osman A. Elnawawy
Indiana University/Purdue University at Indianapolis
Indianapolis, Indiana 46204

for

Holcomb Research Institute
Butler University
Indianapolis, Indiana 46208

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Project Officer

Joseph R. Williams
Extramural Activities and Assistance Division
Robert S. Kerr Environmental Research Laboratory
Ada, Oklahoma 74820

ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ADA, OKLAHOMA 74820

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FOREWORD

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This report describes quality assurance and code testing in ground-water modeling. The quality assurance procedures presented cover both development and application of ground-water modeling codes. An important part of quality assurance is code testing and performance evaluation. The section on code testing and performance evaluation discusses past efforts to test ground-water simulation codes and document their performance and presents the three-level testing procedure developed by the International Ground Water Modeling Center and the Center's approach to developing benchmarks for the first two test levels.

Clinton W. Hall

Clinton W. Hall
Director
Robert S. Kerr Environmental
Research Laboratory

ABSTRACT

This report provides background information on quality assurance and defines the role of quality assurance and quality control in ground-water modeling. A functional and practical quality-assurance methodology is presented which is written from the perspective of the model user and the decision-maker in need of technical information on which to base decisions. An important part of quality assurance is code testing and performance evaluation. A section is included on code testing and performance evaluation presenting the three-level testing procedure developed by the International Ground Water Modeling Center, the development of test problems and related benchmarks for the first two test levels, and a discussion of the implementation of the testing procedure.

BACKGROUND AND REPORT ORGANIZATION

This report describes part of the work performed by the International Ground Water Modeling Center (IGWMC) under a cooperative agreement with the U.S. Environmental Protection Agency entered into by the Center while at Holcomb Research Institute of Butler University, Indianapolis, Indiana. In line with IGWMC's goal to advance the utility of computer modeling in ground-water management, this project aimed at developing a comprehensive set of quality assurance procedures and code testing tools, and at promoting their widespread acceptance by the ground-water professional community.

The agreement included arrangements for IGWMC director Paul K.M.van der Heijde to participate in a special ground-water modeling committee of the Water Science and Technology Board of the National Research Council. The findings of this committee were reported in "Ground Water Models: Scientific and Regulatory Applications", published in 1990 by the National Academy Press, Washington, D.C. In addition, the agreement supported Paul van der Heijde's participation in the Ground Water Modeling Task Group D.18.21.10 of the American Society for Testing and Materials (ASTM).

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Paul K.M. van der Heijde
Golden, Colorado

CONTENTS

CONTENTS – continued

FIGURES

TABLES

1. INTRODUCTION

Ground-water modeling has become an important methodology in support of the planning and decision-making processes involved in ground-water management. The effective application of computer simulation codes in modeling field problems is a qualitative procedure, a combination of science and art. A successful model application requires a combination of knowledge of scientific principles, mathematical methods, and site characterization paired with expert insight in the modeling process, often to be provided within the framework of a multi-disciplinary team effort. As participants at the workshop on "Modeling for Water Management" organized by the European Institute for Water (Como, Italy, May 21-22, 1987) formulated: "Modeling imposes discipline by forcing all concerned to be explicit on goals, criteria, constraints, relevant processes, and parameter values."

Ground-water models provide an analytical framework for obtaining an understanding of the mechanisms and controls of ground-water systems and the processes that influence their quality, especially those caused by human intervention in such systems. For managers of water resources, models may provide essential support for planning and screening of alternative policies, regulations, and engineering designs affecting ground-water. This is particularly evident with respect to ground-water resources development, ground-water protection, and aquifer restoration.

Successful water management requires that decisions be based on the use of technically and scientifically sound data collection, information processing, and interpretation methods, and that these methods are properly integrated. As computer codes are essential building blocks of modeling-based management, it is crucial that before such codes are used as planning and decision-making tools, their credentials must be established, independently of their developers, through systematic testing and evaluation of the codes' characteristics. As is the case in the nuclear industry (Bryant and Wilburn, 1987), software applications in ground-water management have become too prominent for the codes to be developed and maintained in the informal atmosphere that was common in early ground-water modeling software development. Furthermore, the application of ground-water modeling codes to site-specific problems require adherence to systematic, comprehensive procedures and detailed reporting.

In discussing ground-water modeling distinction should be made between model development and model application. Model development consists of three components: (1) research aimed at obtaining a quantitative understanding of the studied ground-water system; (2) software development; and (3) model testing and evaluation. Often, model development, and particularly code development, is driven by immediate and long-term needs of ground-water resources management. Model application is part of a larger set of activities aimed at solving site- or problem-specific issues, and includes such activities as data collection, interpretation and storage, system conceptualization and model design, formulation of alternative problem-solving scenarios and engineering designs, and post-simulation analysis.

Although a consensus may exist as to what ground-water modeling entails, the definition of a "model" per se is somewhat nebulous. In hydrogeology, the term "ground-water model" has become synonymous with conceptual ground-water models, mathematical ground-water models (including analytical and numerical models), computer models, and simulation models. Furthermore, the term "ground-water model" may apply either to a computer code without site-specific data, or to the representation of a site-specific system using such a generic code, together with pertinent data.

In this report a **ground-water model** is defined as a non-unique, simplified, mathematical description of the subsurface component of a local or regional hydrologic system, coded in a computer programming language, together with a quantification of the simulated system in the form of boundary conditions, system and process parameters, and system stresses (van der Heijde *et al.* 1988). The **generalized computer code** usable for different site- or problem-specific simulations is referred to as a **(computer) simulation code** or a **generic simulation model**. A **ground-water modeling study** is defined as the development and use of a ground-water model (*i.e.*, code and data) to solve specific ground-water management problems. Sometimes, such a ground-water model is the result of the application of one or more simulation codes to a generalized ground-water management problem; *e.g.*, in support of promulgating government-mandated regulations. Generalizing such a management problem may be based on the use of concepts and data describing an "average" or "hypothetical" site representing targeted sites.

Sometimes, a model is described in terms of the mathematical solution technique employed. Most commonly used terms are "analytical model", "semi-analytical model", and "numerical model" (van der Heijde et al., 1988). An **analytical model** is a model in which the solution of the mathematical problem (governing equation and boundary conditions) results in a closed-form or analytical expression for the state variable, continuous in the space and time domains. In a **numerical model** a solution for the mathematical problem is found, discrete in both the space and time domains, by using numerical approximations of the governing partial differential equation(s). In a **semi-analytical model** complex analytical solutions are approximated by numerical techniques, resulting in a discrete solution in either the space or time domain.

Developing efficient and reliable software and applying such tools in ground-water management requires a number of steps, each of which should be taken conscientiously and reviewed carefully. Taking a systematic, well-defined and controlled approach to all steps of the model development and application process is essential for its successful utilization in management. Quality Assurance (QA) provides the mechanisms and framework to ensure that decisions are based on the best available data and (modeling-based) analyses.

The following sections provide background information on quality assurance and define the role of QA in ground-water modeling. They present a functional and practical quality-assurance methodology, written from the perspective of the model user and the decision-maker in need of technical information on which to base decisions. An important part of quality assurance is code testing and performance evaluation. The section on code testing and performance evaluation presents the three-level testing procedure developed by the International Ground Water Modeling Center, the development of test problems and related benchmarks for the first two test levels, and a discussion of the implementation of the testing procedure.

2. QUALITY ASSURANCE IN GROUND-WATER MODELING

2.1. QUALITY ASSURANCE DEFINITIONS

Quality assurance in ground-water modeling is the procedural and operational framework put in place by the organization managing the modeling study, to assure technically and scientifically adequate execution of all project tasks included in the study, and to assure that all modeling-based analysis is verifiable and defensible (Taylor, 1985). QA in ground-water modeling is crucial to both model development and model use and should be an integral part of project planning and be applied to all phases of the modeling process.

The two major elements of quality assurance are quality control (QC) and quality assessment. **Quality control** refers to the procedures that ensure the quality of the final product. These procedures include the use of appropriate methodology in developing and applying computer simulation codes, adequate verification and validation procedures, and proper usage of the selected methods and codes. To monitor the quality control procedures and to evaluate the quality of the studies, **quality assessment** is applied (van der Heijde, 1987).

Each project should have a **quality assurance plan** (QA plan), listing the measures planned to achieve the project's quality objectives (van der Heijde, 1989).

"Quality assurance" is a term used in many different disciplines and environments. Its meaning and implementation differs from field to field. For example, there is a significant difference between QA in software engineering, software quality assurance (SQA), and QA in industrial production (Bryant and Wilburn 1987). Also, there are significant differences between data QA (*e.g.*, EPA, 1986) and software QA procedures.

Many modeling studies are performed without adequate QA arrangements being in place. A formal QA plan, part of the overall project plan, is often lacking. QA assessment is frequently postponed until the project reaches its final stage (van der Heijde and Park, 1986). This is especially true for studies where models are applied to solve site-specific problems. However, when policy decisions, affecting large constituencies, are based on modeling assessments, both the simulation code used and its application are often subject to critical review before the study results are accepted. Increasingly, financial and criminal liability in ground-water contamination cases requires modelers to implement rigorous QA procedures in all stages of modeling projects.

2.2. QA IN MODEL DEVELOPMENT

2.2.1. Model Development Process

Model development is closely related to the scientific process of acquiring new, quantitative knowledge about nature through observation, hypothesizing, and verifying deduced relationships, resulting in the establishment of a credible theoretical framework for the observed phenomena. The fundamental understanding of a ground-water system thus is the product of research synthesized by theory.

The object of such research is a prototype natural system containing selected elements of a real world multi-element ground-water system. The selection of a particular prototype system for study is driven by management needs and the researcher's personal interest, and is influenced by the initial conceptualization of the integrated systems based on cursory sampling the real world (Figure 1). The conceptual model of the selected ground-water system forms the basis for determining the causal relationships among various components of the system and its environment. These relationships are defined mathematically, resulting in a mathematical model. If the solution of the mathematical equations is complex or when many repetitious calculations are required, the use of computers is essential. This requires the coding of the solution to the mathematical problem in a programming language, resulting in a computer code. The conceptual formulations, mathematical descriptions and the computer coding constitute the prototype model (Figure 1). Preparation of model documentation should be initialized during the formulation phase of the mathematical model, continued during the code design and program coding phases, and concluded after all other model development steps have been completed.

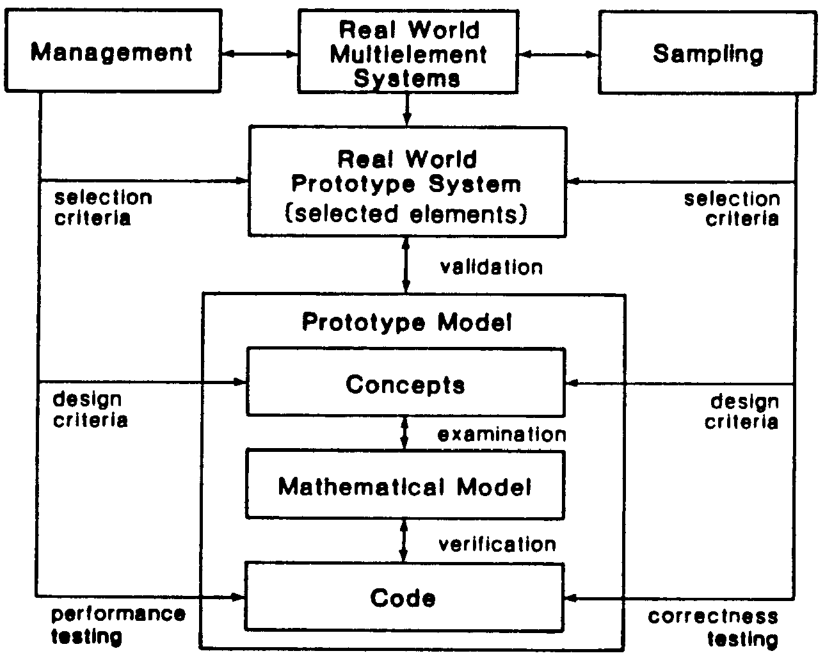


Figure 1. Model development concepts (van der Heijde *et al.*, 1988)

Before a ground-water model is used as a planning and decision-making tool, its credentials must be established through systematic testing of the model's correctness and evaluation of the model's performance characteristics. Of the two major approaches available, the evaluation or review process is rather qualitative in nature, while code testing results can be expressed using quantitative performance measures. Performance characteristics may be expressed in terms of reliability (*e.g.*, convergence and stability of solution algorithms, and absence of terminal failures), efficiency of coded algorithms (in terms of achieved numerical accuracy versus memory requirements and code execution time), and resources required for model setup (*e.g.*, input preparation time). Performance characteristics need to be determined for the full range of parameters and stresses the code is designed to simulate. Ground-water resource managers may be interested in further testing of a code to determine what the consequences are if such a code is used beyond its original design criteria, or beyond the range of applications for which it has already been tested. Through extensive and systematic code testing and model evaluation, confidence in the applicability of the code will increase.

Thus, **code testing** (or **code verification**) is aimed at detecting programming errors, testing embedded algorithms, and evaluating the operational characteristics of the code through its execution on carefully selected example test problems and test data sets. It is important to distinguish between code testing and model testing. Code testing is limited to establishing the correctness of the computer code with respect to the criteria and requirements for which it is designed (*e.g.*, to represent the mathematical model).

Model testing or **(prototype) model validation** is more inclusive (and often more eluding) than code testing, as it represents the final step in determining the validity of the quantitative relationships derived for the real-world prototype system the model is designed to simulate (Figure 1).

2.2.2. QA in Software Development and Maintenance

Software quality assurance (SQA) consists of the application of procedures, techniques, and tools throughout the software life cycle, to ensure that the products conform to pre-specified requirements (Bryant and Wilburn, 1987). This requires, that in the initial stage of the software development project, appropriate SQA procedures (*e.g.*, developing a QA plan, record keeping, establishing a project QA organization), techniques (*e.g.*, auditing, design inspection, code inspection, error-prone analysis, functional testing, logical testing, path testing, reviewing, walk-throughs), and tools (*e.g.*, text-editors, software debuggers, source code comparitors, language processors) need to be identified and the software design criteria be determined. Currently, many ground-water modeling codes have not been subject to such a rigorous SQA approach. Ideally, SQA should be applied to all codes currently in use and yet-to-be-developed codes, be it for either research or resource management.

The use of the software life cycle concept has proven successful in determining the QA requirements of the development, use, and operation of software (Bryant and Wilburn, 1987). The software development life cycle consists of three major phases: the initiation phase, the development phase, and the operation phase (NBS, 1976). According to this concept, the initiation phase is used to define the objectives and requirements for the software and to perform feasibility studies and cost-benefit analysis. In the development phase, software and documentation requirements are determined, program design formulated, and coding implemented and tested.

In the operation phase, the software is used for the purpose for which it has been designed. During this phase the software is maintained, evaluated regularly, and changed as additional requirements are identified. When maintenance is no longer justified (*e.g.*, because of changes in computer environments used, changes in operational requirements, or changes in software design objectives), the end of the software life cycle is reached, a situation applicable to many of the ground-water simulation codes developed in the 1970s. A detailed discussion of the QA requirements for each of these software life cycle phases is given by Bryant and Wilburn (1987).

The most important QA procedures in code development and maintenance are (van der Heijde, 1987):

- documentation of code design and code development;
- verification of program structure and coding;
- validation of complete software product (model validation; see Figure 1);
- documentation of code characteristics, capabilities and use;
- scientific and technical reviews;
- administrative auditing.

To evaluate ground-water modeling codes in a systematic and consistent manner, the International Ground Water Modeling Center (IGWMC) has formulated a model review, verification, and validation procedure (van der Heijde *et al.*, 1985). As part of this procedure, the IGWMC has developed a three-level code testing strategy (see section 3).

If any modifications are made to the simulation code, *e.g.*, to adapt the code for a specific application, the code should be tested again; all QA procedures for code development should again be applied, including record keeping, testing and reporting. The modified code should be test run, where applicable, with the test data sets with which the previous version was tested, and compared with the test results of that earlier version. All new input and output files should be saved for inspection and possible reuse.

2.2.3. Documentation of code design and code development

QA for code development and maintenance implies a systematic approach, starting with the careful formulation of code design objectives, criteria and standards, followed by an implementation strategy. The implementation strategy includes the design of the code structure and a description of the way in which software engineering principles will be applied to the code. In this planning stage, measures will be taken to ensure complete documentation of code design and implementation, record keeping of the coding process, description of purpose and structure of each code segment (functions, subroutines), and record-keeping of the code verification process. An integral part of the code development process is the preparation of user-oriented documentation.

The paper trail for QA in model development consists of reports and files on the development of the model and should include:

- report on the development of the code including the (standardized and approved) programmer's note book;
- verification report including verification (or validation) scenarios, parameter values, boundary conditions and initial conditions used and their source, verification results, and, if applicable, bench marks (data, coding, source);
- nature of the verification grid used, and grid design justification;
- changes and verification of changes made in code after baselining;
- in case of validation, a detailed description of the calibration procedure, if applied.

In addition, depending on the level of QA required, various files should be retained (in hard-copy and, at higher levels, in digital form) including:

- executable image and source code of baselined version of the code;
- input and output for each verification run;
- validation input and output.

2.2.4. Verification of Program Structure and Code

In software engineering, verification is the process of demonstrating consistency, completeness, and correctness of the software (Adrion *et al.*, 1986). ASTM (1984) defines verification as the examination of the numerical technique in the computer code to ascertain that it truly represents the conceptual model, and that there are no inherent problems with obtaining a solution.

In ground-water modeling, the objective of the **code verification** process is twofold: 1) to check the correctness and accuracy of the computational algorithms used to solve the governing equations, and 2) to assure that the computer code is fully operational.

To check the code for correct coding of theoretical principles, for code logic and for major programming errors ("bugs"), the code is run using specially designed problems. This approach to code testing allows for evaluation of reliability (*e.g.*, stability of solution algorithms, absence of terminal failures), efficiency of coded algorithms and internal and external data transfers (*e.g.*, code performance in terms of numerical accuracy versus time of computation, memory use and storage requirements), and the demand for code execution preparation resources (*e.g.*, input preparation time). A well-structured code allows for efficient testing of individual code segments, subroutines, functions and modules, as well as of the overall program structure. This stage of code testing is also used to evaluate the sensitivity of the code to grid design, to various dominant processes, and to a wide selection of parameter values (Huyakorn *et al.*, 1984a; Sykes *et al.*, 1983; Ward *et al.*, 1984; Gupta *et al.*, 1984).

At this point, it is necessary to make a distinction between generic simulation models based on an analytical solution of the governing equation(s) and models which include a numerical solution. Verification of a coded analytical solution is restricted to comparison with independently calculated results using the same mathematical expression, *i.e.*, manual calculations, comparison with the results from computer programs coded independently by third party programmers, or using general mathematical computer software systems such as Mathematica^{R} (Wolfram, 1991) and Mathcad$^{3.0;\ R}$ (Mathsoft, 1991). Verification of a code representing a numerical model might take two forms: (1) comparison with analytical solutions; and (2) code intercomparison between codes, representing the same generic simulation model, using synthetic data sets.

In a frequently used verification approach for numerical models, the test problem describes a system for which the stresses and parameters are defined in every point of the space and time domains, and the response of such a system is described by a closed-form solution to the governing partial differential equation (analytical solution; IGWMC test level 1; see section 3.4). The numerical model to be tested provides solutions to the same equation at a limited number of discrete points in space and time. Assuming that the coding is correct, the differences between the system responses described by the analytical solution and the numerical model are due primarily to the approximate nature of the numerical method involved and to the limitations in computer accuracy, and are generally not randomly distributed. In many instances, the magnitude of these differences is related to the resolution in the discretization used in the computational scheme (Lapidus and Pinder, 1982). Theoretically, if the resolution increases such that the spatial and temporal step sizes approach zero, the differences between the numerical and the closed-form solution should disappear.

It should be noted that, if a computer code implementation of the analytical solutions has been used in this type of testing, the resulting code should be subject to the same rigorous QA as the numerical model.

Although testing numerical models by comparing results for simplified situations with those of analytical models does not guarantee a fully debugged code, a well-selected set of problems ensures that the code's main program and most of its subroutines are being used in the testing, including all of the frequently called ones and those which might for certain sets of field parameters become critical to the code's computational performance. The effectiveness of a verification exercise can be further enhanced by using so-called walk-throughs, a step-by-step analysis of the computer program's operation using the data of the verification problem.

As part of the code verification process, hypothetical, highly simplified problems might be used to test special computational features that are not represented in simple, analytical models (IGWMC test level 2; see section 3.4). Specifically, this type of testing may be aimed at evaluating the code's performance in dealing with irregular boundaries, time varying stresses (sources/sinks), heterogeneity and anisotropy in aquifer properties, and grid orientation and geometry. Such hypothetical problems might be based on the features of a single field site or a generic mixture of features of various sites. The resulting data sets are referred to as **synthetic test data sets**.

The synthetic or hypothetical system used for such a test is defined by synthetic system parameters and system stresses and no independently observed system response is available. Therefore, testing takes place either by evaluating code behavior regarding such aspects as numerical consistency and stability, or by comparing the discretized predictions obtained with the numerical model tested with those obtained with another, preferably well-established, numerical model, using high-resolution spatial and temporal discretization schemes. As the absolute "truth" for these hypothetical problems is unknown, only a comparative verification of a model can be obtained. Using this approach provides a relative **benchmark**. This type of code verification is sometimes referred to as "benchmarking".

If the simulation results in such a code inter-comparison do not deviate significantly from each other, a "relative" or "comparative" validity is established (van der Heijde *et al.*, 1988). However, if significant differences occur, in-depth analysis of the results of simulation runs, performed with both codes, is called for.

The International Ground Water Modeling Center collects coded analytical solutions and two- and three-dimensional synthetic benchmarks for transient flow and solute transport in saturated and unsaturated porous media. Various well-established two- and three-dimensional models are used to derive the benchmark predictions. The design of the benchmark problems draws on known characteristics of the various numerical methods used in solving the linear and non-linear ground-water flow and transport equations.

Most ground-water simulation codes have been verified only with respect to certain segments of their coding, or for a subset of all the conditions they have been designed to simulate. In the past, very few codes have been subject to complete and systematic verification along the principles outlined above.

It should be noted that the code verification stage can (and should) be used to evaluate the operational characteristics of the code, such as the sensitivity of the code to grid design, to various dominant processes, and to a wide selection of parameter values.

Finally, the term "model verification" is sometimes used in conjunction with the calibration of a site-specific model (Anderson and Woessner, 1992; see section 2.3.4).

2.2.5. Model Validation

Much confusion has resulted from equating model validation with code validation and code verification. The term "validation" is defined according to the discipline in which it is used. In terms of software engineering, such as adopted by the National Bureau of Standards, code validation is defined as "the determination of the correctness of the final software product with respect to user needs and requirements" (Adrion *et al.*, 1986). In discussing standard practice for evaluating environmental fate models of chemicals, the American Society for Testing and Materials uses the definition that model validation "is the comparison of model results with numerical data independently derived from laboratory experiments or observations of the environment" (ASTM, 1984).

Van der Heijde (1987) defined the objective of ground-water **model validation** as determining how well a model's theoretical foundation and computer implementation describe actual system behavior in terms of the "degree of correlation" between calculated and independently observed cause-and-effect responses of the prototype real-world ground-water system for which the model has been developed. (Figure 1). This definition applies to a generic simulation model, not to a site-specific ground-water model, although a site-specific model is developed to accomplish validation.

The term "model validation" is also used in site-specific modeling. Anderson and Woessner (1992, p.6) argue that a site-specific model design and application protocol "builds support in demonstrating that a given site-specific model is capable of producing meaningful results, *i.e.*, that the model is valid". In their view the process of model validation encompasses the entire modeling protocol. Moreover, if a post-audit demonstrates that the site-specific model was accurate in its predictions, the model is considered "validated" for that site (Anderson and Woessner, 1992, p.9). They state that "because each site is unique, a model ideally should be validated for each site-specific application."

Various methods exist to quantify or describe qualitatively this degree of correlation (Koch and Link, 1980). It should be noted that the actual measured data of model input, system parameters and system response are samples of the real system and inherently incorporate errors. Thus, model validity established in this manner is always subjective (NRC, 1990).

An additional complexity is that often the data used for field validation are not collected directly from the field but are processed in an earlier study. Therefore, they are subject to inaccuracies, loss of information, interpretive bias, loss of precision, and transmission and processing errors, resulting in a general degradation of the data to be used in the validation process.

There has been some discussion regarding the role of calibration in the validation process. Some authors consider calibration a weaker form of validation, insofar as it tests the ability of the code (and the generic model) to fit the field data after careful adjustments of the physical parameters (Ward *et al.*, 1984). The justification for this viewpoint is that true validation is not possible due to the incompleteness of and uncertainty in the available system parameters and the uncertainty in the observed dependent variables.

The rigorous form of validation is based on model prediction without calibration. The system stresses and system parameters are assumed to be known, together with the system's responses to the stresses present. This approach is a test of the model's ability to fit the experimental data using modeling independent estimates of the parameters. In principle, this is the correct approach to validation. However, unavailability and inaccuracy of field data often prevent applying such a rigid validation approach to actual field systems. Typically, a part of the field data is designated as calibration data, and a calibrated site-model is obtained through reasonable adjustment of parameter values. Another part of the field data is designated as validation data; the calibrated site model is used in a predictive mode to simulate similar data for comparison. The quality of such a test is, therefore, determined by the extent to which the site model is "stressed beyond" the calibration data on which it is based (Ward *et al.* 1984).

From a user point-of-view determining the validity of a generic ground-water model relates to answering such questions as (Figure 1):

- Is the conceptual model valid for the prototype system it represents?
- Does the mathematical model truly represent the conceptual model, the processes involved, and the stresses present for the various design conditions?
- Does the code indeed represent the mathematical framework of the model?
- Will the model be able to truly represent the responses of the prototype system to the site-specific stress scenarios the user intends to investigate?

Therefore, complete model validation requires testing over the full range of conditions for which the model is designed. The development of generic models is an evolutionary process responding to new research results, developments in technology, and changes in user requirements. Model review and validation needs to follow this dynamic process and should be applied each time the model is modified.

For many types of ground-water models, the extensive high-quality data sets required for their validation are lacking. Furthermore, the data sets which are available are often limited with respect to the variety of conditions and stresses that occur in the sampled system. Therefore, testing of models is generally limited to verification, using existing analytical solutions and synthetic benchmarks, to code inter-comparison, and to in-depth post-audits of site-specific model applications (NRC 1990).

The first step in the validation process is the definition of the validation scenarios. Planning and conducting field validation should include the following steps (Hern *et al.*, 1985):

1. define data needs for validation and select an available data set or arrange for a site to study;
2. assess the data quality in terms of accuracy (measurement errors), precision, and completeness;
3. define model performance or acceptance criteria;
4. develop strategy for sensitivity analysis;
5. perform validation runs and compare model performance with established acceptance criteria;
6. document the validation exercise in detail.

Further development of databases for field validation of many types of ground-water models is necessary. These research databases should represent a wide variety of hydrogeological situations and ground-water protection problems, and should reflect the various types of flow, transport, and deformation mechanisms present in the field. The databases should also contain extensive information on hydrogeological, soil, geochemical, and climatological characteristics. With the development of such databases and the adoption of standard model-testing and validation procedures, the reliability of models used in field applications can be improved considerably.

It should be noted that absolute validity of a model does not exist. Whether a model is valid for a particular application can be assessed by applying predetermined performance criteria, sometimes called **validation or acceptance criteria**. If various uses in planning and decision making are foreseen, different performance criteria might be defined. The user should then carefully check the validity of the model for the intended use.

2.2.6. Verification and Validation Criteria

An important aspect of code verification and validation is the definition of informative and efficient measures for use as **evaluation or performance criteria**. Such measures need to characterize accuracy and stability of the solution derived with the numerical model over total space and time domains appropriate for the model, and for the full range of parameter values that might be encountered in the systems for which the model has been developed (van der Heijde, 1990).

Thus far, acceptance of verification and validation tests has been based primarily on visual inspection of graphical representation of the prediction variable for the code tested and the benchmark used (Figure 2). Such inspection, and for that matter, any set of quantitative measures to be derived, should involve the overall goodness-of-fit, including maximum deviation, average deviation, and spreading in deviation, both in absolute terms and relative to the value of the prediction variable. These measures should

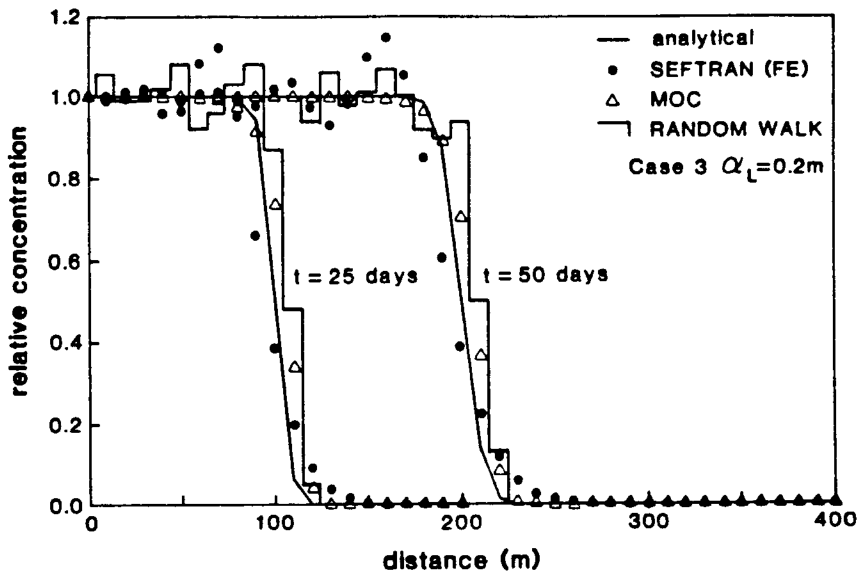


Figure 2. Example of a comparison between an analytical and various numerical solutions (from Beljin 1988).

be applied to both the time and space domains, and to both the full domains and representative parts of the domains. The measures should facilitate evaluation of the model's behavior for different spatial and temporal scales and resolutions, and should reveal oscillations and trends in the deviations of the concerned variable (Figure 3).

Most of the graphical goodness-of-fit determinations use single-dimension graphs, *e.g.*, head versus time or head versus distance. Thus far, multi-dimensional graphs have been used primarily in validation tests, *e.g.*, in the form of contoured deviations. Extending these multi-dimensional graphical techniques to the verification process might significantly enhance our ability to judge the goodness-of-fit (Figure 4).

Donigian and Rao (1986) listed three general procedures used to provide quantitative measures of performance for a code:

- paired -data performance -- the comparison of simulated and observed data for exact locations in time and space;
- time and space integrated, paired-data performance -- the comparison of spatially and temporally averaged simulated and observed data;
- frequency domain performance -- the comparison of simulated and observed frequency distributions.

They selected two statistical models to generate quantitative measures of performance for the ground-water codes under review: standard linear regression statistics estimation of error statistics.

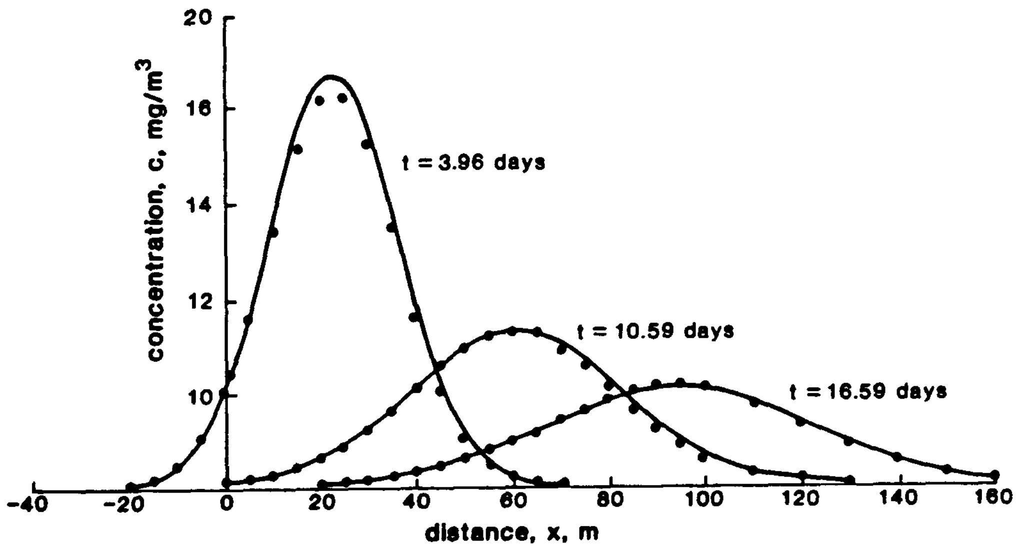


Figure 3. Example of close correspondence between the shape of analytical and numerical solutions over the spatial domain (from Huyakorn *et al.*, 1984a).

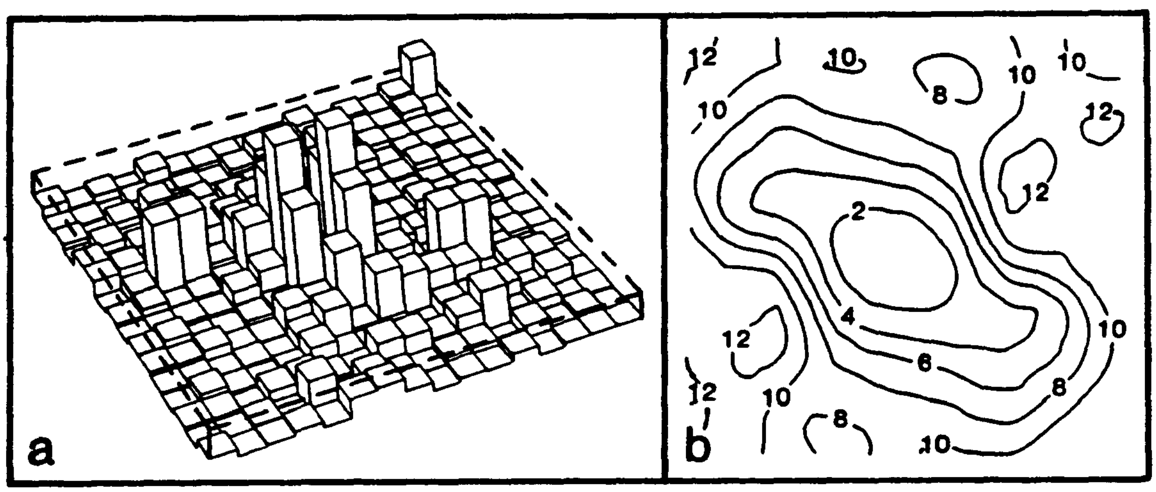


Figure 4. Graphical representations of two-dimensional verification deviations: a) block-diagram, b) contoured deviations.

Each of the three testing levels adopted by the IGWMC requires a different approach to the definition of these measures. At the first two levels of testing, the verification phase, statistical measures are improper, but statistical-like measures might prove useful. For example, ASTM (1984) presents expressions for a deviation coefficient DC, *e.g.*,

$$DC = [\ (x-y)/x\ ]\ 100\%$$

$$DC = \sum_{x=1}^{n} [\ (x_i-y_i)\ /\ x_i\ ]\ 100\%$$

where **x** = predicted value, **y** = measured value, and **n** = total number of computed deviations.

The third level of model testing, the field validation, is similar to the standard data fitting procedure, subject to statistical analysis, and thus open for description by statistical measures such as used by Donigian and Rao (1986).

2.2.7. Software Documentation

Computer code documentation can be defined as the information recorded during the design, development, and maintenance of computer applications as to explain pertinent aspects of a data processing system, including purposes, methods, logic, relationships, capabilities, and limitations (Gass, 1979). It is the principal instrument for those involved in a modeling effort, such as code developer, code maintenance staff, computer system operators and code users, to communicate regarding all aspects of the software. The main purposes of software documentation are given by Gass (1979) as:

- to record technical information that enables system and program changes to be made quickly and effectively;
- to enable programmers and system analysts, other than software originators, to use and to work on the programs;
- to assist the user in understanding what the program is about and what it can do;
- to increase program sharing potential;
- to facilitate auditing and verification of program operations, *i.e.*, code evaluation;
- to provide managers with information to review at significant developmental milestones so that they may determine that project requirements have been met and that resources should continue to be expended;
- to reduce the disruptive effects of personnel turnover;
- to facilitate understanding among managers, developers, programmers, operators, and users by providing information about maintenance, training, and changes in and operation of the software;
- to inform other potential users of the functions and capabilities of the software, so that they can determine whether it serves their needs.

Detailed guidelines for the preparation of comprehensive software documentation is given by the Federal Computer Performance Evaluation and Simulation Center (FEDSIM, 1981). This publication discusses the structure recommended for four types of manuals providing model information for managers, users, analysts, and programmers. According to FEDSIM (1981) the manager's summary manual should contain a model description, model development history, an experimentation report, and a discussion of current and future applications. Currently ASTM (American Society for Testing and Materials) is developing a standard ground-water code description for this specific purpose (Ritchey, 1992). The user's manual should consist of an extended model description, model input data description and format, type of output data provided, code execution preparation instructions, sample model runs, and a trouble-shooting guide. The programmer's manual should include model specifications, model description, flow charts, description of routines, data base description, source listing, and error messages. Finally, the analysts manual should present a functional description of the model, model input and output data, and code verification and validation information. The code itself should be well-structured and internally well-documented; where possible self-explanatory parameter, variable, subroutine and function names should be used.

Typically, ground-water modeling code documentation should include a description of the theoretical framework represented by the generic model on which the code is based, code structure and language standards applied, and code use instructions regarding model setup and code execution parameters.

Good documentation includes a complete treatment of the equations on which the generic model is based, of the underlying assumptions, of the boundary conditions that are incorporated in the model, of the method and algorithms used to solve the equations, and of the limiting conditions resulting from the chosen approach. The documentation must also include user's instructions for implementing and operating the code, and for preparing data files. It should present examples of model formulation (*e.g.*, grid design, assignment of boundary conditions), complete with input and output file descriptions, and include an extensive code verification and validation report. Finally, programmer-oriented documentation should provide instructions for code modification and maintenance.

While documentation should commence at the very beginning of a software development project, it is often left until the project is otherwise complete (Gass, 1979). This, in turn, makes documentation more difficult because it requires searching old records and fading memories. A frequently cited reason for incomplete documentation is that the model originally was a research tool and that it was subsequently elevated to forming the core of a policy evaluation.

2.2.8. Scientific and Technical Reviews

Generally, the complete scientific and technical review process is qualitative in nature and comprises (van der Heijde *et al.*, 1985; Bryant and Wilburn, 1987):

- examination of model concepts, governing equations, and algorithms chosen;

- evaluation of documentation and general ease-of-use;
- inspection of program structure and program logic;
- error-prone analysis;
- examination of the computer coding.

If verification or validation runs have been made, the review process should include evaluation of these processes.

To facilitate thorough review of the generic model, detailed documentation of the model and its developmental history is required, as is the availability of the source code for inspection. In addition, to ensure independent evaluation of the reproducibility of the verification and validation results, the computer code should be available or at least accessible for use by the reviewer, together with files containing the original test data used in the code's verification and validation.

Model development review should be performed by an experienced team consisting of at least a scientist knowledgeable in theoretical aspects of ground-water modeling and a software engineer. Increasingly, the theoretical framework of a model is so complex that review should be performed by a multi-disciplinary team (hydrodynamics, hydrogeology, geochemistry, contaminant chemistry, aquatic microbiology, and stochastic and numerical analysis) rather than by individuals. Because review is rather subjective in nature, selection of the reviewers is a sensitive and critical process.

Model Examination--

Model examination determines whether anything fundamental was omitted in the initial conceptualization of the prototype system. Such a procedure determines whether the concepts underlying the model adequately represent the nature of the system under study, and identifies the processes and actions pertinent to the model's intended use. The examination also determines whether the equations representing the various processes are valid within the range of the model's applicability, whether these equations conform mathematically to the intended range of the model's use, and whether the selected solution approach is the most appropriate. Finally, model examination determines the appropriateness of the selected initial and boundary conditions, and establishes the applicability range of the model.

For complex models, detailed examination of the implemented algorithms is required to determine whether appropriate numerical schemes have been adopted to represent the model. This step should disclose any inherent numerical problems such as non-uniqueness of the numerical solution, inadequate definition of numerical parameters, incorrect or non-optimal values used for these parameters, numerical dispersion, numerical instability such as oscillations or divergent solution, and problems regarding conservation of mass (ASTM, 1984).

In addition, the specific rules for proper application of the model should be analyzed from the perspective of its intended use. Examples of such rules are:

- data assignment according to node-centered or block-centered grid structure for the finite-difference method;

- size and shape of elements in the integrated finite-difference and finite-element methods;
- grid size variations;
- treatment of singularities such as wells;
- approach to vertical averaging in two-dimensional horizontal models or layered three-dimensional models;
- inclusion of approximate solutions in the analytical element method;
- treatment of boundary conditions.

Consideration is also given to the ease with which the mathematical equations, the solution procedures, and the final results can be physically interpreted.

Computer Code Inspection--

Part of the model review process is the inspection of the computer code. In this inspection attention is given to the manner in which modern programming principles have been applied with respect to code structure, compliance with programming standards, efficient use of programming languages, and internal documentation. This step might reveal undetected programming or logic errors, hard to detect in verification runs.

Evaluation of Generic Model Documentation--

Documentation of a generic model is evaluated through visual inspection, comparison with existing documentation standards and guidelines, and through its use as a guide in preparing for and performing verification and validation runs. A discussion of what constitutes good documentation has been presented in section 2.2.7.

Evaluating Ease of Use--

The data files provided by the model developer are used to evaluate the operation of the code and the user's guide through a test-run process. In this stage special attention is given to the rules and restrictions ("tricks"; *e.g.*, to overcome restrictions in applicability) necessary to operate the code, and to the code's ease-of-use aspects (van der Heijde and Beljin, 1988; see section 2.7.2.).

2.2.9. Post-Audits

An important role in determining the validity of a generic simulation model might be reserved for post-audits. Although post-audits are used primarily to determine the success rate of a model application, positive results of a well-executed post-audit analysis contribute to the acceptability of the model's predictive ability and may be considered as a form of code validation, even when used in conjunction with calibration (*e.g.*, Anderson and Woessner, 1992). To use post-audits successfully, conceptualization, assumptions, and system parameters and stresses should be evaluated, and if necessary, updated, and the model rerun to facilitate comparison of predictions with recent, observed system responses.

2.3. QA IN MODEL APPLICATION

2.3.1. QA Requirements in Model Application

The application of a generic simulation model to a site-specific problem is often called "model application" or "(computer/simulation) code application". The application of a generic model to site-specific conditions should follow a well-structured model application protocol. Such protocols are described by Mercer and Faust (1981), van der Heijde *et al.* (1988) and Anderson and Woessner (1992), among others. Quality assurance in this type of ground-water studies follows the same pattern as is discussed for generic model development projects and consists of using appropriate data, data analysis procedures, modeling methodology and technology, administrative procedures and auditing. It should be noted that, to a large extent, the quality of a modeling study is determined by the expertise of the modeling and quality assessment teams.

Quality assurance in code application addresses all facets of the modeling process, including such issues as:

- correct and clear formulation of problems to be solved;
- project description and objectives;
- type of modeling approach to the project;
- if modeling is the best available approach and if so, if the selected code is appropriate and cost-effective;
- conceptualization of system and processes, including hydrogeologic framework, boundary conditions, stresses, and controls ;
- detailed description of assumptions and simplifications, both explicit and implicit (to be subject to critical peer review);
- data acquisition and interpretation;
- code selection considerations, or justification for modifying an existing code or developing a new one;
- model preparation (parameter selection, data entry or reformatting, gridding);
- the validity of the parameter values used in the model application;
- protocols for parameter estimation and model calibration to provide guidance, especially for sensitive parameters;
- level of information in computer output (variables and parameters displayed; formats; layout);
- identification of calibration goals and evaluation of how well they have been met;
- the role of sensitivity analysis;
- post-simulation analysis (including verification of reasonableness of results, interpretation of results, uncertainty analysis, and the use of manual or automatic data processing techniques, as for contouring);
- establishment of appropriate performance targets (*e.g.*, 6-foot head error should

be compared with a 20-foot head gradient or drawdown, not with the 250-foot aquifer thickness!); these targets should recognize the limits of the data;

- presentation and documentation of results;
- evaluation of how closely the modeling results answer the questions raised by management.

QA for model application should include complete record-keeping of each step of the modeling process. The paper trail for QA should consist of reports and files addressing the following items:

- assumptions;
- parameter values and sources;
- boundary and initial conditions;
- nature of grid and grid design justification;
- changes and verification of changes made in code;
- actual input used;
- output of model runs and interpretation;
- validation (or at least calibration) of model.

As is the case with code development QA, all data files, source codes, and executable versions of computer software used in the modeling study should be retained for auditing or post-project re-use (in hard-copy and, at higher levels, in digital form) including:

- version of the source and executable image of the code used;
- calibration input and output;
- verification input and output;
- application input and output (*e.g.*, for each of the scenarios studied).

If any modifications are made to the code used in the modeling study, the code should be tested again according to a standard testing protocol; the code should be subject to the full QA procedure for code development, including accurate record keeping and reporting. All new input and output files should be saved for inspection and possible re-use together with existing files, records, codes, and data sets.

An increasing number of costly decisions are made in part based on the outcome of modeling studies. In the light of major differences noted in comparative studies on model application (*e.g.*, McLaughlin and Johnson, 1987; Freyberg, 1988) and the general lack of confidence in modeling results, effective quality assurance might go so far as to require that the analysis is done by at least two independent modeling teams. In that case, a third modeling team or a review panel should review and compare the results of both modeling efforts and assess the importance and nature of differences present.

A detailed discussion of QA aspects of particular modeling procedures is presented below.

2.3.2. Data Collection

An important (sometimes preliminary) step in a modeling project is data collection. Quality assurance in this stage of the project defines steps to be taken in the acquisition, review, collation, conversion and synthesis of technical data collected in preparation of model input, and for deriving preliminary technical conclusions.

Data received by the project team may be in one of many forms available and at different levels of applied review and documentation (QA). To assure traceability, records of receipt with information on source and description of documentation should be filed along with the original data sheets and files. During additional data processing, records of such actions and subsequent findings need to be kept. Examples of such data processing are unit conversions, contouring, node allocation, etc. A reviewer needs to be able to judge the conversions to be defensible. Record-keeping should include example calculations and conversions, and software references for data processing (*e.g.*, name of software, provider, version).

2.3.3. Model Formulation

In the model formulation or design stage attention is given to many aspects of the system and possible avenues of analysis. It includes system conceptualization (*i.e.*, definition of the hydrogeological framework, relevant processes and the boundary conditions present) and model conceptualization (*i.e.*, what does the project team consider justifiable in simplifying the system in a manner consistent with the objectives of the modeling study). QA in this stage requires documenting the analysis of all relevant issues such as: the interaction between ground-water and surface water; governing constitutive relationships and equations of state; determination of temporal scale (steady-state versus transient); if the system is saturated and/or unsaturated; the dimensionality of the model; boundary conditions; and the initial state of system.

After the decision to use a model has been made, an appropriate code is selected by matching a detailed description of the modeling needs with well-defined, quality-assured characteristics of existing codes, while taking into account the objectives of the study and the limitations in the personnel and material resources of the modeling team (van der Heijde, 1987). If a good match between model requirements and code characteristics cannot be found, releasing some of the matching criteria, modification of an existing code or the development of a new code may be considered. A separate section discusses in detail model selection procedures and emphasizes choosing QA codes.

In case a code is selected that has to be obtained from elsewhere, special care applies to the code transfer and implementation. Here, QA means evaluation of completeness of documentation and computer files, documenting transfer media formats, and filing of receipt notices and acceptance sign-offs.

One of the critical steps in applying a ground-water model is designing the grid (Mercer and Faust, 1981). Generally, the finer the grid the more accurate the solution. Various rules might apply to gridding process, dependent on the model selected (van der Heijde *et al.*, 1988). Examples are found in: 1) the location of grid nodes near or at wells or the center of well fields; 2) designing a fine grid where a high level of accuracy is important, where detailed analysis is required (resolution, not accuracy at issue), or where large changes in spatial characteristics occur (this might influence accuracy in other areas of model); and 3) aligning the grid axis with the principal directions of hydraulic conductivity or other anisotropic parameters. Other rules apply to particular methods, such as the treatment of irregular boundaries in finite-difference grids, and the use of small grid cells next to large elements etc.

Other considerations in the gridding process are:

- relationship between spatial scale and discretization;
- trade-offs between (relative) accuracy and discretization;
- the role of spatial averaging and aggregation in reaching project objectives;
- variant accuracy requirements in space and time.

The next step in model application is the preparation of an input file by assigning nodal or elemental values and other data pertinent to the execution of the selected computer code.

2.3.4. Model Calibration and Verification

Calibration is the process of adjusting model inputs until the resulting predictions give a reasonable good fit to observed data (NRC 1990). Most calibrations are performed under steady-state conditions, but may also involve a second calibration to a transient data set. Commonly, calibration is started with the best estimates of values for model input based on measurements and subsequent data analysis. The results of the initial simulations may be used to improve the concepts of the system or to modify the values of the parameters. The success of model calibration is dependent on the validity of the underlying model formulation; if the model's structure ignores important sources, geological heterogeneities, physical processes, or chemical reactions, parameter estimation and model calibration will be reduced to a fitting exercise that forces available inputs to compensate (usually inadequately) for a proper formulation (NRC 1990).

Often, more data may be needed during the calibration process. In some cases the code is used initially to design a data collection program. The newly collected data may be used both to improve the conceptualization of the system and to prepare for the predictive simulations.

Model inputs subject to modification during calibration include:

- constitutive coefficients and parameters (*e.g.*, hydraulic conductivity, dispersion coefficients and partition coefficients);
- forcing terms (*e.g.*, sources and sinks for water or contaminants);
- boundary conditions (specified heads, concentrations, and fluxes).

During calibration sensitivity analysis is performed to assist in identifying which elements of the model input are most critical to the outcome of the calibration procedure. The degree of allowable adjustment of any parameter is generally directly proportional to the uncertainty of its value or specification and limited to its expected range of values or confidence interval (Konikow and Patten, 1985).

Usually, the model is considered calibrated when it reproduces historical data within some acceptable level of accuracy, determined prior to the calibration exercise. It should be noted that a good fit to historical data does not guarantee good predictions, particularly if the historical fit is based on a small amount of data, or if it does not test the model capabilities that are required for making predictions (NRC 1990).

Calibration is often accomplished through a trial-and-error adjustment of the model input data. Because a large number of interrelated factors influence model output, this may become a highly subjective procedure (Konikow and Patten, 1985). Automatic parameter identification procedures may help to eliminate some of this subjectivity. The hydrological experience and judgment of the modeler continues to be a major factor in calibrating a model both accurately and efficiently.

An important QA aspect of calibration is the use of calibration targets (Anderson and Woessner 1992). For example, for flow, field-measured values of heads and fluxes (*e.g.*, base flow, spring flow, infiltration from a losing stream, and evapotranspiration from the water table) form the *sample information* or *calibration values*. The calibration value with its associated error forms the *calibration target*, which should be determined before calibrating the model. The associated error might consist of:

- measurement error
- scaling error (representativeness of measurement for model variable)
- interpolation error (from transferring measured information to nodal values)

Additional calibration information for a flow model can be obtained from velocities and solute distributions. Such additional calibration information might increase the likelihood to obtain a "unique" solution (NRC, 1990).

Calibration measures commonly used may be qualitative or quantitative in nature. Qualitative measures of calibration progress may be based on:

- comparison between contour maps of measured and simulated variable, providing information on the spatial distribution of the error;
- contouring the calibration error (residuals);
- graphic representation of calibration error per cell or element (comparable to a three-dimensional bar-graph);
- scatterplot of measured versus simulated variables; deviation of points from the straight line should be randomly distributed (might include confidence intervals for the linear regression);

- tabulation of measured and simulated variables, and their deviations for each node.

Quantitative measures, often referred to as *calibration criteria*, include (Anderson and Woessner 1992):

- The *mean error (ME)* is the mean difference between measured heads and simulated heads:

$$ME = \frac{1}{n}\sum_{i=1}^{n} (h_m - h_s)_i$$

  with n the number of calibration values. The ME can be represented in a graph against various values of the calibrated parameter. Both negative and positive differences are incorporated in the ME and may cancel out each other.

- The *mean absolute error (MAE)* is the mean absolute value of the differences in measured and simulated heads:

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |(h_m - h_s)_i|$$

- The *root mean squared (RMS) error* or the *standard deviation* is the average of the squared differences in measured and simulated heads:

$$RMS = [\frac{1}{n}\sum_{i=1}^{n} (h_m - h_s)_i^2]^{0.5}$$

An overall assessment of the success of calibration may be expressed using *calibration levels* (Anderson and Woessner 1992):

level 1: simulated value falls with target (highest degree of calibration);
level 2: simulated value falls within two times the associated error of the calibration target;
level 3: simulated value falls within three times the associated error of the calibration target;
level n: simulated value falls within *n* times the associated error of the calibration target (lowest degree of calibration).

As the set of parameters used in the calibrated model may not accurately represent field values, the calibrated parameters may not represent the system under a different set of boundary conditions or hydrologic stresses. **Model verification** will help establish greater confidence in the calibration and the predictive capabilities of the calibrated model (Anderson and Woessner, 1992).

A site-specific model is considered "verified" if its accuracy and predictive capability have been proven to lie within acceptable limits of error by tests independent of the calibration data. In general, model verification is performed using a transient data set, *e.g.*, the response of heads to drought or long-term pumping. If only a single time-series is available, the series may be split in two sub-series, one for calibration (*e.g.*, representing the response of the system to natural cyclic variations in stress), and another for verification (*e.g.*, representing the response of the system to a significant changed stress condition such as caused by irrigation development). If such data are not available, verification may be performed using a second "independent" steady-state data set (*i.e.*, not used previously for calibration). If the parameters are changed during the verification, this exercise becomes a second calibration and the first calibration needs to be repeated to account for the changes. The second exercise cannot be considered "verification" anymore.

From a QA point of view, adherence to a well-defined model calibration procedure is critical. Reporting should include description of calibration targets, measures of calibration, calibrated variables, calibration assessment (*i.e.*, comparing calibration measures with calibration targets according to an established classification and evaluation of reasonableness of calibrated variables), and if performed, model verification results.

2.3.5. Sensitivity Analysis

An important characteristic of a model is its sensitivity to variations or uncertainty in input parameters. Sensitivity analysis is used to identify those parameters most influential in determining the accuracy and precision of model predictions. This information is of importance to the user, as he must establish required accuracy and precision in the model application as a function of data quantity and quality (Hern, *et al.* 1985). Sensitivity analysis defines quantitatively or semi-quantitatively the dependence of a selected model performance assessment measure (or an intermediate variable) on a specific parameter or set of parameters (Intera, 1983). Sensitivity analysis can also be used to decide how to simplify the simulation model (*e.g.*, processes involved, dimensionality, spatial and temporal variability, boundary conditions, etc.) and to improve the efficiency of the calibration process.

Model sensitivity can be expressed as the relative rate of change of selected output caused by a unit change in the input. If the change in the input causes a large change in the output, the model is sensitive to that input. Sensitivity analysis methods are mostly non-statistical, or even intuitive in nature. In this context the use of a sensitivity index as described by Fjeld et al. (1987) is of interest.

Sensitivity analysis is typically performed by changing one input parameter at a time and evaluating the effects on the distribution of a dependent variable, *e.g.*, hydraulic head. Nominal, minimum, and maximum values for the selected input parameter are specified. The distribution of the dependent variable is determined for its nominal value, resulting in C_t^{nom}. The minimum and maximum values of a given parameter are then substituted for its nominal value, yielding bounds on the dependent variable, *i.e.*, C_t^{pmin} corresponding to the minimum value of parameter p, and C_t^{pmax} corresponding to the maximum value of parameter p. The sensitivity index S_t may be defined as (Fjeld et al. 1987):

$$S_t = \frac{C_t - C_t^{nom}}{C_{nom}^{max}}$$

where C_t is either C_t^{pmin} or C_t^{pmax}. C_{max}^{nom} is the maximum instantaneous value of the dependent variable based upon nominal values of the parameter (*i.e.*, the nominal value of the dependent variable at the maximum time).

It should be noted that if models are coupled, as in multimedia transport of contaminants, the propagation of errors and the increase in uncertainty through the subsequent simulations must be analyzed as part of the sensitivity analysis.

Although a detailed sensitivity analysis can be laborious and time-consuming, it is usually feasible to carry out a small scale exploratory analysis that focuses on a few critical inputs identified, most likely by intuition. Sensitivity analysis should be performed initially at the beginning of calibration to design a calibration strategy. After the calibration is completed a more elaborate sensitivity analysis is performed to quantify the uncertainty in the calibrated model caused by uncertainty in the estimates of aquifer parameters, stresses, and boundary conditions.

Well-documented sensitivity analysis provides reviewers an excellent opportunity to evaluate many aspects of the simulations performed during the scenario analysis stage. Therefore, results of a sensitivity analysis should be qualitatively discussed (Anderson and Woessner 1992).

2.3.6. Scenario Analysis

The main objective of most model applications is scenario analysis and subsequent screening of the proposed alternative scenarios in support of management's decision-making. Therefore, the scenario analysis step should be carefully executed and extensively documented. Important elements of such documentation include code execution options used, a complete set of input data (type, format), and an overview of the immediate (non-manipulated or -postprocessed) results of the simulations.

2.3.7. Interpretation and Presentation of Results

QA in this stage includes inspection of the form of the results, and of the meaning and reasonableness of computational results and post-simulation analysis. Performing control calculations and post-simulation validation (see post-audits) of predictions are major means in the QA framework.

It should be noted that there is a significant difference between validation of the predictions made with deterministic models and those obtained with stochastic models. The validation of mathematical models for uncertainty analysis, *e.g.*, in performance assessment, must confirm the probability distribution calculations for each scenario evaluated. The calculated probabilities predict the behavior of the scenario performance measure, that would result if the governing parameters are allowed to vary within the range of plausible values (Brandstetter and Buxton, 1987). Re-sampling studies must be conducted by repeatedly and randomly selecting parameter values from a range of plausible values. Calculations need to be made with each new set of parameters.

2.3.8. Post-Audits

Another important QA procedure is found in post-audit studies. Whenever an opportunity exists to obtain further field information regarding the system being modeled, refinements and improvements in the model should be made and previous analysis modified. Sometimes, such an opportunity is offered in the form of post-audits. A post-audit is an evaluation of the correctness of the initial predictions, conducted several years after the original modeling study is completed (Anderson and Woessner, 1992). If the model's predictions were accurate, the model might be considered "valid" for the specific site and the actual stresses. A post-audit requires new field observation for the predicted variable, collected after the system has had a chance to adjust to the foreseen changes. Studies by Konikow (1986), Person and Konikow (1986), and Lewis and Goldstein (1982), among others, have demonstrated the need to evaluate model-based predictions when new information becomes available or after a period of time when the effects of the predicted changes in the system become evident.

2.4. QA ORGANIZATION STRUCTURE

QA is the responsibility of both the project team (quality control and internal auditing) and the contracting or supervising organization (quality assessment). QA should not drive or manage the direction of a project nor is QA intended to be an after-the-fact filing of technical data.

There are two levels in the QA framework within the organization that carries out a software development or model application study: 1) a permanent organization, complete with QA management policies, goals and objectives; and 2) project QA organization where general QA policies and assignments are detailed towards project objectives. Upper levels of management need to recognize that QA is a vital part of software development and modeling studies. Such recognition by upper management must be translated into a commitment through policies that set quality goals, establish QA functions, and authorize necessary resources in terms of people, funding and equipment to perform the tasks (Bryant and Wilburn, 1987).

The QA organization should have a charter with each element of the organization defined, and its responsibility outlined. The persons responsible for QA should be independent from those responsible for software development or model application. The QA organization must not be subordinate in any way to product development or delivery (Bryant and Wilburn, 1987).

Competent staffing is the key to a successful QA program. QA staff must have the respect of the project staff with whom they work. They must understand how the work, whose quality they are assuring, is actually accomplished. Implementation of a successful QA program requires that all individuals involved understand what QA means, why it is being done, how they will benefit, what is expected of them, what are the responsibilities for each individual, and that good QA will help rather than hinder the modeling process (Bryant and Wilburn, 1987). They should be convinced of the usefulness of QA and the importance given to it by management.

Successful QA, as is the case with the successful completion of a project, is dependent on the capabilities of the modeling team. A good modeling team is multi-disciplinary, includes highly trained and widely experienced senior staff, and has effective internal communication. Such a team is managed by persons that have an overview of the different disciplines involved in the project, and who are able to translate management's questions into technical project objectives, and explain modeling results to management.

2.5. QA PLANS

At the beginning of a model development or application project a project plan should be made containing a complete set of QA procedures, called the **QA plan**. These QA procedures comprise a list of the measures required to achieve prescribed quality objectives. The QA plan needs approval before initiation of technical work. Major elements of such a QA section of the project plan or QA plan are:

- formulation of QA objectives and required quality level in terms of validity, uncertainty, accuracy, completeness, and comparability;
- development of operational procedures and standards for performing adequate software development and model application studies;
- establishing a paper trail for QA activities in order to document that standards of quality have been maintained;
- QA milestones for internal and external auditing and review procedures.

The QA plan should also specify individual responsibilities for achieving these goals and outline procedures for remedial or corrective action in case problems are detected in the quality assessment stage.

An illustrative example of a generic computer software maintenance and quality assurance plan is given in Wilkinson and Runkle (1986); its implementation for the high-level waste management program at Sandia National Laboratories is discussed in Harlan and Wilkinson (1988). The plan contains requirements for software storage and documentation, as well as a brief description of the software maintenance process. The Sandia National Laboratories has established a computerized software management system for implementing the QA plan. This system aims at: 1) being a repository for current and previously used versions of the software (to allow traceability and retrievability); 2) a repository for documentation including reports, documentation of errors, modifications and enhancements, results of verification simulations, etc. In this context, retrievability is defined as the capability to access previous versions of software developed over a reasonable period of time even though they may not be executable due to hardware and/or system software changes over that period of time; traceability is the ability to identify the actual configuration of the software used in the calculations (Wilkinson and Runkle 1986).

The Sandia QA plan was prepared in accordance with the "Draft Quality Assurance Plan for Operational Software" of the U.S. Nuclear Regulatory Commission (Codell and Silling, 1984), and aimed at satisfying NRC's NUREG-0856 (Silling 1983). It includes a description of the preparation and filing of standard forms for software testing, manuscript review, software problem reports, computer code summary descriptions, update logs (including data and version), and software update description.

A typical model application QA plan provides a description of the preparation, review, and filing of standard forms for all major activities in the project, and of all relevant project data, analyses, and products (reports, electronic files, maps, etc.). It should also present the chain-of-responsibilities in the project, and the QA organization adopted. Examples of the forms included are: 1) checklists for all elements of the modeling procedure adapted (see table 1); 2) forms for data and software transfers from third parties; 3) use of standardized project notebooks (containing relevant handwritten or word-processed notes detailing conceptualization assumptions, data evaluation, code implementation, model setup, input file preparation, post processing, etc.); 4) forms for data, simulation and report review; and 5) standardized software problem reports and computer code summary descriptions (including data and version). All forms should include space for date of filing, and for QA approvals.

2.6. QA ASSESSMENT

Quality assessment consists of two elements: auditing and technical review (van der Heijde, 1987). Audits are procedures designed to assess the degree of compliance with QA requirements, commensurate with the level of QA prescribed for the project. Compliance is measured in terms of traceability of records, accountability (approvals from responsible staff), and fulfillment of commitments in the QA plan. Technical review consists of independent evaluation of the technical and scientific basis of a project, and of the usefulness of the project results.

QA assessment not only involves checking if procedures have been applied correctly, but also establishing quantitatively the overall success of the project in meeting its original objectives.

Various phases of quality assessment exist for both model development and application. First, review and testing in case of software development or review and performing control calculations by the responsible researcher, and sometimes by other staff not involved in the project, or by invited experts from outside the organization. Also to be considered is the quality assessment by the organization for which the project has been carried out. Again, three levels can be distinguished for project or product review or testing: 1) review or testing by the project officer or project monitor; 2) review or testing by technical experts within the funding or controlling organization, who were not involved in the project; and 3) review or testing by an external peer review panel (van der Heijde, 1987).

Quality assessment generally takes the form of technical and administrative reviews. Review comments can be presented in the form of a memorandum or report, or as annotations in the margin in a certified copy of the reviewed documents. In case this review leads to important recommendations for corrective action or additional studies, follow up activities by the project team, and additional review need to be arranged and documented.

It should be noted that, like in software development, reviewing model application projects increasingly involve various scientific and engineering disciplines. For such projects, establishing a multi-disciplinary review team or panel might be the most appropriate approach.

Table 1: Assessment Framework for Ground-Water Model Applications (EPA 1992)

Modeling Application Objectives

1 Management's decision objectives and the modeling objectives should be clearly specified up-front.

2 Management's decision objectives should be based upon existing information about the physical characteristics of the site (e.g., hydrogeologic system) and the source and location of the contamination.

3 The function of the model (e.g., data organization, understanding the system, planning additional field characterization or evaluation of remediation alternatives) should be defined during the development of the modeling objectives.

Table 1 - continued

4	The potential solutions to be evaluated (e.g., containment and remediation solutions) should be identified prior to the initiation of the modeling.
5	The level of analysis required (e.g., numerical model, analytical model or graphical techniques) should be determined during the definition of the modeling objectives.
6	Management, in consultation with a professional ground-water scientist, should specify the time period (e.g., one year, ten years or hundreds of years) for which model predictions are required.
7	The level of confidence (quantitative or qualitative) required of the modeling results should be specified.
8	Performance targets (e.g., allowable head error) for the model application should be specified up-front.
9	An analysis should be performed of the incremental costs associated with expanding these study objectives (e.g., expanding the size of the study area, the number of remedial technologies modeled or the performance targets of the model) and the consequent incremental improvement in supporting management's decision objectives.
10	Management's decision objectives should be reaffirmed throughout the modeling process.
11	The modeling objectives should be reviewed, after the development of the conceptual model and prior to the initiation of the modeling, to ensure that they support management's decision objectives.
12	The level of analysis required should be reviewed during the course of the project and, if necessary, modified.
13	The function of the model should be reviewed during the course of the project and, if necessary, modified.
Project Management	
14	The individuals who are actually performing the modeling, managing the modeling effort and performing the peer review should have the ground-water modeling experience required for the project. Specifically, for their role on the project, each should have the appropriate level of:

- formal training in modeling and hydrogeology;
- work experience modeling physical systems;
- field experience characterizing site hydrogeology; and
- modeling project management experience.

15 These individuals should be organized as a cohesive modeling team with well defined roles, responsibilities and level of participation.

16 The organization of the team should be appropriate for the application.

17 An independent quality assurance (QA) process should be established at the beginning of the project.

18 This QA process should include ongoing peer review of the:
- modeling objectives development;
- conceptual model development;
- model code selection;
- model setup and calibration;
- simulation of scenarios; and
- post simulation analysis.

19 This QA process should be implemented.

20 A procedure should be established up front for documenting the model application.

21 The documentation should include a discussion of the:
- general setting of the site;
- physical systems of interest;
- potential solutions to be evaluated;
- modeling objectives and time frame for model predictions;
- quality assurance and peer review process;
- composition of the modeling team;
- data sources and data quality;
- conceptual model: hydrostratigraphy, ground-water flow system, hydrologic boundaries, hydraulic properties, fluid sources and sinks, loading and areal extent of contaminant source, and contaminant transport and transformation processes;

- selection of the computer code: description of the code, reliability, usability, transportability, performance, public domain versus proprietary models, limitations, and related applications;
- ground-water model construction: code modifications, model grid, hydraulic parameters, boundary conditions, and simplifying assumptions;
- calibration, sensitivity analysis, and verification;
- predictive simulations: scenarios, implementation of the scenarios, and discussion of the results of each run;
- uncertainty analysis;
- discussion of results related to management's information needs as formulated in the decision objectives;
- executive summary (in terms of the decision objectives);
- references; and
- input and output files.

22 The documentation should provide the information required for an independent reviewer to complete a post application assessment.

Conceptual Model Development

23 An initial conceptual model of both the local and regional hydrogeological system should be developed prior to any computer modeling.

24 The conceptual model should be based upon a quantification of field data as well as other qualitative data that includes information on the:

- aquifer system (distribution and configuration of aquifer and aquitard units): thickness and continuity of relevant units, areal extent, and interconnections between units;
- hydrologic boundaries: physical extent of the aquifer system, hydrologic features that impact or control the ground-water system, ground-water divides, and surface water bodies;
- hydraulic properties (including, where relevant, homogeneous and isotropic characteristics): transmissivity, porosity, hydraulic conductivity, storativity, and specific yield;
- sources and sinks: recharge to the aquifer (e.g., infiltration), evapotranspiration, drains, ground-water discharges (e.g., flow to surface water bodies), and wells (e.g., water supply, injection or irrigation wells, horizontal wells);

- fluid potential (i.e., the potentiometric surface, the magnitude and direction of the hydraulic gradient within each model layer);
- contaminant: source, loading, areal extent, physical properties, chemical interactions, and biotransformations;
- soils.

25 The quantity, quality and completeness of the field data should be analyzed as part of the development of the conceptual model.

26 If there are data gaps (e.g., missing water level or hydraulic conductivity information), additional field work and other attempts to fill in these gaps should be documented.

27 If there are data gaps, the tradeoff should be analyzed between the cost of acquiring additional data and the consequent improvement in meeting management's decision objectives.

28 The data sources should be documented.

29 The quality of the data should be examined and documented and the influence of their quality on the project's results should be assessed.

30 Any and all potential interactions with other physical systems (e.g., surface water systems or agricultural systems) should be evaluated, prior to the beginning of the modeling, by means of a water budget, a chemical mass balance or other analytical techniques.

31 The manner in which existing and future engineering (e.g., wells, slurry walls) must be represented in the numeric or analytic model should be explicitly incorporated into the conceptual model.

32 Sufficient contaminant sources should be identified to account for the contaminant mass in the plume.

33 A clear statement of the location, type and state of the boundary conditions; justification of their formulation; and the source(s) of information on the boundary conditions should be included as part of the conceptual model.

34 All conceptual model parameters and reasonable parameter ranges should be specified prior to beginning the calibration of the numerical model.

Table 1 - continued

Model (code) Selection

35 The selected model (code) should be described with regard to its flow and transport processes, mathematics, hydrogeologic system representation, boundary conditions and input parameters.

36 The reliability of the model (code) should be assessed including a review of:

- peer reviews of the model's theory (e.g., a formal review process by an individual or organization acknowledged for their expertise in ground-water modeling or the publication of the theory in a peer-reviewed journal);
- peer reviews of the model's code (e.g., subject to a formal review process by an individual or organization acknowledged for their expertise in assessing ground-water computer models);
- verification studies (e.g., evaluation of the model results against laboratory tests, analytical solutions or other well accepted models);
- relevant field tests (i.e., the application and evaluation of the model to site specific conditions for which extensive data sets are available); and
- the model's (code) acceptability in the user community as evidenced by the quantity and type of use.

37 The usability of the model (code) should be assessed including the availability of:

- the model's binary code;
- the model's source code;
- pre- and post-processors;
- existing data resources;
- standardized data formats;
- complete user instruction manuals;
- sample problems;
- necessary hardware;
- transportability across platforms; and
- user support.

38 The tradeoff should be analyzed between model (code) performance (e.g., accuracy and processing speed) and the human and computer resources required to perform the modeling.

39 The model (code) should be in the public domain or at least readily accessible to all interested parties. If not, the modelers should explain how the inaccessibility would not detract from the study objectives and the regulatory process.

40 The assumptions in the model (code) should be analyzed with regard to their impact upon the modeling objectives.

41 Any and all discrepancies between the modeling requirements (i.e., as indicated by the decision objectives, conceptual model and available data) and the capabilities of the selected model should be identified and justified. The modelers should explain why the modeling objectives and/or the conceptual model did or did not need to be modified. For example, the implications of the selected code supporting one, two or three dimensional modeling; providing steady versus unsteady state modeling; or requiring simplifications of the conceptual model should be discussed.

42 If the modeling objectives are modified due to such discrepancies, those modifications should be documented.

43 If the model source code is modified, the following tests should be performed and the testing methodology and results should be justified:

- reliability testing (see criteria #36);
- usability evaluation (see criteria #37);
- performance testing.

Model Setup And Input Estimation

44 The overall grid resolution (e.g., average spacing of 100 feet versus 1000 feet) should be analyzed with respect to the dependent variable accuracy required to meet management's objectives. For example, the grid should be fine enough to allow the hydraulic gradient to be accurately represented.

45 The finite element or finite difference grid design should be analyzed with respect to the modeling objectives such as the need to locate or model wells accurately, existing and future engineering or contaminant sources and plumes.

46 The grid should be designed with respect to the physical system. For example:

- the main grid orientation should be aligned with the principal directions of hydraulic conductivity and/or transmissivity;
- a finer grid should be used in areas where results were needed (e.g., in the area of highest pollution or drawdown) or areas having large: changes in transmissivity, changes in hydraulic head, or concentration gradients; and

- a coarser grid should be used where data are scarce and for those parts of the study area that are not of particular interest.

47 The grid spacing and time step size should be analyzed with respect to numerical accuracy. For example:

- If a finite difference model with variable grid spacing was used, the grid should be expanded towards distant boundaries by less than a factor of 2;
- If a finite element model was used, the following should be analyzed with regard to their impact on the numerical accuracy of the model application: length to width ratio of each element, size difference between neighboring elements, and the Peclet number ($P_e = v \bullet \Delta X/D$);
- the Courant number ($C_r = v \bullet \Delta t/\Delta X$) should be ≤ 1.

  where:

  D = Dispersion Coefficient $[L^2/T]$

  Δt=Time Step [T]

  V = Velocity [L/T]

  ΔX = Grid spacing [L]
- If Random Walk particle tracking was used, the grid spacing and particle mass should be analyzed with respect to the contaminant resolution required.

48 The mapping of the location of the boundary conditions on the grid should be evaluated. For example:

- the boundaries should be located far enough away from the areas of interest to dampen any instability in the model;
- the manner in which the boundaries are represented in the grid should ensure the fineness of the grid, the accuracy of the geometry and the accuracy of the boundary conditions; and
- for finite element grids, internal and external boundaries should coincide with element boundaries.

49 Well nodes should be located near the physical location of the wells.

50 The data sources, the data collection procedures and the data uncertainty for the model input data should be evaluated and documented in the project report or file.

51 All model inputs should be defined as to whether they are measurements, estimates or assumptions including:

Table 1 - continued

- the constitutive coefficients and parameters (i.e., parameters that are not generally observable but must be inferred from observations of other variables, for example the distribution of transmissivity and specific storage);
- the forcing terms (e.g., sources and sinks of water and dissolved contaminants);
- the boundary conditions; and
- the initial conditions.

52 The input estimation process whereby data are converted into model inputs (e.g., spatial and temporal interpolation and extrapolation or Kriging) should be described and the spatial location and the associated values of the data used to perform the interpolation should be shown on a map or provided in a table.

53 The uncertainty associated with the input estimation process should be specified, explained and documented.

54 The model should be calibrated.

55 If the model is not calibrated, the reasoning for not calibrating the model should be explained.

56 The criteria being used to terminate the calibration process (i.e., the definition of an adequate match between observed and modeled values) should be justified with regard to the modeling objectives.

57 The calibration should be performed in a generally acceptable manner. Specifically:

- a sensitivity analysis should be performed to determine the key parameters and boundary conditions to be investigated during calibration;
- the calibration should include a calculation of residuals between simulated and measured values;
- the calibration should include an evaluation of both spatial and temporal residuals;
- the calibration should be performed in the context of the physical features (e.g., were residuals analyzed with respect to the pattern of ground-water contours including mounds or depressions or indications of surface water discharge or recharge).

58 If a water budget is developed, the results and their use in calibrating the model should be explained.

Table 1 - continued

59 All changes in initial model parameter values due to calibration should be justified as to their reasonableness.

60 Any discrepancies between the calibrated model parameters and the parameter ranges estimated in the conceptual model should be justified.

61 If the conceptual model is modified as a result of the model calibration, all changes in the conceptual model should be justified. Whenever feasible the calibrated model should be verified with an independent set of field observations.

Simulation Of Scenarios

62 For each modeling scenario, the model inputs and the location of features in the model grid should be justified. For example:

- if a pumping well was not located at a node, the allocation of well discharges among neighboring nodes should be justified;
- if a slurry wall is a remedial alternative, the representation in the model of the wall's geometric and hydraulic properties should be justified;
- if cleanup times are calculated, all assumptions about the location, quantity and state of the contaminants should be justified;
- when a remedial action, such as extraction wells, affects the flow, such effects should be determined, including the downgradient distance to the stagnation point and the lateral reach of each modeled extraction well.

Post Simulation Analysis

63 The success of the model application in simulating the site scenarios should be assessed.

64 This assessment should include an analysis of:

- whether the modeling simulations were realistic;
- whether the simulations accurately reflected the scenarios;
- whether the hydrogeologic system was accurately simulated; and
- which aspects of the conceptual model were successfully modeled.

65 The sensitivity of the model results to uncertainties in site specific parameters and the level of error in the model calibration should be examined and quantified. For example, the modeling scenarios should be simulated for the range of possible values of the more sensitive hydrogeologic

Table 1 - continued

	parameters. Moreover, the range of error in the model calibration should be considered when drawing conclusions about the model results.
66	The post-processing should be analyzed to ensure that it accurately represents the modeling results and interpolation and smoothing methods should be documented, where appropriate.
67	The post-processing results should be analyzed to ensure that they support the modeling objectives.
68	The final presentation should effectively and accurately communicate the modeling results.
69	When feasible, a post audit of the model should be carried out or planned for in the future.
Overall Effectiveness	
70	Any difficulties encountered in the model application should be documented.
71	The model application should provide the information being sought by management for decision making.
72	The model application results should be acceptable to other relevant parties.
73	The model application should support a timely and effective regulatory decision.
74	Those aspects of the modeling effort that, in hindsight, might have been done differently should be documented.

2.7. QA AND CODE SELECTION

2.7.1. Code Selection Process

In the model application process, code selection is a critical step in ensuring an optimal trade-off between project effort and result. The result is generally expressed as the expected effectiveness of the modeling effort in terms of forecast accuracy. The effort is ultimately represented by the project costs. Such costs should not be considered independently from those of field data acquisition. For a proper assessment of modeling cost, such measures as choice between the development of a new code or the acquisition of an existing code, the implementation, maintenance, and updating of the code, and the development and maintenance of databases, need to be considered.

As code selection is in essence matching a detailed description of the modeling needs with well-defined characteristics of existing codes, selecting an appropriate code requires formulation of the modeling needs as well as systematic characterization of existing simulation codes. Code credibility is a major problem in model use; therefore, special attention should be given in the selection process to ensure the use of qualified simulation codes that have undergone adequate review and testing. Selecting an appropriate model is crucial to the success of a modeling project.

2.7.2. Formulation of Modeling Needs

To select a simulation code efficiently, management-oriented criteria need to be developed for evaluating and accepting such models. To obtain such criteria, the management objectives to be addressed and the level of analysis sought (based among others on the sensitivity of the project for incorrect or imprecise answers or risk involved), should be known. Furthermore, adequate knowledge of the physical system under study should be present, and an analysis of the constraints in human and material resources available for the study should be completed. The set of chosen selection criteria should be based on:

- trade-offs between costs of running a code (including data acquisition for the required level of analyses) and accuracy;
- a profile of model user and a definition of required user-friendliness;
- accessibility in terms of effort, cost, and restrictions;
- acceptable temporal and spatial scale and level of aggregation.

Based on these considerations, the user needs to formulate the code characteristics relevant to the problem under study, and prioritize these characteristics for mapping on the characteristics of existing codes. Code characteristics, often focussed on in the selection process, include the purpose of the model, the nature of the ground-water system represented, and the mathematical method(s) employed. Furthermore, the user may be interested in the correctness of the model, the completeness of documentation, and the quality, performance, and usability of the software. Other information the user may find relevant to code selection include the computer system it runs on and the conditions for its use.

2.7.3. Description of Code Characteristics

There are various types of ground-water models, designed to simulate different types of ground-water systems, and able to compute different system variables. To be able to identify the main attributes of a particular model a descriptive system is needed using standardized, well-defined model descriptors. As part of the development of a data base of ground-water modeling code descriptions (MARS: Model Annotation Search and Retrieval), the International Ground Water Modeling Center has developed such a systematic list, containing hundreds of hierarchically grouped descriptors (van der Heijde and Williams, 1989). The level of detail adopted for this descriptive system allows the user to identify simulation codes of interest, and to perform a preliminary usability assessment.

The description of the simulation codes covers the purpose of the model, the nature of the ground-water system represented and the mathematical method(s) employed. Furthermore, it addresses the correctness of the model, the completeness of documentation, and the quality, performance, and usability of the software. Other information included in the descriptive system MARS concerns the computer system on which the software runs and the conditions for its use.

Before a final selection is made, the user should obtain code documentation and assess code characteristics in detail. Also, the user should be aware of general performance characteristics of the various numerical methods available. Each method has its strengths and weaknesses, often related to the type of terms included in the governing equations, the boundary conditions applicable, and the parameter distribution of interest. For example, Kinzelbach (1987) evaluated two-dimensional tracer solute transport codes, representing four major solution approaches. He demonstrated that standard finite difference and finite element methods yield unreliable results if discretization conditions are not met. Particle tracking methods, *e.g.* the method of characteristics and the random walk method, show oscillations and demixing problems.

If the accuracy of the computations to be made with the selected model is very critical, one has to evaluate the code's documentation and related publications for verification tests, specifically addressing the type of situations expected to be encountered at the field site. An example of such verification can be found in Khoury *et al.* (1989). They used the USGS MOC code to analyze the design of a reservoir. A naturally occurring clay layer should provide the impermeable base for the reservoir. However, this clay layer is absent in one corner of the reservoir, where the clay layer pinches out, and in an area adjacent to the maximum height dam section. The area upstream of the dam is to be remediated using a compacted clay blanket. Concern persisted that leakage from the reservoir could generate excessive piezometric mounding in the confined aquifer underlying the clay layer, which in turn could impact the dam design and valley stability, and could cause other problems. To assess the applicability and accuracy of the code, its predictions for an analogous problem with a simplified asymmetric geometry were compared against an analytical solution (Khoury *et al.*, 1989), and against the solution obtained with a proprietary two-dimensional finite element code.

2.7.4. Code Selection Criteria

The major criteria in selecting a code are: 1) that the code is suitable for the intended use; 2) that the code is reliable; and 3) that the code can be applied efficiently. If different problems must be solved, more than one code might be needed, or a code might be used in more than one capacity. In such cases, the model requirements for each of the problems posed have to be clearly defined at the outset of the selection process. To a certain extent this is also true for modeling the same system in different stages of the project. Often, a code is selected in an early stage of a project to assist in problem scoping and system conceptualization. Limitations in time and resources and in data availability might initially force the formulation of a "simple" model. Growing understanding of the system and data availability might lead to a succession of models of increasing complexity and subsequent selection of different codes. In such cases, flexibility of the candidate code, or the availability of a set of integrated codes of different levels of sophistication, might become an important selection criterion.

As mentioned above, the major criteria in selecting a code are its suitability for the identified tasks, its reliability, and its efficiency. The reliability of a code is defined by the level of quality assurance applied during its development, and by its verification, field validation, and performance evaluation. The reliability of codes should be established by applying a widely accepted review and testing procedure (see section 2.2.). Such a procedure has not yet been adopted, although various organizations have established their own procedures (*e.g.*, Wilkinson and Runkle, 1986; van der Heijde, 1987). In addition, discussions have started within the Section on Ground-water Models of Subcommittee D-18.21 of the American Society for Testing and Materials (ASTM) to develop standard guidance in ground-water simulation code selection.

A code's efficiency is determined by the availability of its source or run-time version and of its documentation, and by its usability, portability, modifiability, and economy with respect to human and computer resources required for its operation.

Acceptance of a simulation code should be based on technical and scientific soundness, its efficiency, and legal and administrative considerations. A model's efficiency is determined by the rapid access to its code, availability of good documentation, access to user support, and by its reliability, credibility, usability, portability, modifiability, runtime resource utilization, and overall economy. A brief discussion of some of these criteria is given below and follows a more extended treatment in van der Heijde and Beljin (1988). This latter publication includes also a proposed rating system for each of these criteria.

Availability--

A generic simulation model is defined as available, if the program code associated with it can be obtained either as source code or as an executable, compiled version, or if the program can be accessed easily by potential users. Ground-water software is either in the *public domain* or has *proprietary* status. In the United States, most software developed by federal or state agencies or by universities through funding from such agencies is available without restrictions in its use and distribution, and is therefore considered to be in the public domain. In other countries the situation is often different, with most software having a proprietary status, even if developed with government support, or its status is not well-defined. There, the computer code can be obtained or accessed under certain restrictions of use, duplication, and distribution.

Codes developed by consultants and private industry are often proprietary. This may also be true of software developed by some universities and private research institutions. Proprietary codes are in general protected by copyright law. Although the source codes of some generic models have appeared in publications such as textbooks, and are available on tape or diskette from the publisher, their use and distribution might be restricted by the publication's copyright.

Further restrictions occur when a code includes proprietary third-party software, such as mathematical or graphic subroutines. For public domain codes, such routines are often external and their presence on the host-computer is required to run the program successfully.

Between public domain and proprietary software is a somewhat grey area of so-called freeware or user-supported software. Freeware can be copied and distributed freely, but users are encouraged to support this type of software development with a voluntary contribution. In ground-water modeling, this type of distribution is rarely used.

For some codes developed with public funding, distribution restrictions are in force, as might be the case if the software is exported, or when an extensive maintenance and support facility has been created. In the latter case, restrictions are in force to avoid use of non-quality-assured versions, to prevent non-endorsed modification of source code, and to facilitate efficient code update support to a controlled user group.

User support--

If a particular code is selected for a site-specific problem, the user may encounter technical problems in running the code on the available computer system. Such a difficulty may result from:

- compatibility problems between the computer on which the code was developed and the user's computer;
- coding errors in the original program;
- user errors in data input and code execution.

User-related errors can be reduced by becoming more familiar with the code. Here the user benefits from good documentation. If, after careful code selection, problems in implementation or execution occur and the documentation fails to provide answers, the user needs help from someone who is knowledgeable about the code's operation and familiar with its use. Such assistance, called software implementation and execution support or software user support, cannot replace the need for proper training in code use and modeling in general; requests for support from code developers may assume such extensive proportions that user support becomes a consulting service or on-the-job training. This potentiality is generally recognized by code developers, but not always by the users of the software.

Credibility--

A major issue in the use of ground-water simulation codes is their credibility. A code's credibility, and that of the theoretical framework it represents, is based on its proven reliability, and on its acceptance by users (based in part on the number of successful applications). Modelers and ground-water managers often have the greatest confidence in those simulation codes most frequently applied. This notion is reinforced when successful, peer-reviewed applications are published. As reliability of a program is related to the localized or terminal failures that can occur because of software errors (Yourdon and Constantine, 1979), it is assumed that most such errors, originally present in a widely used program, have been detected and corrected. Yet no computer program is without programming errors, even after a long history of use and updating. Some errors will never be detected and do not, or only slightly, influence the program's utility. Other errors show up only under exceptional or untested circumstances. Decisions based on the outcome of simulations will be viable only if the codes used have undergone adequate review and testing (see section 2.2). However, relying too much on field validation (if present), or on frequency of code application may exclude certain scientifically sound, well-documented and thoroughly tested codes, even those most efficient for solving the problem at hand.

It may be argued that if a code is used by a large number of people, this demonstrates significant user confidence. Such extensive use often reflects the code's applicability to different types of ground-water systems, and its capability to address various management questions. It might also imply that the code is relatively easy to use (see *Usability*). Finally, if a code has a large user base, many opportunities exist to discuss particular applications with knowledgeable colleagues.

Usability--

Various problems can be encountered when a simulation code is implemented on the user's computer system. Such difficulties may arise from hardware incompatibilities or coding of user errors in code installation, data input, or program execution. Programs that facilitate rapid understanding and knowledge of their operational characteristics and which are easy to use are called user-friendly and are defined by their usability (van der Heijde and Beljin, 1988). In such programs, emphasis is generally placed on extensive, well-edited documentation; easy input preparation and code execution, preferably through the use of (intelligent) pre-processors with on-line help systems; and well-structured, informative output. Adequate code support and maintenance also enhance the code's usability.

Portability--

Programs that can be easily transferred from one execution environment to another are called portable. To evaluate a program's portability, both software and hardware dependency need to be considered. If the program needs to be altered to run in a new computer environment, its modifiability is important.

Modifiability--

In the course of a computer program's useful life, the user's experiences and changing management requirements often lead to changes in functional specifications for the software. In addition, scientific developments, changing computing environments, and the persistence of errors make it necessary to modify the program. If software is to be used over a period of time, it must be designed so that it can be continually modified to keep pace with such events. A code that is difficult to modify is called fragile and lacks maintainability. Such difficulties may arise from global, program-wide implications of local changes (van Tassel, 1978).

Runtime Resource Utilization--

Runtime resource utilization refers to the computational resources needed to perform the modeling computations. The main resources comprise of type and number of hardware devices and system software required, computer core memory (RAM) use, program execution (CPU) time, input/output processing (I/O) time, and mass storage requirements. Computer core memory use is often predefined in the code by the programmer. In other cases, the user determines core use indirectly by specifying the problem setup. Program execution and I/O time, together with mass storage space needs, may be measured by running a suite of representative benchmarks.

2.7.5. QA in Code Selection

It should be realized that a perfect match rarely exists between desired characteristics and the characteristics present in available generic models. Many of the selection criteria deemed important for a particular application are subjective or often weakly justified, often because there are insufficient data in the selection stage of the project to establish the importance of certain characteristics of the system to be modeled. If a match is hard to obtain, reassessment of these criteria and their relative weight in the selection process is necessary. Hence, code selection is very much an iterative process, the success of which depends on expert judgment.

Quality assurance in code selection follows the same pattern as discussed in the QA aspects of code development and model application. The principal elements of code selection QA are: 1) carefully following the step-by-step selection procedure as described above; 2) detailed reporting on the adherence to this procedure; and 3) documenting the considerations, assumptions, and decisions made at each step. Specifically, detailed justification should be presented why the code selected is adequate for the problem under study, and the limitations of the selected code in regard to the problem under study should be discussed.

Further information on ground-water model selection is presented in (Rao *et al.* 1981; Kincaid *et al.* 1984; Boutwell *et al.* 1985; Simmons and Cole 1985). An overview of ground-water models available is given in van der Heijde and Beljin (1988), van der Heijde *et al.* (1988) and van der Heijde and Elnawawy (1992).

2.8. QA CLOSURE

Literally, quality assurance assures the quality of the product (code, model) or activity of concern (modeling). A more workable description is that QA (in modeling) guarantees that the quality of the model-based analysis and advice (to decision-makers) satisfies quantitative quality criteria or measures. As the principle idea behind QA is accountability, and the main mechanism is maintaining records (hardcopy and electronic files, reports) of all activities and results, a more proper term might be quality documentation.

Taken in a broad sense, QA provides a methodological and administrative framework to do the best we can within the limitations of our current understanding of nature and available technology.

That QA always assures acceptable quality of a code development project or a modeling study is an idle hope. However, adequate QA can provide safeguards against faulty codes or improper modeling. Regulators and decision-makers should understand that there is no way to guarantee that modeling-based advice is entirely correct, nor that the simulation code used (or any scientific model or theory, for that matter) can ever be proven, verified or validated in the strictest sense of these terms. Rather, a model can only be invalidated by disagreement of its predictions with independently derived observations regarding real systems.

It should be noted that a major role of QA/QC is to provide communication between the modeler and his/her peers, and between modeler and decision-maker, giving the latter a sense of the accuracy, uncertainty, and reliability of the modeler's advice. Therefore, QA should not apply to the work of junior modelers only, but should also be adhered to by expert modelers.

There are various cautions to be made. QA should never become so stifling that experienced modelers are discouraged to take new avenues not previously explored, or that an inappropriately large part of the budget of a project is consumed by responding to bureaucratic requirements. When QA regulations become bureaucratic red tape, the time and cost of QA may take away precious resources from the data collection and problem analysis activities. Furthermore, the risk is present that QA deteriorates and becomes only a checklist installing false confidence in modeling results.

3. CODE TESTING AND EVALUATION PROCEDURES

3.1. INTRODUCTION

The usefulness of predictive simulations based on ground-water models is often limited by our inability to indicate and quantify the reliability of such model results. Researchers have developed various techniques to assess confidence levels for model predictions, so that water resources managers can account for uncertainties in the decision-making process. For example, Freeze *et al.* (1990) present a methodology based on the application of decision analysis to engineering design in a hydrogeological environment. The methodology involves the coupling of a decision model based on a risk-cost-benefit objective function, a simulation model for ground-water flow and contaminant transport, and an uncertainty model that encompasses both geological uncertainty and parameter uncertainty.

One of the areas of concern is the credibility of the simulations codes used and the generic models they represent. As discussed in the previous section, an important aspect of the credibility of a simulation code is its reliability. The reliability of codes is established by applying a comprehensive, systematic review and testing procedure. The quality assurance aspects of such a procedure have been discussed in section 2.2. The following section presents a systematic code verification and performance testing protocol, based on the use of analytical solutions and synthetic data sets as benchmarks. Although the report provides some example test problems, it does not contain actual benchmarks. A comprehensive set of benchmarks for two- and three-dimensional ground-water flow and transport models will be presented in a follow-up report.

3.2. LITERATURE REVIEW

Starting in the early days of computer-based simulation of ground-water systems, verification of codes have been part of code development activities (*e.g.*, Pinder and Bredehoeft, 1968; Prickett and Lonnquist, 1971; Pinder and Frind 1972). More recently, such code verification by the code developers have become quite elaborate (Ward *et al.*, 1984; Reeves *et al.*, 1986; Gupta *et al.*, 1987; Sims *et al.*, 1989; Faust *et al.*, 1990; Zheng, 1990).

In some cases, verification of codes and evaluation of their performance have been performed by test teams, independent of the code developing team (*e.g.*, Beljin, 1988; Watson and Brown, 1985). Often, such third-party testing is initiated by a regulatory agency to determine, if the code is acceptable for use within a certain regulatory framework. The need for comprehensive verification and validation of ground-water simulation codes is illustrated by the success of a series of international cooperative programs: INTRACOIN, HYDROCOIN, and INTRAVAL. These studies attempted to evaluate conceptual and mathematical models for ground-water flow and radionuclide transport in the context of performance assessment of repositories for radioactive waste (Nicholson *et al.*, 1987; INTRAVAL, 1990). They were performed by participating modeling groups from different countries, coordinated by the Swedish Nuclear Power Inspectorate (SKI). The individual teams were supported by government agencies in their country. The first project, the International Nuclide Transport Code Intercomparison study, INTRACOIN, ran from 1981-1986. This was succeeded by the Hydrologic Code Intercomparison study, HYDROCOIN, completed in 1990. A third project, INTRAVAL (International Project to Study Validation of Geosphere Transport Models) was initiated in 1987 and is still active. These studies tested the numerical accuracy of computer codes, the validity of the underlying conceptual models, and different techniques for sensitivity and uncertainty analysis.

The INTRACOIN study consisted of a comparison of twenty-two different computational codes describing transport of radionuclides in geologic media (INTRACOIN, 1984). This comparison was performed at three levels aimed at establishing: 1) the numerical accuracy of the codes; 2) the capabilities of the codes to describe in-situ measurements; and 3) the quantitative impact of various physical phenomena on the nuclide transport calculations in a typical repository scenario assessment. Using the terminology defined in section 2 of this report, INTRACOIN Level 1 concerns verification of the simulation code, Level 2 concerns validation of the generic model, and Level 3 concerns performance evaluation through analysis of the sensitivity of the code for perturbations in field parameters and boundary stresses.

At INTRACOIN Level 1, researchers verified the codes either by comparing computational results from numerical models with existing analytical solutions, or by intercomparison of the computational results from codes utilizing different numerical methods (INTRACOIN, 1984). This study was limited to one-and two-dimensional far-field radionuclide geosphere transport models; although a few of the participating codes could handle three-dimensional problems, the study did not include a three-dimensional test case because "too few of the participating codes were able to treat such problems" (INTRACOIN, 1984, p. 11). The seven test problems ranged from simple one-dimensional transport in a porous medium with constant parameters to two-dimensional transport in a fractured medium with diffusion into the rock matrix:

- one-dimensional advection-dispersion, constant migration parameter (*i.e.*, ground-water velocity, retention factors and dispersivity are held constant), and constant leach-rate;
- one-dimensional advection-dispersion in a layered medium (piece-wise constant migration parameters);
- one-dimensional advection-dispersion with continuously varying parameters;
- two-dimensional advection-dispersion with constant retention factors and dispersivity:
    - – parallel flow field and radial dispersion;
    - – two-dimensional flow field and radial dispersion (flow field between two wells;
- one-dimensional advection-dispersion with diffusion into the rock matrix;
- two-dimensional advection-dispersion with matrix diffusion:
    - – parallel flow field and radial dispersion;
    - – two-dimensional flow field and radial dispersion; and
- one-dimensional advection-dispersion with linear mass transfer kinetics and constant

migration parameters.

The twenty-two codes involved were divided into five groups: 1) one-dimensional advection-dispersion models, 2) one-dimensional advection-dispersion models with piece-wise constant parameters, 3) models including matrix diffusion, 4) models including non-linear chemical effects, and 5) combined models including equations for hydrology and heat transport. The fifth group of models incorporated equations for hydrology and heat transport which were not included in the test objectives of the INTRACOIN study. Also, models for ground-water flow, transport in the biosphere and dose calculations, and "near-field" models were not included (INTRACOIN, 1984). In general, each code was run only for selected problems; only the first problem was used by almost all test teams. Code comparison was performed using three criteria:

- the nuclide concentrations at the end of the migration path as a function of time;
- maximum concentrations, the times for the maxima, and the times when the concentration is half the maximum concentration; and
- execution time (CPU time) and the time for one-single precision floating point multiplication at the computer installation.

The comparative results were presented in the tabular and graphic form.

The results of the various INTRACOIN Level 1 test problems showed generally good agreement among the participating codes (INTRACOIN, 1984). Result variations were attributed to a variety of causes. Some of the codes use algorithms primarily designed to handle predominantly advective or predominantly dispersive problems, and can thus not be expected to give unconditionally reliable results in all ranges of parameter values. Using a low Peclet number ($Pe<10$) will accommodate a sensitive intercomparison for this issue. However, most of the deviating results have been explained either by discrepancies in the implementation of boundary conditions, discrepancies in the implementation of input data, or considered the result of truncation errors (coarse discretization in space or time domain). The study concluded that carefully designed benchmarks combined with convergence test studies, varying the discretizations of the model domain, will contribute significantly to the quality assurance of numerical codes. Specifically, the study considered the development of rigorous and well-programmed analytical solutions of "uttermost importance" in the quality assurance process. It was recommended to perform future benchmark studies using firmly designed test cases, with: 1) stringent definition of boundary conditions and their numerical implementation; 2) stringent definition of the discretization of continuously varying properties; and 3) parameters values chosen such as to give an optimal sensitivity in the comparison. Furthermore, it is necessary that accuracy measures be defined for such studies. It was noted that codes based on the discrete parcel random walk algorithm or on particle tracking seem to need "finger tip feeling" from the user in order to yield reliable results.

INTRACOIN (1986) presents the results of the validation using in-situ measurements (INTRACOIN Level 2) and sensitivity analysis (INTRACOIN Level 3) activities. The capabilities of the codes to describe in-situ measurements were evaluated by comparing various concepts of physico-chemical radionuclides transport in geologic media with field experiments, complemented by laboratory data. Two carefully-selected field experiments were chosen for comparison with model calculations, one in a fractured medium, and one in a porous medium. The researchers involved in INTRACOIN Level 2 testing concluded that in general the participating codes could reproduce field experiment results reasonably well, but that there is an urgent need for better and more-detailed experiments if a reasonable level of validation is expected (INTRACOIN, 1986). In this context it was considered crucial that future validation sites need to be well-characterized with respect to heterogeneities and flow channels. The report recommended that field experiments should be performed which are directly designed for the purpose of validation in order to reduce the degrees in freedom in interpreting the experimental situation.

The Hydrologic Code Intercomparison study, HYDROCOIN, was established as a flow-oriented complement to the INTRACOIN study. The project, initiated in 1984, focused on analytical and numerical methods used to simulate ground-water flow (HYDROCOIN, 1988). The objective of HYDROCOIN was:"...to obtain improved knowledge of the influence of various strategies for groundwater modeling for the safety assessment of final repositories for nuclear waste..." The study aimed to assess three issues: 1) the impact of different solution algorithms on ground-water flow calculations; 2) the capabilities of different models to describe field and laboratory experiments; and 3) the impact of incorporating various physical processes in the ground-water flow calculations. HYDROCOIN used the same three levels of code evaluation as formulated for the INTRACOIN study.

At HYDROCOIN Level 1, the numerical accuracy of the codes was determined by comparing the computational results with analytical solutions or by code intercomparison in the same manner as previously described for INTRACOIN. Seven hypothetical test cases were developed:

1) transient flow from a borehole in a permeable medium containing a single fracture (analytical solution);
2) steady-state flow in a two-dimensional domain containing two permeable fracture zones intersecting each other;
3) partially saturated flow through a sequence of alternating high and low permeability sedimentary rocks;
4) thermal convection for a system where the heat is evolved from a spherical source with a decaying heat output (analytical solution);
5) fluid flow and salt transport in a two-dimensional domain in which the fluid density depends on the salt concentration;
6) steady-state flow in a (weakly) three-dimensional domain, representing a generic bedded-salt geological setting; and
7) steady-state flow through a shallow land-burial site in argillaceous media.

The test cases were designed primarily to yield sensitive tests for the models rather than to represent realistic waste repository scenarios.

Twenty-nine simulation codes have been subjected to these test scenarios. The computed entities used for the comparisons included the distribution of ground-water pressure, salt concentration and temperature, and flow velocities and trajectories. The HYDROCOIN (1988) report concluded that for the four linear test cases (cases 1, 2, 6 and 7) agreement between the calculated primary entities was satisfactory. Deviations observed were explained in terms of the use of different discretization densities in time and space, or as a result of the use of element types with different numerical characteristics. However, the agreement between calculated velocity fields and trajectories was less convincing than that of the scalar entities. As this was considered primarily a product of the differences in post-processing algorithms used by the various teams, the selection of such algorithms should be subject to additional scrutiny. The mildly non-linear case (Case 4) was easy to solve, and good agreement was achieved between the calculated primary scaler entities . The two strongly non-linear cases (Cases 3 and 5) revealed many problems in the simulations, specifically Case 3. Here, the permeability contrast specified resulted in the moisture content to be discontinuous in the domain. Finally, the report concluded that test results are highly dependent on appropriate discretization in space and time. The HYDROCOIN study participants found no definite difference between the results of finite-differences and finite-elements when applied correctly. It was pointed out that it is easier to model a complex geometry domain accurately using finite-elements, yet finite-difference solvers are less expensive to run than finite-element solvers. A more detailed discussion of the actual testing of a number of codes is given by U.S. Nuclear Regulatory Commission (1988). This latter report provides details regarding the setup of the models for the different test cases, grid design, selection of iteration criteria, and implementation of boundary conditions and singularities, among others.

At HYDROCOIN Level 2 testing, the capabilities of the participating models to describe field measurements and laboratory experiments were evaluated (HYDROCOIN 1990). At the beginning of this phase, an extensive search was launched for data sets from relevant experiments. In the ideal data set, measured values for all model parameters should be present in order to reduce the freedom in interpretation of the data. However, no such an ideal data set could be found. The five experiments and field sites selected represent a variety of spatial and temporal scales, several processes of importance, and various media of interest. These five case studies were analyzed using twenty-two participating codes.

In performing the case studies the participating study teams encountered problems related to complexities in the ground-water system, allowing alternative formulations for relevant hydrologic processes or hydrogeologic structures and the representation of flow parameter heterogeneity. Furthermore, the study teams experienced significant difficulties in interpretation of experimental data. Specifically, major differences appeared between the participating modeling teams in the interpretation and formulation of the boundary conditions. In spite of these difficulties, eventually the models were "tuned" to simulate the experimental results of the five test cases. Several conceptual models and parameter sets yielded comparable results, and deviations between experimental findings and modeling results found plausible explanations.

In 1987 a third project began, the International Project to Study Validation of Geosphere Transport Models (INTRAVAL). The focus of this project is the validity of model concepts. It uses the results of laboratory and field experiments and the results of natural analogue studies to study analytically the model validation process (INTRAVAL, 1990).

Other benchmarking, validation, and verification studies have been performed, yet not with as systematic an approach as used in the INTRACOIN, HYDROCOIN, and INTRAVAL studies. Potter *et al.* (1987) conducted a verification study of numerical models for variably saturated flow through a heterogeneous media. They examined the steady-state performance of six flow models employing different numerical methods. The methods included were: (1) finite-difference single formulation; (2) finite-difference double formulation; (3) finite-element single formulation employing linear bases; (4) finite-element double formulation employing linear bases; (5) continuous finite-element formulation employing Hermitian bases; and (6) a Darcian-continuous finite-element formulation employing Hermitian bases. These numerical models were compared with two newly-developed, steady-state analytical solutions to the Richard's equation for flow through a variably-saturated, heterogeneous soil column. The authors found the accuracy for the double formulation finite-difference and finite-element methods significantly higher than for single formulation models. Comparing finite-difference to the finite-element results, the finite-difference method was found to be notably more accurate. The Darcian-continuous finite-element model showed a significant increase in accuracy over the continuous model and over the other models. The study concluded that for the cases explored, using a finite-difference solution may be the most logical choice considering accuracy, complexity, parameter estimation, and knowledge of the physical characteristics of the specific system. According to the authors, "finite-difference concepts are simple, straightforward, and understood by a wider audience than are the finite-element procedures" (Potter *et al.*, 1987, p. 442).

Two studies evaluated computer-coded models designed to simulate the fate of pesticides in the vadose zone. Watson and Brown (1985) performed a comprehensive evaluation of the SESOIL model (Bonazountas and Wagner, 1984) and Carsel *et al.* (1986) evaluated the PRZM model (Carsel *et al.*, 1984). The studies are discussed by Donigian and Rao (1986), illustrating the testing and evaluating of unsaturated zone flow and solute transport models. In reference to the definitions in this report, the Watson and Brown study includes both verification and validation. They performed verification through comparison of SESOIL model predictions of the leaching of aldicarb from a soil column to ground water, with predictions by Jones *et al.* (1983) using three other models: PRZM (Enfield *et al.*, 1982), PESTAN, and PISTON (Donigian and Rao, 1986, p. 104). Verification also included comparing SESOIL results with those from an analytical solution. Validation was performed by comparison of the SESOIL model predictions with relevant published field data. The study by Carsel *et al.* (1986) can be described as (partial) validation performed by comparing the PRZM model results with available field data. As Donigian and Rao (1986) point out, the Carsel *et al.* (1986) study is a good example of the problems encountered in model performance testing using field data not collected specifically for model evaluation, but rather as monitoring data. Often, these field data sets lack certain type of data important for model evaluation. Also, many field tests are of short duration. With regard to validation, Donigian (1983) recommends making conditions under which the model operates as close as possible to the actual field conditions when the observed data were collected, and to be aware of model assumptions and limitations in representing field conditions. He suggests that model testing should be performed with an "informed skepticism" and a questioning approach, in order to use the models as tools to aid decision making.

A study performed by Hecox *et al.* (1989) calibrated and verified a quasi-three-dimensional flow and solute transport model. This model consisted of the internally linked flow and transport codes PLASM (Prickett and Lonnquist, 1971) and RANDOM WALK (Prickett *et al.*, 1981). The study intended to use the model to assess understanding of flow and transport mechanisms, to aid in the design of a remedial system, and to predict future plume movement directions and concentrations. Flow verification consisted of comparing actual and simulated aquifer pumping test drawdowns, as well as actual and simulated seasonal recharge water level fluctuations. The solute transport verification consisted of comparing actual and observed solute front movement rates and concentration distributions for one slightly-retarded and two distinctly-retarded compounds (Hecox *et al.*, 1989). As the Hecox report describes, the flow verification of drawdown was accomplished through a three week pumping test, and the flow verification of seasonal recharge water level fluctuations was accomplished through simulating drainage. Results were reasonably close to observed levels for each flow verification, and differences were explained rationally. The runs for solute transport verification were made using three distinct plumes. Calibration for solute transport focussed on the retardation factor only. The report argues that because the simulations showed a reasonable agreement with the observed plumes without calibration for dispersivity or porosity, the model has been verified.

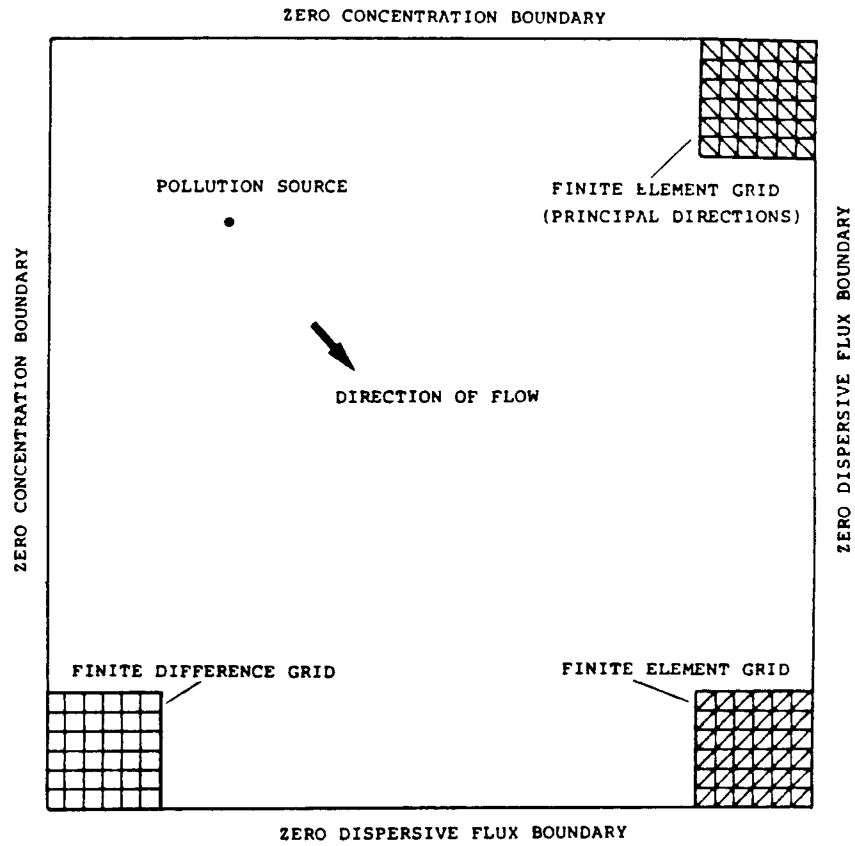
Kinzelbach (1987) compared four major numerical solution methods by applying typical representative two-dimensional code implementations to a number of test cases using equal discretization of the space and time. The codes selected represent the following approaches:

- an explicit finite difference formulation with central or upwind spatial differences;
- a finite element formulation with triangular elements and linear interpolation with forwards differencing in time;
- the method of characteristics (MOC); and
- the random walk method with the option of adding complete velocity terms according to the Ito-Fokker-Planck theory.

The test cases (Figure 5) were selected on basis of expected numerical problems with one or more of the numerical solution techniques. The first test case featured a permanent solute source in axiparallel flow with a Peclet number of 0.5 in longitudinal direction and a time step in accordance with the Courant criterion. In the explicit finite difference model and in the MOC model the time step was chosen to also comply with the Neumann stability criterion. Test case 2 used dispersivity values resulting in a Peclet number smaller than 2. For the third test case the flow field was rotated 45° with respect to the coordinate axes and a high dispersivity anisotropy was chosen. Finally, test cases 4 and 5 treat the permanent source with a single well 1000 m downstream of the source. The difference between cases 4 and 5 is the choice of dispersivity values. The results were presented in graphic form by using concentration versus longitudinal or transverse distance, contoured concentration distributions in space, and breakthrough curves plotting concentration versus time.

Varying data for individual test cases					
Test case	1	2	3	4	5
Pumping rate Q	0	0	0	3400 m^3/d	3400 m^3/d
Longitudinal dispersivity α_L	100 m	10 m	100 m	100 m	10 m
Transverse dispersivity α_T	10 m	1 m	1 m	10 m	1 m

Common data for all test cases	
Pore velocity u	1 m/d
Thickness of flow m	25 m
Source strength $\dot{M}$	120 kg/d
Effective porosity n_e	0.17
Grid distance (x-direction) Δx	50 m
Grid distance (y-direction) Δy	50 m



TEST CASES 1, 2, 4, 5

TEST CASE 3

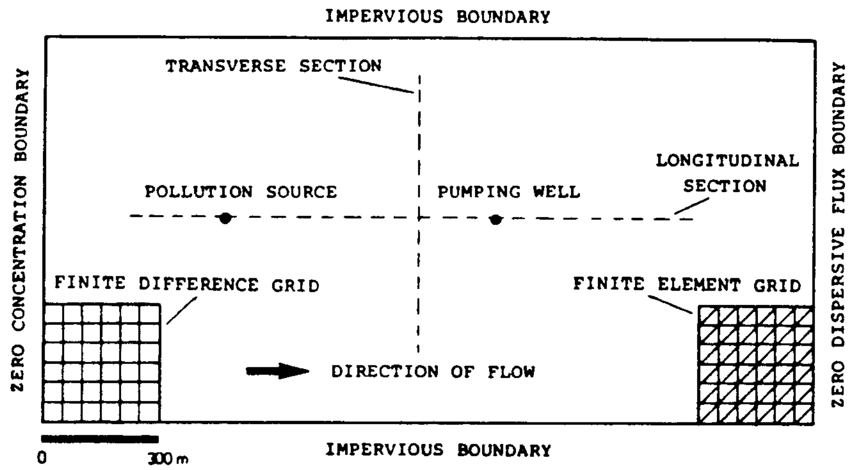


Figure 5. Test problems for two-dimensional solute transport models (from Kinzelbach, 1987)

In the mid 1980s the International Ground Water Modeling Center developed a three-level ground-water simulation code testing procedure. The procedure and methodology have been presented in van der Heijde *et al.* (1985) and applied by Huyakorn *et al.* (1984a) and Beljin (1988) to two-dimensional flow and solute transport codes. At the first level, the code is verified by testing against analytical solutions for highly schematized and simplified systems (IGWMC Level 1). The second level aims at testing code features specifically designed to cope with problems for which no closed-form analytical solutions exist (IGWMC Level 2). Here, verification is attempted by using complex, synthetic data sets representing hypothetical or strongly simplified real-world systems, specially designed for testing specific types of models or code features (*e.g.*, in the neighborhood of singularities [wells] and discontinuities in the parameter field [flow barriers, abrupt changes in hydrogeology]). At the third level, the model (and its code) is validated against independently obtained field or laboratory data (IGWMC Level 3).

The study of Huyakorn *et al.* (1984a) applied the IGWMC testing approach to the two-dimensional finite element code SEFTRAN (Huyakorn *et al.*, 1984b). In Level 1 testing, six analytical solutions were used. The problems were selected to allow verification of several distinct features of the Galerkin formulation and its coding. For each problem, a range of realistic values of the flow and transport parameters was selected to evaluate the code's numerical behavior under various potential application conditions. The six problems considered range from a simple one-dimensional problem to a relatively complex two-dimensional problem involving transport in a nonuniform flow field:

- transport of a retarding solute in a semi-infinite column with a first-type (Dirichlet) inlet boundary condition;
- transport of a retarding and decaying solute in a semi-infinite column with a third-type (Cauchy) inlet boundary condition;
- transport from a continuous point source in a uniform ground-water flow field;
- transport of a slug released from a point source in a uniform ground-water flow field;
- transport in a radial flow field created by an injection well; and
- transport in a nonuniform flow field created by a recharging-discharging well pair.

For each of the problems, the report provides a detailed problem statement, test objectives, input specification, spatial and temporal discretization and simulation results. As expected, the code displayed significant numerical problems for simulations with high Peclet numbers (Figure 5), a coarse grid discretization (Figure 6), and a doublet (recharging-discharging well pair) with small dispersivity values (Figure 7).

In level 2 testing of the code, two hypothetical field situations were used. The problems included an irregular geometry and complex boundary conditions as well as heterogeneous and anisotropic system characteristics. The first situation involves a cross-section analysis of contaminant transport in an unconfined aquifer system located underneath a landfill. The second situation involves an areal analysis of contaminant transport from a disposal pit to a pumping well. Test objectives included:

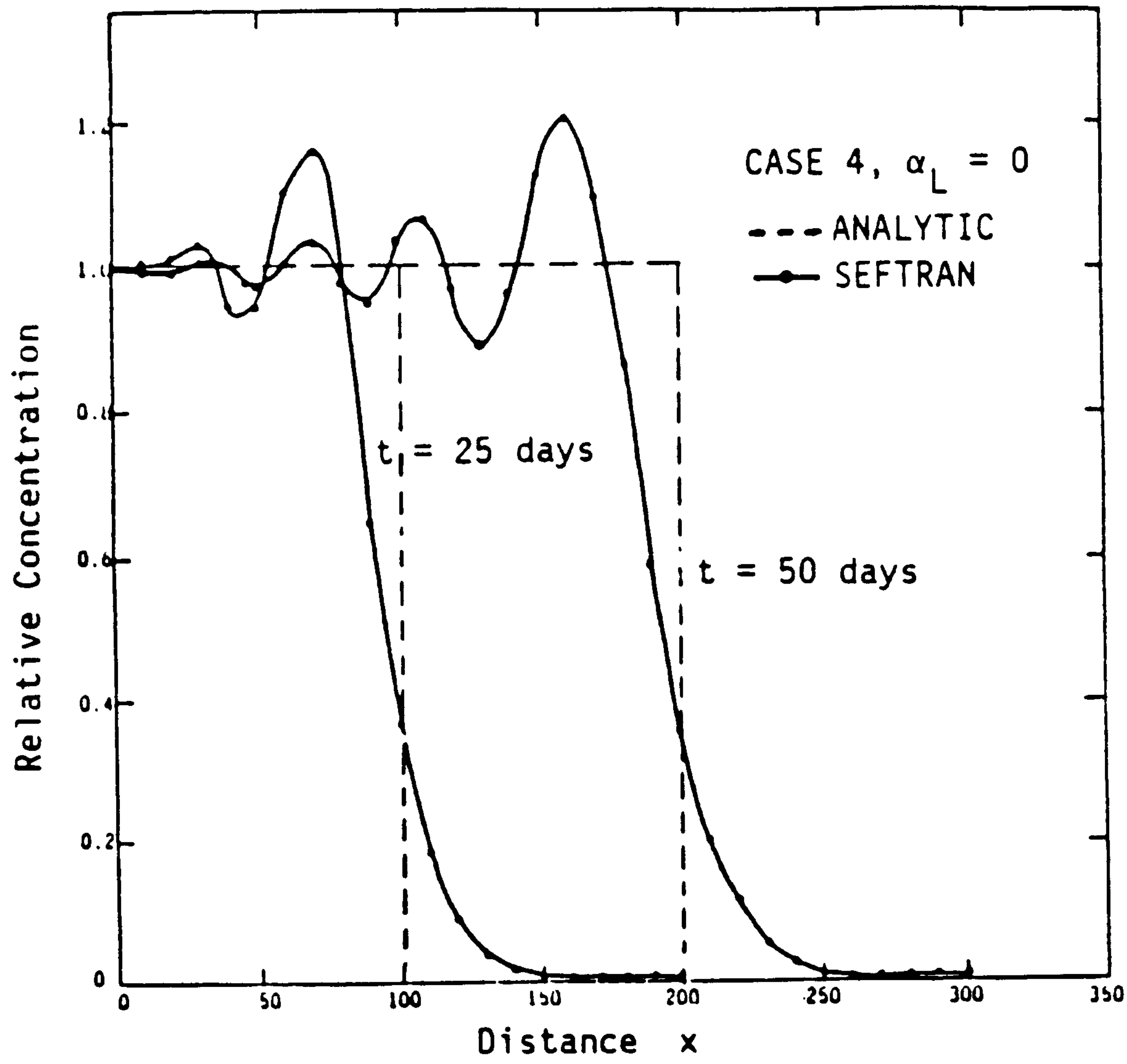


Figure 6. Comparison of analytical and numerical solutions for problem 1.1, case 4 with Pe = ∞ (*i.e.*, pure advection) (from Huyakorn *et al.*, 1984a).

- to determine the ability of the code to accommodate irregular geometry and zonal variations of aquifer properties;
- to evaluate the ability of the code to handle associated, time-dependent flow and transport problems; and
- to assess the efficiency with which the code can represent a region of complex geometry.

The evaluation of these test objectives was limited to a rather intuitive, qualitative assessment of the reality of the simulation results, and by examining the numerical solution for irregular behavior.

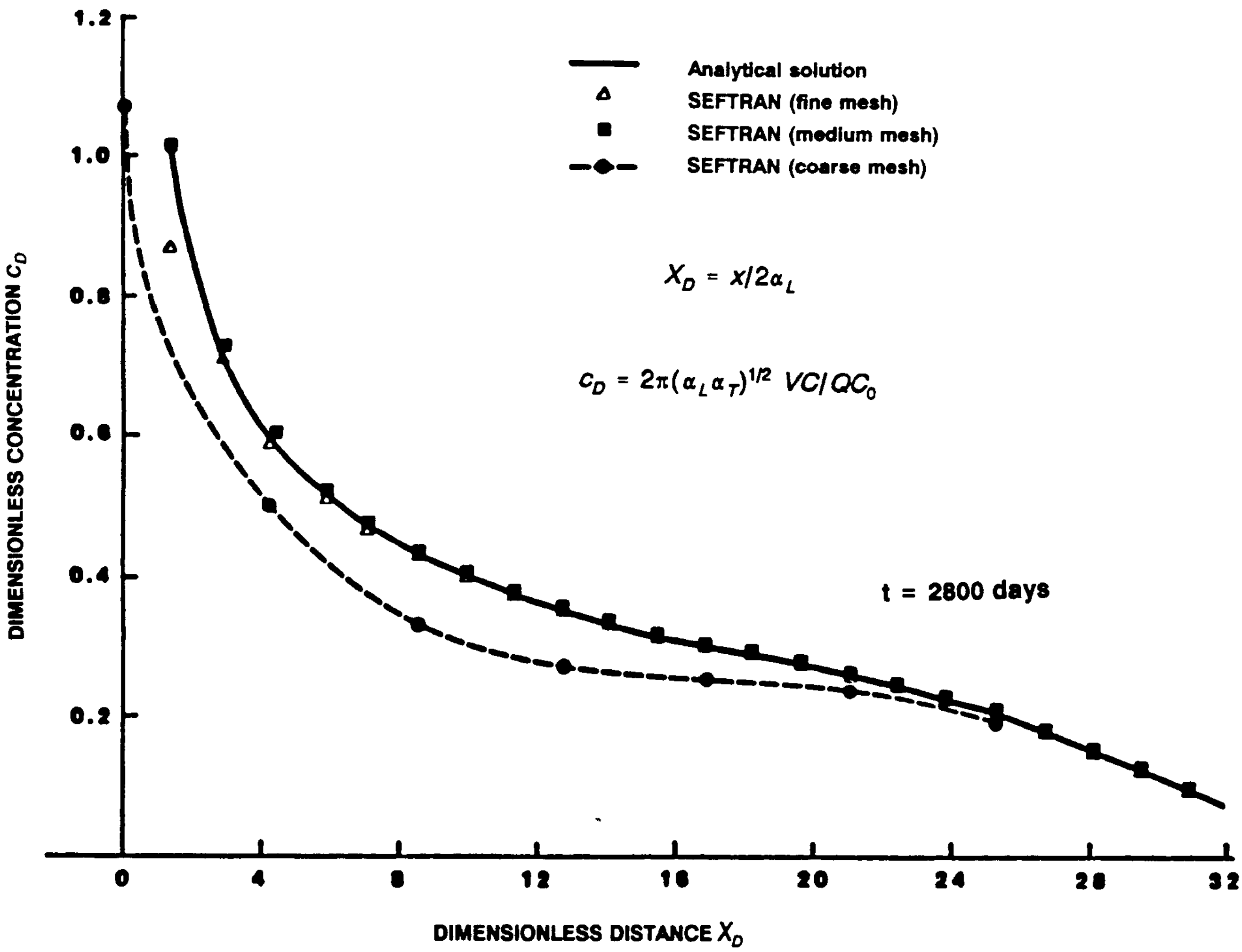


Figure 7. Concentration distributions along x-axis showing comparison of analytical and numerical solutions for problem 1.3, case 1 (from Huyakorn *et al.*, 1984a).

For Level 3 testing Huyakorn *et al.* (1984a) used the experimental data set describing the movement of a chloride plume at the Canadian Air Forces Base Borden Landfill, Ontario, Canada. The simulation results obtained by the study team were compared with field observations and predictions made by other modeling teams.

Beljin (1988) applied the IGWMC testing approach to three two-dimensional solute transport models, representing different numerical solution techniques. The code SEFTRAN (Huyakorn *et al.*, 1984b) represents a form of the finite element technique, the USGS 2D-TRANSPORT/MOC/KONBRED code combines the method of characteristics with a finite difference solution technique (Konikow and Bredehoeft, 1978), and RANDOM WALK (Prickett *et al.*, 1981) uses a finite difference approximation for flow and a random walk particle movement technique for transport. The numerical accuracy of the computational algorithms was verified by comparing simulation results with five analytical solutions for solute transport.

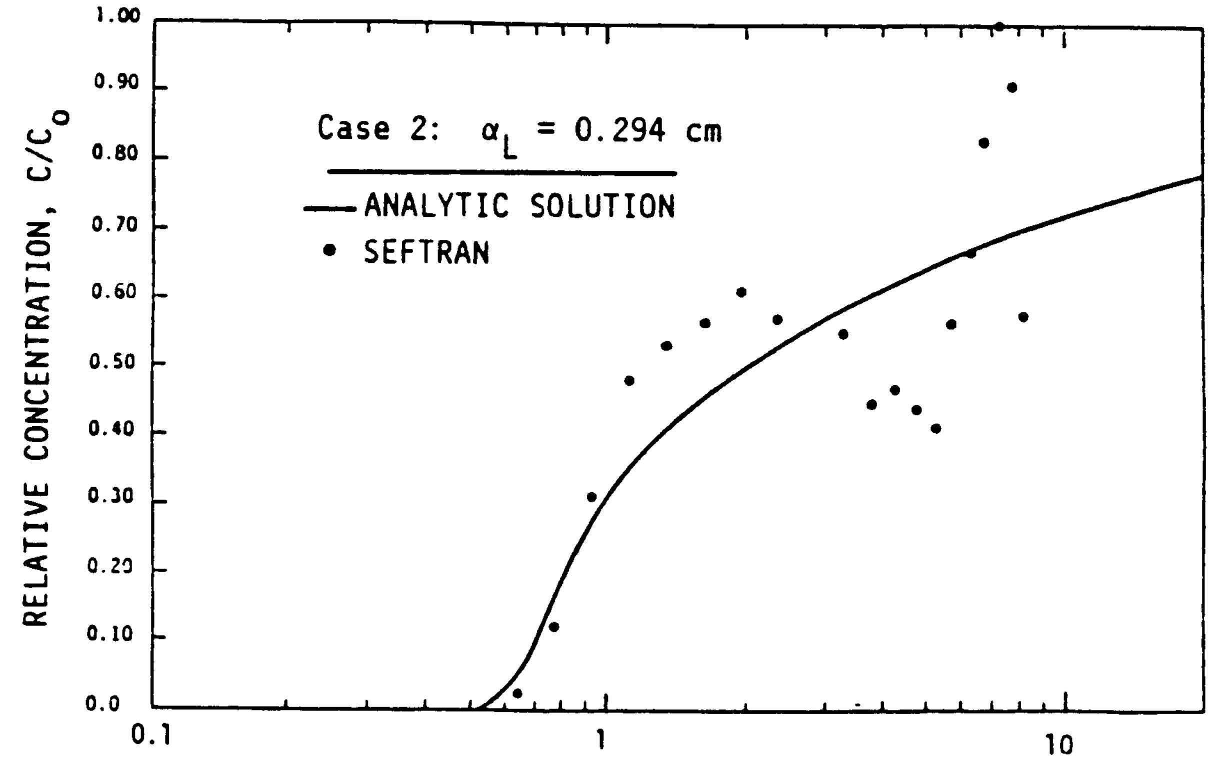


Figure 8. Time versus concentration at the pumped well showing comparison of analytical and numerical solutions for problem 1.6, case 2 (from Huyakorn *et al.*, 1984a).

Verification was also used to evaluate the sensitivity of each code to various parameters as well as to time and space discretization. For each test problem, specific test objectives, the mathematical formulation, and the data sets used are given. Beljin (1988) selected the first five of the six Level 1 test problems formulated by Huyakorn *et al.* (1984a). The numerical results of the codes were compared with the analytical solutions in both tabular and graphical representations. Graphical display of the results was in the form of relative concentration versus distance for a particular time since the start of the release (see Figure 8), and relative concentration versus time for a particular distance from the source (see Figure 9). The report expressed the goodness-of-fit both qualitatively and quantitatively. Qualitatively, it is described by such attributes as "poor," "reasonable," "acceptable," "good," and "very good." Quantitavely, the goodness-of-fit is expressed by the root-mean-squared error between the analytically and numerically computed values of concentration.

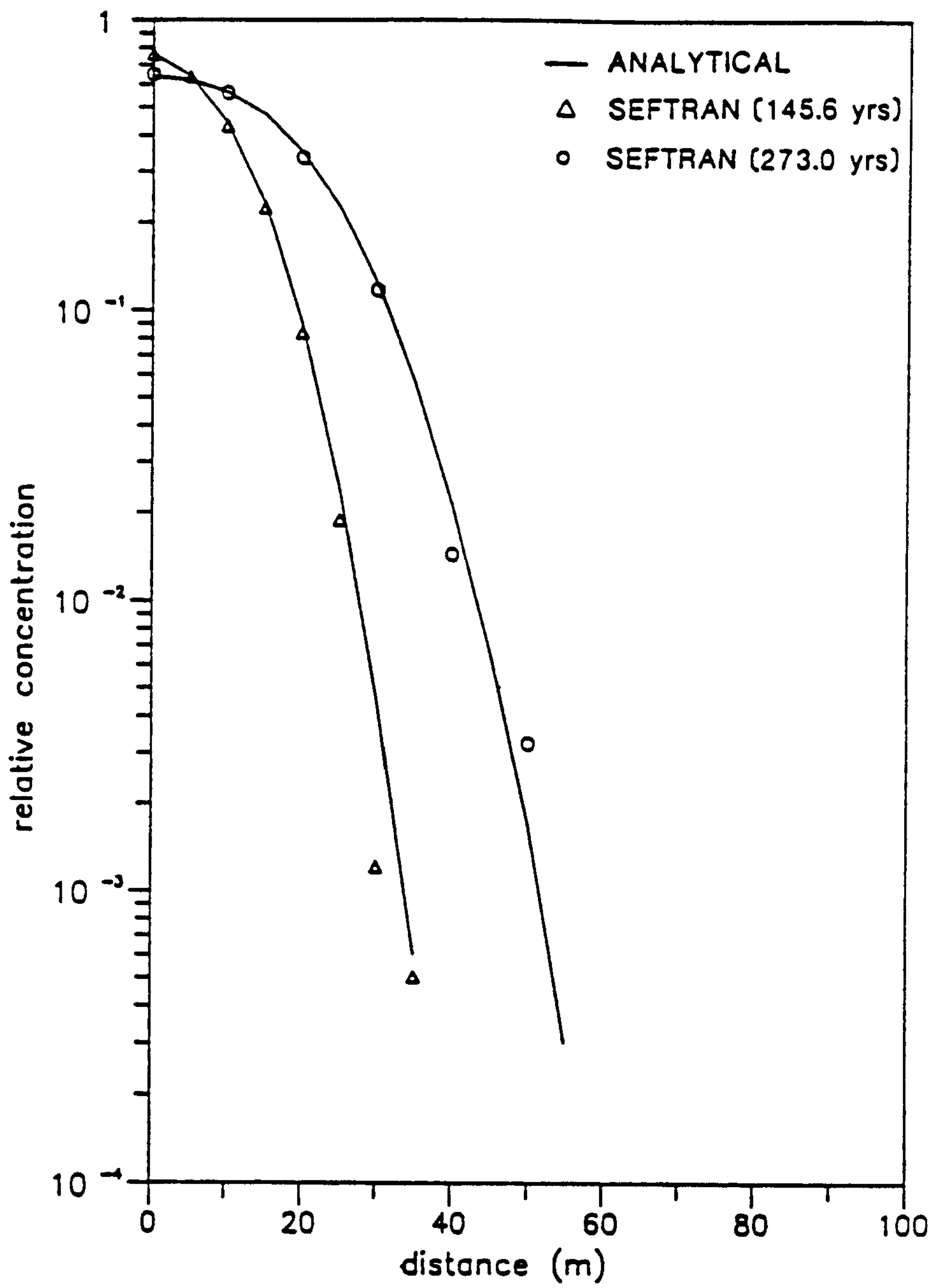


Figure 9. Comparison of analytical and numerical solutions for problem BM-1.2; relative concentration versus distance (from Beljin, 1988).

3.3. THE NEED FOR COMPARATIVE CODE TESTING

Although the preceding literature review illustrates some of the work now under way in code testing, a more systematic code testing approach is needed, together with unified and consistent guidelines and

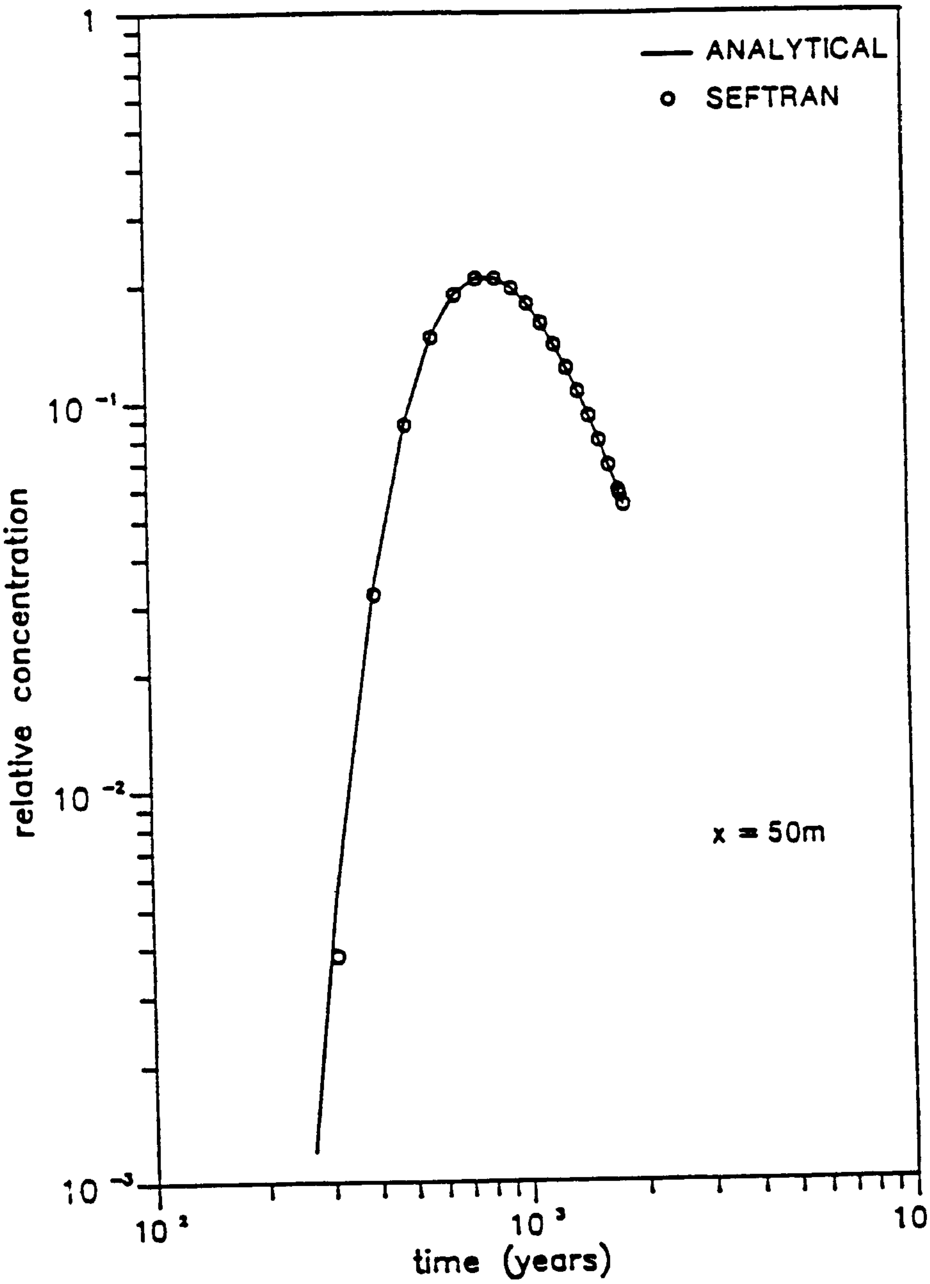


Figure 10. Comparison of analytical and numerical solutions for problem BM-1.2; relative concentration versus time (from Beljin, 1988).

procedures (Donigian, 1983). Such a testing approach should provide benchmark problems (*i.e.*, problem description, data set, and solution), applicable to a wide range of code types, and addressing all potential code performance problem areas. Furthermore, such a testing approach should provide quantitative and qualitative measures for evaluation of the verification and validation progress, and for establishing code performance characteristics. It should be noted that when a code is subjected to such a systematic and comprehensive procedure, the opportunity exists to evaluate the code's documentation and operational characteristics.

As pointed out in Streile and Simons (1986), since few experimental investigations have tested the multi-dimensional theories and conceptualizations, research aimed at verifying and validating the simulation models is urgently needed. Engesgaard and Christensen (1988), in their study of chemical transport models, also support further verification and validation studies of transport processes and chemical transformations in such models. It is their assertion that further efforts should be directed toward model testing studies rather than toward the development of more complex models. It is generally believed the credibility of current capabilities of computer models should be established before extending those capabilities.

3.4. TESTING STRATEGY AND EXAMPLE BENCHMARK PROBLEMS

In testing a code, it should be subject to a step-wise evaluation of its performance at simulating increasingly complex problems. The IGWMC testing strategy attempts to do this by focusing first on Level 1 testing, and, if successfully completed, continuing with Level 2 testing. Eventually, if an adequate field or laboratory data set is available, the code's (and its underlying theoretical model) might gain further credibility by being subject to Level 3 testing.

For saturated flow codes focus of the testing will be the computation of the distribution of hydraulic head (in space and time), head gradients, global water balance and individual boundary fluxes, flow velocity patterns (direction and magnitude), flow path lines, capture zones, and travel times. For solute transport codes such evaluations will concern the concentration distribution in the aquifer (in space and time), global mass balance (per species), and breakthrough curves at observation points and sinks (wells, streams).

At Level 1, the code is analyzed for its individual capabilities and functions. Test problems are designed to verify the operation of these functions (functionality testing). For flow simulating codes, such functions include the code's capabilities to handle boundary geometry and conditions, flow towards drains, flow from and towards streams, etc. Among others, flow fields are evaluated for numerical symmetry, and numerical solutions for iteration progress. For solute transport, concentration distributions in time and space are evaluated with respect to symmetry, numerical accuracy, and efficiency of the solution procedure. As most numerical solute transport models require calculation of the velocity field at each time step, special attention needs to be given to evaluate the accuracy of the direction and magnitude of the velocities used in the transport part of the code. This requires Level 1 benchmarks that not only provide the hydraulic head distribution, but also calculate the velocity distribution.

The Level 1 benchmarks for the numerical models range from simple calculations based on gradient analysis, Darcy's law and mass balances to complex analytical solutions. At this test level, not only the model's algorithms are checked but also its sensitivity for grid orientation and resolution, and time discretization. A review of coded analytical solutions for solute transport useful for Level 1 testing is included in Appendix A. In addition to the sources of information on analytical solution mentioned in Appendix A, analytical solutions for saturated flow may be found in Harr (1962), TNO (1964), Edelman (1972), Huisman (1972), Bear (1979), and Strack (1989). Analytical solutions for unsaturated flow can be found in Potter *et al.* (1987). Additional analytical solutions for solute transport are given in Lester *et al.* (1986) and Wexler (1992).

At Level 2, the code is applied to hypothetical problems designed to study specific code behavior, *e.g.*, around singularities and discontinuities in the parameter field and near irregularities in the internal and boundary geometries. Due to the absence of analytical solution to provide "ground truth", the code's test results are checked for unexpected or unexplained behavior and code intercomparison is used to obtain a relative measure of performance. This form of checking can be used to study the influence of a number of factors on code behavior. Such factors include various hydrogeologic conditions (such as aquifer stratification and heterogeneities), physico-chemical processes and ranges of their respective parameters, boundary and initial conditions, large variations in the gradient of the dependent variable, *(e.g.*, solute fronts), and sources and sinks. Some of the different conditions are summarized in Table 2.

As is the case on Level 1, at Level 2 grid orientation and resolution effects, as well as associated numerical dispersion and oscillations, are included in the evaluations. For this purpose, the test problems will be solved using a critical range of Peclet and Courant numbers. Accurate numerical solutions will be generated using codes that are known to effectively handle these critical conditions, high resolution numerical grids, and small time steps. This approach is based on the idea that the smaller the discretization is in space and time, the better the approximate numerical solution will represent the real (unknown) solution of the governing partial differential equation (Huyakorn and Pinder, 1983). The benchmarks will be developed in a step-wise fashion, going from coarse resolution grids and large time steps to higher resolution grids and smaller time steps. After each run, computational differences will be monitored (as well as the execution time). When further refinement, *e.g.*, with a factor 2, does not provide significant changes in the computational results, the benchmark is established. The high-resolution synthetic data sets and their solutions will be made available to model developers and users as benchmarks. To establish a benchmark at Level 2, the code selected needs to have successfully completed the Level 1 and Level 2 testing. Furthermore, successful field applications increase the credibility of the code, and the acceptance of benchmarks established with it. Examples of Level 2 test problems are given in Table 3 and Table 4.

Table 2. Typical field conditions for which model representation should be tested.

Boundary conditions

- specified head (constant or varying in time)
- recharge (from precipitation or as interflow; constant or varying in time)
- no flow
- specified flow
- head dependent flow (*e.g.*, streams, reservoirs, drains, spring flows, evapotranspiration)
- specified concentration
- specified solute flux
- concentration dependent solute flux

Sources/sinks

- wells (individual wells, wellfields)
- drains (open drains, subsurface drains)
- ponds, impoundments, lakes
- excavations, open mine pits
- point solute sources
- areal solute sources of limited extent
- non-point solute sources (*e.g.*, chemicals introduced by precipitation)

Aquifer conditions

- confined
- leaky-confined
- phreatic
- heterogeneity (*e.g.*, single aquifers, aquifer-aquitard systems, aquifers with low permeable discontinuous lenses, pinchouts of aquifers and confining beds, scale dependency, highly contrasted neighboring parameter zones)
- anisotropy (hydraulic conductivity, dispersivity)

Flow characteristics

- uniform flow field
- steady-state, symmetrically curved stream-lines
- non-steady flow field
- varying density
- porous media flow
- discrete fractures
- dual porosity

Transport processes

- advection-dominated transport
- advective-dispersive transport
- retardation (linear equilibrium adsorption)
- first-order decay

Table 3. Synthetic Data Set 1 (see Figure 11)

<u>*General Aspects*</u>:	This problem concerns the transport of a contaminant plume from a continuous areal source of limited extent into a generic but realistic unconfined ground-water system bound by a ground-water divide, two impermeable parallel rock outcrops and a fully penetrating stream.

(continued...)

Table 3 -- continued

Objectives: This problem verifies the capability of a transport code to simulate transport in a non-uniform, unconfined flow field, *i.e.* it tests for both the flow and transport simulating modules of the code. Grid orientation and resolution effects are explored in this stationary problem. Three types of grid orientation are used: (1) parallel to the main flow direction(s), (2) under a 45 degree angle with the main flow direction, and (3) under a 60 degree angle with the main flow direction. The problem will be run: (1) with only areal recharge and the solute source, (2) with only an active well and the solute source, and (3) with both areal recharge and an active well.

Assumptions:

- aquifer is homogeneous and isotropic with respect to hydraulic conductivity
- ground-water flow is steady
- fluid density and viscosity are constant
- solute source does not affect flow field

Specification of Parameters

A single pumping well (400 m^3/d) and a contaminant source are located in an aquifer measuring 200 m by 200 m wide and 21 m thick (for dimensions and location of source and location of well see figure 11. The following physical parameters are used in conducting the simulation:

$K_x = K_y = K_z = 1.0$ m/d (hydraulic conductivity for fine to medium sand)
$\theta = 0.35$ (porosity in fairly uniform sand)
$D^* = 1 \times 10^{-4}$ m^2/d (molecular diffusion coefficient)

dispersivity values

	α_L	α_{TH}	α_{TV}	
1	1.0	0.1	0.01	α_L = longitudinal dispersivity
2	1.0	0.01	0.01	α_{TH} = transverse horizontal dispersivity
3	1.0	0.01	0.001	α_{TV} = transverse vertical dispersivity
4	1.0	0.5	0.1	
5	5.0	0.1	0.1	

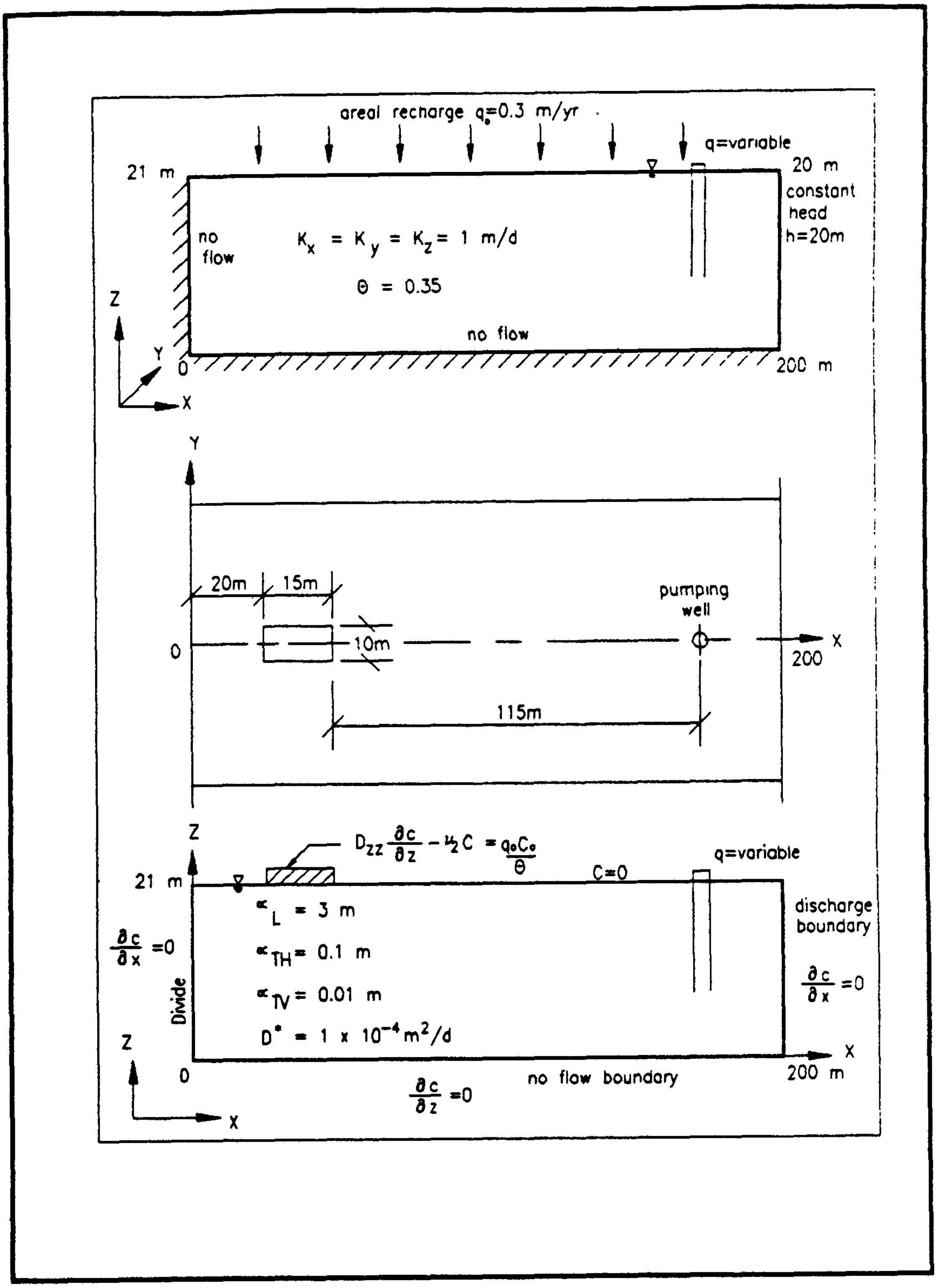


Figure 11. Synthetic data set 1: Movement of a contaminant plume from a continuous source in a non-uniform, unconfined flow field.

Table 4. Synthetic Data Set 2 (see Figure 12)

General Aspects: This problem involves the movement of a contaminant in an areally recharged unconfined aquifer composed of a fine silty sand, within which is located a discontinuous 2 m medium-grained sand layer. The boundaries are identical in nature to those of synthetic data set 1. This problem is based on Sudicky (1989).

Objectives: This problem verifies the capability of a transport code to simulate transport in a non-uniform, unconfined flow field, with heterogeneous aquifer properties in the vertical direction, *i.e.*, it tests for both flow and transport in a layered aquifer with lenses of high permeability. Grid orientation scenario is identical to the one used in synthetic data set 1.

Assumptions:

- aquifer is isotropic with respect to hydraulic conductivity
- ground-water flow is steady
- fluid density and viscosity are constant
- solute source does not affect flow field

Specification of Parameters

A contaminant source is located in an unconfined aquifer measuring 250 m by 250 m wide (for dimensions and location of source, location of boundaries and boundary conditions see Figure 12). The following physical parameters are used in conducting the simulation:

$K_{x1} = K_{y1} = K_{z1} = 5 \times 10^{-4}$ cm/s (hydraulic conductivity for fine silty sand)
$K_{x2} = K_{y2} = K_{z2} = 1 \times 10^{-2}$ cm/s (hydraulic conductivity for medium-grained sand)
$\theta = 0.35$ (porosity in fairly uniform sand)
$D^* = 1.34 \times 10^{-5}$ cm^2/s (molecular diffusion coefficient)

dispersivity values

	α_L	α_{TH}	α_{TV}
1	1.0	0.1	0.01
2	1.0	0.01	0.01
3	1.0	0.01	0.001
4	1.0	0.5	0.1
5	5.0	0.1	0.1

α_L = longitudinal dispersivity
α_{TH} = transverse horizontal dispersivity
α_{TV} = transverse vertical dispersivity

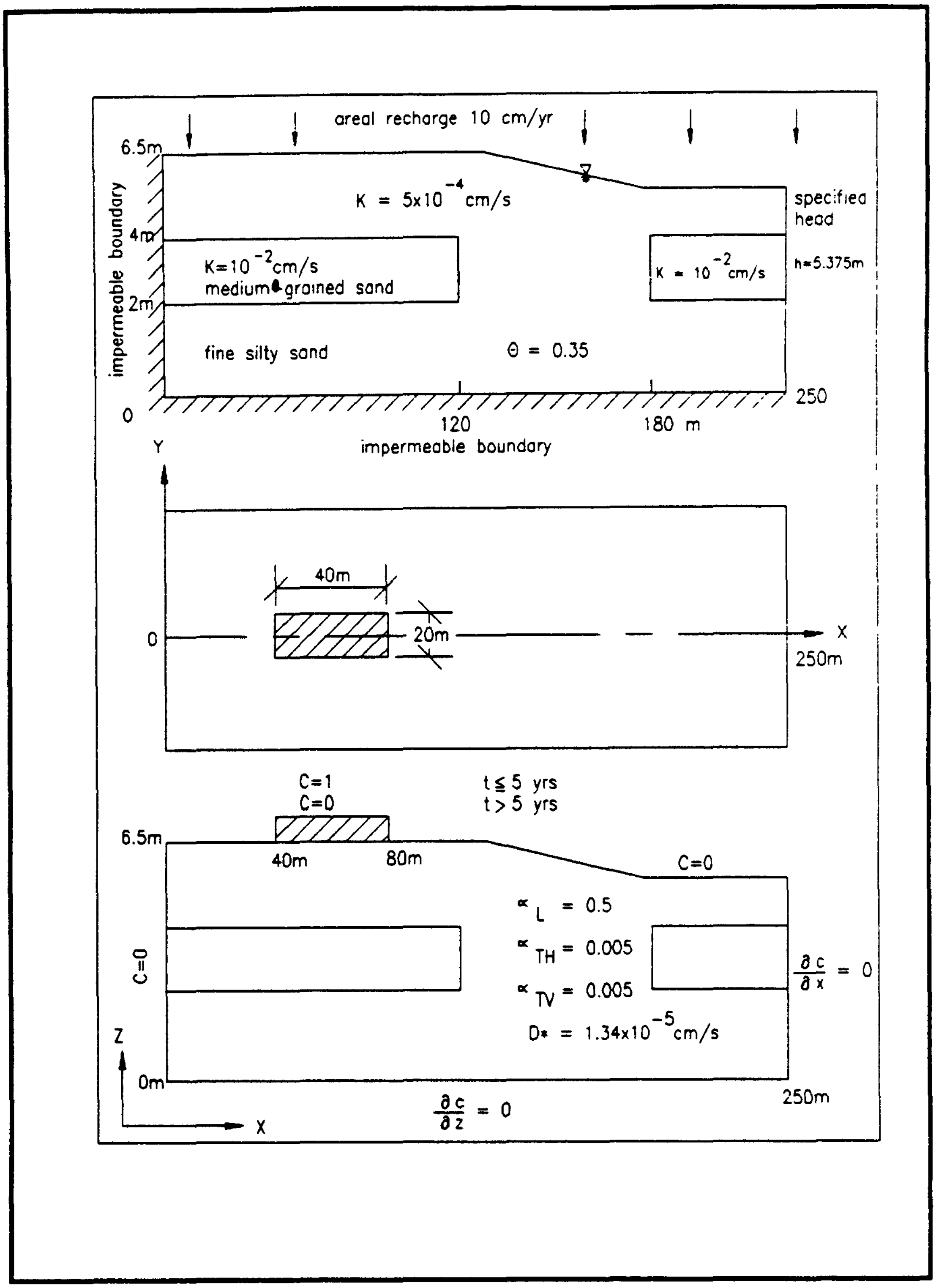


Figure 12. Synthetic data set 2: Contaminant transport in a heterogeneous aquifer

As discussed before, there should be a logical progression in the sequence of test problems. The "code tester" should evaluate the results of each test before proceeding with the next test. If necessary, the current test problem needs to be repeated with different input values to explore the code's behavior under various parameter and stress conditions (*i.e.*, performance evaluation). Table 5 presents such a sequence designed for testing of three-dimensional solute transport codes.

Table 5. Test scenario for three-dimensional solute transport codes.

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1. Solute transport in a steady-state uniform flow field in a large homogeneous isotropic aquifer (analytical solutions are available);

2. Solute transport in a non-uniform steady-state flow field in a large homogeneous aquifer (analytical solutions available);

3. Solute transport in a non-uniform flow field in a large homogeneous aquifer (analytical solutions not available):
   - 3.1. steady-state flow field with:
     - 3.1.1. different solute source patterns
     - 3.1.2. different boundary conditions
     - 3.1.3. different boundary conditions, combined with sources and sinks (for flow and solute transport)
   - 3.2. non-steady flow field with:
     - 3.2.1. sources and sinks (for flow and solute transport)
     - 3.2.2. different boundary conditions
     - 3.2.3. both

4. Non-uniform flow field in a heterogeneous anisotropic aquifer (no analytical solutions available):
   - 4.1. layered system
     - 4.1.1. steady-state flow field with:
       - 4.1.1.1. sources and sinks
       - 4.1.1.2. different boundary conditions
       - 4.1.1.3. both
     - 4.1.2. non-steady flow field with:
       - 4.1.2.1. sources and sinks
       - 4.1.2.2. different boundary conditions
       - 4.1.2.3. both

continued.....

Table 5 – continued

4.2. lens heterogeneities

- 4.2.1. steady-state flow field with:
  - 4.2.1.1. sources and sinks
  - 4.2.1.2. different boundary conditions
  - 4.2.1.3. both
- 4.2.2. non-steady flow field with:
  - 4.2.1.1. sources and sinks
  - 4.2.1.2. different boundary conditions
  - 4.2.1.3. both

4.3. random heterogeneities

- 4.3.1. steady-state flow field with:
  - 4.3.1.1. sources and sinks
  - 4.3.1.2. different boundary conditions
  - 4.3.1.3. both
- 4.3.2. non-steady flow field with:
  - 4.3.2.1. sources and sinks
  - 4.3.2.2. different boundary conditions
  - 4.3.2.3. both

4. CONCLUSIONS

There is a urgent need for comprehensive, systematic testing of all types of ground-water models and for the establishment of a verification and validation protocol. Ground-water management decisions should be based on the use of technically and scientifically sound methods of data collection, information processing, and interpretation. Because few experimental investigations have tested multidimensional theories, conceptualization, and associated computer codes, it is extremely important to conduct further research aimed at developing and executing verification and validation studies for prominent ground-water models. It may be argued that from a ground-water management point-of-view further efforts should be directed towards model testing studies rather than toward the development of more complex models.

In recent years, the IGWMC has developed a testing procedure and methodology for model evaluation as part of its efforts to implement a comprehensive quality assurance program. The current project attempts to systematically analyze the scientific considerations and collect the technical elements for implementation of such a methodology. The next step is the application of this comprehensive methodology to actual computer codes.

5. REFERENCES

Adrion, W.R., M.A. Branstad, and J.C. Cherniasky. 1986. Validation, Verification and Testing of Computer Software. In: S.J. Andriole (ed.), Software Validation, Verification, Testing and Documentation, pp. 81-131, Petrocelli Books, Princeton, New Jersey.

American Society for Testing and Materials (ASTM). 1984. Standard Practices for Evaluating Environmental Fate Models of Chemicals. Annual Book of ASTM Standards, E 978-84, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Anderson, M.P., and W.W. Woessner. 1992. Applied Groundwater Modeling: Simulation of Flow and Advective Transport. Academic Press, Inc., San Diego, California.

Bear, J. 1979. Hydraulics of Groundwater. McGraw-Hill, New York, New York.

Beljin, M.S. 1988. Testing and Validation of Models for Simulating Solute Transport in Groundwater. GWMI 88-11. International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

Bonazountas, M., and J. Wagner. 1984. SESOIL: A Seasonal Soil Compartment Model. Arthur D. Little, Inc., Cambridge, Massachusetts.

Boutwell, S.H., S.M. Brown, B.R. Roberts, and D.F. Atwood. 1985. Modeling Remedial Actions at Uncontrolled Hazardous Waste Sites. EPA/540/2-85/001, U.S. Environmental Protection Agency, OSWER/ORD, Washington, D.C.

Brandstetter, A, and B.E. Buxton. 1987. The Role of Geostatistical, Sensitivity and Uncertainty Analysis in Performance Assessment. In: Proceedings of the '87 DOE/AECL Conference on Geostatistical, Sensitivity and Uncertainty Methods for Groundwater Flow and Radionuclide Transport Modeling, September 15-17, 1987. CONF-870971. U.S. Department of Energy, Washington, D.C.

Bryant, J.L., and N.P. Wilburn. 1987. Handbook of Software Quality Assurance Techniques Applicable to the Nuclear Industry. NUREG/CR-4640, Office of Nuclear Reactor Regulation, U.S. Nuclear Regulatory Commission, Washington, D.C.

Carsel, R.F., W.B. Nixon, and L.G. Balentine. 1986. Comparison of Pesticide Root Zone Model Predictions with Observed Concentrations for the Tobacco Pesticide Metalaxyl in Unsaturated Zone Soils. Environmental Toxicology and Chemistry, 5(4):345-353.

Carsel, R.F., C.N. Smith, L.A. Mulkey, J.D. Dean, and P. Jowise. 1984. User's Manual for the Pesticide Root Zone Model (PRZM): Release 1. EPA-600/3-84-109, U.S Environmental Protection Agency, Environmental Research Laboratory, Athens, Georgia.

Codell, R. and S. Silling. 1984. Draft Quality Assurance Plan for Operational Software. Memorandum 3110/DC/84/09/20/0, Division of Waste Management, U.S.Nuclear Regulatory Commission, Washington, D.C.

Donigian, Jr., A.S. 1983. Model Predictions vs. Field Observations: The Model Validation/Testing Process. In: R.L. Swann and A. Eschenroeder (eds.), Fate of Chemicals in the Environment, ACS Symposium Series 225, American Chemical Society, Washington, D.C.

Donigian, Jr., A.S. and P.S.C. Rao. 1986. Example Model Testing Studies. In: S.C. Hern and S.M. Melancon (eds.), Vadose Zone Modeling of Organic Pollutants, pp. 103-131, Lewis Publishers, Chelsea, Michigan.

Edelman, J.H. 1972. Groundwater Hydraulics of Extensive Aquifers. Bulletin 13, International Institute for Land Reclamation and Improvement, Wageningen, The Netherlands.

Enfield, C.G., R.F. Carsel, S.Z. Cohen, T. Phan, and D.M. Walters. 1982. Approximating Pollutant Transport to Ground Water. Ground Water, 20:711-722.

Engesgaard, P. and Th.H. Christensen. 1988. Review of Chemical Solute Transport Models. Nordic Hydrology, NOHYBB 19(3):183-216.

Faust, C.R., P.N. Sims, C.P. Spalding, P.F. Andersen, and D.E. Stephenson. 1990. FTWORK: A Three-Dimensional Groundwater Flow and Solute Transport Code. WRSC-RP-89-1085, Westinghouse Savannah River Company, Aiken, South Carolina.

Federal Computer Performance Evaluation and Simulation Center (FEDSIM). 1981. Computer Model Documentation Guide. NBS Special Publication 500-73, Institute for Computer Science and Technology, National Bureau of Standards, U.S. Department of Commerce, Washington, D.C.

Fjeld, R.A., B.L. Sill, and B.B. Looney. 1987. The Sensitivity Index as a Screening Tool in the Analysis of Ground-Water Contaminant Transport. In: B.E. Buxton (ed.), Geostatistical, Sensitivity, and Uncertainty Methods for Ground-Water Flow and Radionuclide Transport Modeling, pp. 323-325. Battelle Press, Columbus, Ohio.

Freeze, R.A., J. Massman. L. Smith, T. Sperling, and B. James. 1990. Hydrogeological Decision Analysis: 1. A Framework. Ground Water 28(5):738-766.

Freyberg, D.L. 1988. An Exercise in Ground-Water Model Calibration and Prediction. Ground Water

26(3):350-360.

Gass, S.I. 1979. Computer Model Documentation: A Review and an Approach. NBS Special Publication 500-39, Institute for Computer Science and Technology, National Bureau of Standards, U.S. Department of Commerce, Washington, D.C.

Gupta, S.K., C.R. Cole, F.W. Bond, and A.M. Monti. 1984. Finite-Element Three-Dimensional Ground-Water (FE3DGW) Flow Model: Formulation, Computer Source Listings, and User's Manual. BMI/ONWI-548, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio.

Gupta, S.K., C.R. Cole, C.T. Kincaid, and A.M. Monti. 1987. Coupled Fluid, Energy, and Solute Transport (CFEST) Model; Formulation and User's Manual. BMI/ONWI-660, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio.

Harlan, C.P., and G.F. Wilkinson. 1988. High-Level Waste Management Code Maintenance and Quality Assurance. SAND87-2254/UC-70. Sandia National Laboratories, Albuquerque, New Mexico.

Harr, M.E. 1962. Groundwater and Seepage. McGraw-Hill, New York, New York.

Hecox, G.R., J. Rohde, and Z. Tuta. 1989. Methods and Field Audit Results of a Remedial Design Using a Verified Ground Water Model. In: Proceedings, 4th International Conference on Solving Ground Water Problems with Models, February 7-9, 1989, Indianapolis, Indiana. National Ground Water Association, Dublin, Ohio.

Hern, S.C., S.M. Melancon, and J.E. Pollard. 1985. Generic Steps in the Field Validation of Vadose Zone Fate and Transport Models. In: Hern, S.C., and S.M. Melancon (eds.), Vadose Zone Modeling of Organic Pollutants, pp.61-80. Lewis Publishers, Inc., Chelsea, Michigan.

Huisman, L. 1972. Groundwater Recovery. Macmillan Publishing Co., London, United Kingdom.

Huyakorn, P.S. and Pinder, G.F. Computational Methods in Subsurface Flow. Academic Press, New York, New York 1983.

Huyakorn, P.S., A.G. Kretschek, R.W. Broome, J.W. Mercer, and B. H. Lester. 1984a. Testing and Validation of Models for Simulating Solute Transport in Groundwater: Development, Evaluation, and Comparison of Benchmark Techniques. GWMI 84-13, International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

Huyakorn, P.S., R.W. Broome, A.G. Kretschek, and J.W. Mercer. 1984b. SEFTRAN: A Simple and Efficient Transport Code. GeoTrans, Inc., Herndon, Virginia.

HYDROCOIN Work Group. 1988. The International Hydrocoin Project, Level One: Code Verification. Swedish Nuclear Power Inspectorate (SKI), Stockholm, Sweden.

HYDROCOIN Work Group. 1990. The International Hydrocoin Project, Level Two: Model Validation. Swedish Nuclear Power Inspectorate (SKI), Stockholm, Sweden.

Intera Environmental Consultants, Inc. 1983. A Proposed Approach to Uncertainty Analysis. ONWI-488, Battelle Memorial Institute, Columbus, Ohio.

INTRACOIN Work Group. 1984. International Nuclear Transport Code Intercomparison (INTRACOIN) Study: Final Report Level One - Code Verification. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

INTRACOIN Work Group. 1986. International Nuclear Transport Code Intercomparison (INTRACOIN) Study: Final Report Levels Two and Three - Model Validation and Uncertainty Analysis. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

INTRAVAL. 1990. An International Project to Study Validation of Geosphere Transport Models, Progress Report 5. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Jones, R.L., P.S.C. Rao, and A.G. Hornsby. 1983. Fate of Aldicarb in Florida Citrus Soils: 2. Model Evaluation. In: Proceedings, NWWA/U.S.EPA Conference on Characterization and Monitoring of the Vadose (Unsaturated) Zone, Las Vegas, Nevada. National Water Well Association, Dublin, Ohio.

Khoury, M.A., H.A. Simons, and J.W. Scarrow. 1989. Modeling Aquifer Mounding beneath the Manasquan Reservoir. In: Proceedings, Conference Solving Ground Water Problems with Models, Indianapolis, Indiana, February 7-9, 1989. pp. 715-734. National Water Well Association, Columbus, Ohio.

Kincaid, C.T., J.R. Morrey, and J.E. Rogers. 1984. Geo-hydrological Models for Solute Migration; Vol. 1: Process Description and Computer Code for Selection. EA 3417.1, Electric Power Research Institute, Palo Alto, California.

Kinzelbach, W. 1987. Methods for the Simulation of Pollutant Transport in Ground Water -- A Model Comparison. In: Proceedings, Conference on Solving Ground Water Problems with Models, Denver, Colorado, February 10-12, 1987. pp. 656-674. National Water Well Association, Dublin, Ohio.

Koch, Jr., G.S., and R.F. Link. 1980. Statistical Analysis of Geological Data. Dover Publications Inc., New York, New York.

Konikow, L.F., 1986. Predictive Accuracy of a Ground-Water Model--Lessons from a Post-Audit. Ground

Water 24(2):677-690.

Konikow, L.F., and J.D. Bredehoeft. 1978. Computer Model of Two Dimensional Solute Transport and Dispersion in Ground Water. Techniques of Water-Resources Investigations, Book 7, Chapter C2. U.S. Geological Survey, Reston, Virginia.

Konikow, L.F. and E.P. Patten, Jr. 1985. Groundwater Forecasting. In: M.G. Anderson and T.P. Burt (eds.), Hydrologic Forecasting, pp. 221-270. John Wiley and Sons, Ltd., Chichester, United Kingdom.

Lapidus, L., and G.F. Pinder. 1982. Numerical Solution of Partial Differential Equations in Science and Engineering. John Wiley and Sons, New York, New York.

Lester, B.H., P.S. Huyakorn, H.O. White, Jr., T.D. Wadsworth, and J.E. Buckley. 1986. Analytical Models for Evaluating Leachate Migration in Groundwater Systems. Report by GeoTrans, Inc., Herndon, Virginia, for U.S. Environmental Protection Agency, Office of Solid Waste, Washington, D.C.

Lewis, B.D. and F.J. Goldstein. 1982. Evaluation of a Predictive Ground-Water Solute Transport Model at the Idaho National Engineering Laboratory, Idaho. Water Resources Investigations 82-25, U.S. Geological Survey, Reston, Virginia.

Mathsoft. 1991. Mathcad®3.0 User's Guide Windows Version. Mathsoft, Inc., Cambridge, Massachusetts.

McLaughlin, D., and W.K. Johnson. 1987. Comparison of Three Groundwater Modeling Studies. ASCE Journal of Water Resources Planning and Management 113(3):405-421.

Mercer, J.W., and C.R. Faust. 1981. Ground Water Modeling, National Water Well Association, Dublin, Ohio.

National Bureau of Standards (NBS). 1976. Guidelines for Documentation of Computer Programs and Automated Data Systems. FIPS 38, Federal Information Processing Standards Publications, U.S. Department of Commerce, Washington, D.C.

National Research Council (NRC), Committee on Ground Water Modeling Assessment, Water Science and Technology Board. 1990. Ground Water Models: Scientific and Regulatory Applications. National Academy Press, Washington, D.C.

Nicholson, T.J., T.J. McCartin, P.A. Davis, and W. Beyeler. 1987. NRC Experiences in HYDROCOIN: An International Project for Studying Ground-Water Flow Modeling Strategies. In: Proceedings, GEOVAL 87, April 4-9, 1987, Stockholm. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.

Person, M. and L.F. Konikow. 1986. Recalibration and Predictive Reliability of a Solute-Transport Model of an Irrigated Stream-Aquifer System. Journal of Hydrology 87:145-165.

Pinder, G.F. and J.D. Bredehoeft. 1968. Application of the Digital Computer for Aquifer Evaluation. Water Resources Research 4(5):1069-1093.

Pinder, G.F., and E.O. Frind. 1972. Application of Galerkin's Procedure to Aquifer Analysis. Water Resources Research 8(1):108-120.

Potter, S.T., E.B. Richie, and R.R. Schnabel. 1987. Verification of Numerical Models - Variably Saturated Flow Through a Heterogeneous Media. In: Proceedings, Conference on Solving Ground Water Problems With Models, Denver, Colorado, February 10-12, 1987. pp. 424-443. National Water Well Association, Dublin, Ohio.

Prickett, T.A. and C.G. Lonnquist. 1971. Selected Digital Computer Techniques for Groundwater Resource Evaluation. Bulletin 55, Illinois State Water Survey, Champaign, Illinois.

Prickett, T.A., T.G. Naymik, and C.G. Lonnquist. 1981. A 'Random-Walk' Solute Transport Model for Selected Ground Water Quality Evaluations. Bulletin 65, Illinois State Water Survey, Champaign, Illinois.

Rao, P.S.C., R.E. Jessup, and A.C. Hornsby. 1981. Simulation of Nitrogen in Agro-Ecosystems: Criteria for Model Selection and Use. In: Nitrogen Cycling in Ecosystems of Latin America and the Caribbean; Proceedings of International Workshop, Cali, Colombia, March 16-21, 1981, pp.1-16.

Reeves, M., D.S. Ward, N.D. Johns, and R.M. Cranwell. 1986. Theory and Implementation for SWIFT II, The Sandia Waste-Isolation Flow and Transport Model for Fractured Media; Release 8.84. NUREG/CR-3328, SAND83-1159, Sandia National Laboratory, Albuquerque, New Mexico.

Ritchey, J.D. 1989. Standards for Ground Water Modeling: What and Why. In: Proceedings, Conference on Solving Ground Water Problems with Models, Indianapolis, Indiana, February 7-9, 1989, P. 869-878. National Water Well Association, Dublin, Ohio.

Silling, S.A. 1983. Final Technical Position on Documentation of Computer Codes for High-level Waste Management. NUREG/CR-0856-F, Off. of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commission, Washington, D.C.

Simmons, C.S., and C.R. Cole. 1985. Guidelines for Selecting Codes for Groundwater Transport Modeling of Low-Level Waste Burial Sites. Volume 1: Guideline approach. PNL-4980 Vol. 1. Battelle Pacific NW Laboratory, Richland, Washington.

Sims, P.N., P.F. Andersen, D.E. Stephenson, and C.R. Faust. Testing and Benchmarking of a Three-Dimensional Groundwater Flow and Solute Transport Model. In: Proceedings, Conference on Solving Ground Water Problems with Models. Indianapolis, Indiana, February 7-9, 1989. National Water Well Association, Columbus, Ohio.

Strack, O.D.L. 1989. Groundwater Mechanics. Prentice-Hall, Englewood Cliffs, New Jersey.

Streile, G.P., and C.S. Simmons. 1986. Subsurface Flow and Transport of Organic Chemicals: An Assessment of Current Modeling Capability and Priority Directions for Future Research (1987-1995). PNL-6043, Battelle Pacific Northwest Laboratory, Richland, Washington.

Sudicky, E.A. 1989. The Laplace Galerkin Technique: A Time-Continuous Finite Element Theory and Application to Mass Transport in Groundwater. Water Resources Research 24(8):1833-1846

Sykes, J.F., S.B. Pahwa, D.S. Ward, and R.B. Lantz. 1983. The Validation of SWENT, a Geosphere Transport Model. In: R. Stepleman *et al.* (eds.), Scientific Computing. IMACS/North-Holland Publishing Company, New York, New York.

Taylor, J.K. 1985. What is Quality Assurance? In: J.K. Taylor and T.W. Stanley (eds.), Quality Assurance for Environmental Measurements, pp.5-11. ASTM Special Technical Publication 867, American Society for Testing and Materials, Philadelphia, Pennsylvania.

TNO-Central Organization for Applied Scientific Research. 1964. Steady Flow of Ground Water Towards Wells. Proceedings and Informations No. 10, Committee for Hydrological Research TNO, The Hague, The Netherlands.

U.S. Environmental Protection Agency (EPA). 1986. Information on Preparing Quality Assurance Narrative Statements. RSKERL-QA-2, Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

U.S. Environmental Protection Agency (EPA). 1992. Compendium of Model Information. OSWER Models Management Initiative: Pilot Project on Groundwater Modeling, Office of Solid Waste and Emergency Response, Washington, D.C.

U.S. Nuclear Regulatory Commission. 1988. NRC Model Simulations in Support of the Hydrologic Code Intercomparison Study (HYDROCOIN); Level 1-Code Verification. NUREG-1249, Vol. 1. Office of Nuclear Regulatory Research, Washington, D.C.

van der Heijde, P.K.M., P.S. Huyakorn, and J.W. Mercer. 1985. Testing and Validation of Ground Water Models. In: Proceedings, Conference on Practical Applications of Groundwater Models, Columbus, Ohio, August 19-20, 1985. National Water Well Association, Dublin, Ohio.

van der Heijde, P.K.M., and R.A. Park. 1986. U.S. EPA Groundwater Modeling Policy Study Group, Report of Findings and Discussion of Selected Groundwater Modeling Issues. International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

van der Heijde, P.K.M. 1987. Quality Assurance in Computer Simulations of Groundwater Contamination. Environmental Software 2(1):19-28.

van der Heijde, P.K.M., and M.S. Beljin. 1988. Model Assessment for Delineating Wellhead Protection Areas. EPA 440/6-88-002, Office of Ground-Water Protection, U.S. Environmental Protection Agency, Washington, D.C.

van der Heijde, P.K.M., A.I. El-Kadi, and S.A. Williams. 1988. Groundwater Modeling: An Overview and Status Report. EPA/600/2-89/028. U.S. Environmental Protection Agency, Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

van der Heijde, P.K.M. 1989. Quality Assurance and Quality Control in Groundwater Modeling. GWMI 89-04. International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

van der Heijde, P.K.M., and S.A. Williams. 1989. Design and Operation of the IGWMC Model Information Database MARS (Model Annotation Search and Retrieval System). GWMI 89-03, International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

van der Heijde, P.K.M. 1990. Quality Assurance in the Development of Groundwater Models. In: K. Kovar (ed.), "Calibration and Reliability in Groundwater Modeling." Proceedings ModelCARE 90, 271–278. The Hague, The Netherlands, September 3–6, 1990. IAHS Publication 195, Wallingford, United Kingdom.

van der Heijde, P.K.M., and O.A. Elnawawy. 1992. Compilation of Ground-Water Models. GWMI 91-06. International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado.

van Tassel, D. 1978. Program Style, Design, Efficiency, Debugging, and Testing, 2nd ed. Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

Ward, D.S., M. Reeves, and L.E. Duda. 1984. Verification and Field Comparison of the Sandia Waste-Isolation Flow and Transport Model (SWIFT). NUREG/CR-3316, Office of Nuclear Safety and Safeguards, U.S. Nuclear Regulatory Commission, Washington, D.C.

Watson, D.B., and S.M. Brown. 1985. Testing and Evaluation of the SESOIL Model. Anderson-Nichols

Company, Inc., Palo Alto, California.

Wexker, E.J. 1992. Analytical Solutions for One-, Two-, and Three-Dimensional Solute Transport in Ground-Water Systems with Uniform Flow. Techniques of Water-Resources Investigations, Book 3, Chapter B7. U.S. Geological Survey, Washington, D.C.

Wilkinson, G.F. and G.E. Runkle. 1986. Quality Assurance (QA) Plan for Computer Software Supporting the U.S. Nuclear Regulatory Commission's High-Level Waste Management Program. NUREG/CR-4369, Office of Nuclear Safety and Safeguards, U.S Nuclear Regulatory Commission, Washington, D.C.

Wolfram, S. 1991. Mathematica: A System for Doing Mathematics by Computer; Second Edition. Addison-Wesley Publishing Co., Redwood City, California.

Yourdon, E. and L.L. Constantine, 1979. Structured Design: Fundamentals and Systems Design. Prentice-Hall, Englewood Cliffs, New Jersey.

Zheng, C. 1990. MT3D: A Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reaction of Contaminants in Groundwater Systems. S.S. Papadopulos & Associates, Inc. Rockville, Maryland.

APPENDIX

Review of Three-dimensional Analytical Models for Solute Transport in Ground-Water Systems

Review of Three-dimensional Analytical Models for Solute Transport in Ground-Water Systems

Milovan S. Beljin, Ph.D.
Groundwater Research Center
University of Cincinnati
Cincinnati, Ohio 45221

Prepared for:
International Ground Water Modeling Center
Holcomb Research Institute
Butler University
Indianapolis, Indiana 46208

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Disclaimer

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Contents

List of Figures

List of Symbols

Roman

a	Dispersivity of porous medium, $[L]$
a_{ijkl}	Component of $a, [L]$
a_L	Longitudinal dispersivity of isotropic porous medium, $[L]$
a_T	Transversal dispersivity of isotropic porous medium, $[L]$
B	Saturated thickness of the aquifer, $[L]$
	Length of the vertical line source, $[L]$
C	Concentration of the solute, $[M/L^3]$
C'	Concentration of the solute in the injected fluid, $[M/L^3]$
C_i	Initial concentration of the solute, $[M/L^3]$
C_0	Concentration of the solute at the inlet boundary, $[M/L^3]$
C_{max}	Maximum (peak) concentration of the solute, $[M/L^3]$
D_{ij}	Coefficient of dispersion, $[L^2/T]$
D_L	Coefficient of longitudinal dispersion, $[L^2/T]$
D_T	Coefficient of transversal dispersion, $[L^2/T]$
D^*	Coefficient of molecular diffusion, $[L^2/T]$
g	Gravitational acceleration, $[L/T^2]$
K_d	Distribution coefficient, $[L^3/M]$
L	Length of the horizontal line source,
	Side length of the cubical source, $[L]$
M	Total mass of pollutant released, $[M]$
$\dot{M}$	Mass flux, dM/dt, $[M/T]$
M_s	Mass release rate, $[M/T]$
n	Porosity, $[-]$
n_i	Component of the unit vector

N Number of items

R_d Retardation factor, [−]

S Concentration of species adsorbed on solid, $[M/M]$

t Time, $[T]$
$t_{1/2}$ Half-life of solute, $[T]$
t_0 Time of source activity, $[T]$
T_{ij} Transmissivity tensor, $[L^2/T]$

V Ground-water (seepage) velocity, $[L/T]$

x Cartesian coordinate, $[L]$
x_s Distance to center of line source in x-direction, $[L]$
X Contaminant source dimension in x-direction, $[L]$

y Cartesian coordinate, $[L]$
y_s Distance to center of line source in y-direction, $[L]$
Y Contaminant source dimension in y-direction, $[L]$

z Cartesian coordinate, $[L]$
z_s Distance to center of line source in z-direction, $[L]$
Z Contaminant source dimension in z-direction, $[L]$

Greek letters

α Aquifer compressibility, $[LT^2/M]$
β Fluid compressibility, $[LT^2/M]$
λ Decay constant, $[1/T]$
μ Dynamic viscosity of the fluid, $[M/LT]$
ρ_l Fluid density, $[M/L^3]$
ρ_b Bulk density of the porous medium, $[M/L^3]$
ρ_s Soil particle density, $[M/L^3]$
τ Dummy variable of integration

Mathematical Operators and Special Functions

$\delta()$	Dirac delta function
erf	Error function
$erfc$	Complementary error function
J_n	Bessel function of the first kind and order n
Y_n	Bessel function of the second kind and order n
K_0	Modified Bessel function of the second kind and order zero
$T()$	Degradation function
X_i	Green's function in x-direction
Y_i	Green's function in y-direction
Z_i	Green's function in z-direction

1 Introduction

Concern over the increasing problem of ground-water pollution has created a need for better accuracy in predicting contaminant migration through porous media. Mathematical modeling has been recognized as an important tool in predicting such migration. Currently, two modeling methods are available, analytical and numerical; both provide a means for ground-water investigations and for evaluating monitoring programs and remedial actions. Advances in analytical modeling of the flow of ground water dominated technical literature during the 1950s, and 1960s. A number of analytical solute transport models were developed during the 1960s and 1970s (Bear, 1979; Cleary and Adrian, 1973; Hunt 1983; Huyakorn et al., 1987). Although progress in analytical modeling continues, especially in modeling of solute transport, during the last two decades attention was largely diverted to numerical modeling (Bear and Verruijt, 1987).

Modeling is an iterative process with several phases that can be defined as (Walton, 1988): (1) collection of data; (2) definition of the problem; (3) design of a conceptual model; (4) formulation of a model; (5) programming of a model; (6) specification of the structure of the model (specification of initial and boundary conditions, geometry of the model, parameters, etc.); (7) the model sensitivity study; (8) model calibration; (9) model runs; and (10) analysis of simulation results. Modeling development should be a sequential process progressing from simple conceptual models to sophisticated representation of ground-water systems.

During the early phase of a ground-water contamination study, analytical models offer an inexpensive way to evaluate the physical characteristics of a ground-water system. Widespread availability of microcomputers and other graphic devices enables investigators to conduct a rapid preliminary analysis of ground-water contamination and sensitivity analyses. However, several of assumptions regarding the ground-water system are necessary to obtain an analytical solution for the transport problem, including a constant ground-water velocity, constant dispersion coefficients, constant physical parameters, and a simplified geometry for the system. Although these simplifying assumptions do not necessarily dictate that analytical models cannot be used in "real-life" situations, they do require sound professional judgment and experience in their application to field situations. Walton (1979) argues that with appropriate recognition of hydrogeologic controls, there are many practical ways to circumvent analytical difficulties posed by complicated field conditions. When modeling complex field problems, numerical models are more realistic and adaptable than analytical models. Nonetheless, it is also true that in many field situations few data are available; hence, complex numerical models are often of limited use. When sufficient data has been collected, numerical models may be used for predictive evaluation and decision assessment. This can be done during the later phase of the study. Analytical models should be viewed as a useful complement to numerical models.

Because analytical models give an exact solution of the governing equation, they are quite useful for designing and verifying numerical models. As a partial check for correct computer programming, the code is applied to problems for which analytical solutions exist. Because an analytical solution is exact to any required degree of numerical accuracy, it is a useful reference for testing and verifying the accuracy of the algorithm used in the numerical model.

In addition to their value as practical tools, analytical models have proven useful in understanding basic principles of solute transport and thus are an excellent educational tool. Use of the analytical models on microcomputers is popular in university classrooms and for teaching short courses on basics of ground-water hydrology and introductory courses on ground-water modeling

A large portion of the literature on solute transport modeling is devoted to one- and two-dimensional models (Cleary and Ungs, 1978; Bear, 1979; Hunt, 1983). For example, an excellent review of one-dimensional solute transport models can be found in van Genuchten and Alves (1982). It has been recognized that many field situations require the use of three-dimensional models. The increasing effort in development and use of three-dimensional numerical models requires more effort in verifying the models with three-dimensional analytical models. The objectives of this report are to review and inventory available three-dimensional analytical solute transport models that can be used for research and practical application, as well as for model verification.

Concern over the fate of nuclear waste buried in a geological formation has created a need for better prediction of transport of radionuclides in ground-water systems. Because ground-water models are the only tool available for this type of prediction, a number of analytical and numerical models have been developed during the past decade (Chambre et al., 1982; Codell et al., 1982; Herbert, 1984; Gureghian, 1987). Many of the solutions for transport of radionuclides in porous media can be readily applied for contaminant transport. The present report brings these model types to the attention of ground-water specialists outside of the nuclear waste industry.

This report contains several sections: (1) introduction, (2) literature review, (3) general theory of solute transport in porous media, (4) listing of models, (5) conclusions, and (6) recommendations and future needs. Each model is completely described mathematically by presenting its governing equation, initial and boundary conditions, and the solution. An effort was made to list all the assumptions associated with the model. In addition, information about computer codes availability is provided. Special attention is given to future research needs and software development. The bibliography contains the most comprehensive literature list available on analytical three-dimensional solute transport models.

Although different authors use different mathematical notation, this reports attempts to present all equations in a consistent manner, using one notation system. If the reader is interested in more detailed information about a particular solution (e.g., solution technique, example problems, etc.), in addition to the reference, the original equation number and page number are given.

The solutions of the three-dimensional advective-dispersive equation are given in order of difficulty, from a simple instantaneous point source in an infinite aquifer to a volumetric source in a finite-depth aquifer. Appendix A provides a summary reference table of all reviewed models. The table includes the model name, list of processes, source configuration, boundary conditions, type of release, and references.

Many of the solutions presented have been used only for research. Scientists have utilized the solutions by coding them into computer programs (codes) using a higher computer language (FORTRAN, BASIC, C, or PASCAL) or symbolic packages (MATHCAD™ or MATHEMATICA™). As research codes, most of these are not readily available nor fully documented. Hence, it is not surprising how few codes are available for practical use in comparison to the number of one- and two-dimensional codes. Some of the solutions presented in the report that have been coded and are available as public domain or proprietary programs for use on microcomputers, are listed in the quick reference table (Appendix A).

2 Literature Review

The compiled list of models in the report has been extracted from existing literature. This section describes briefly the development of the three-dimensional analytical models in their chronological order. The complete mathematical description of the models is presented in section 4.

Walton (1979; 1988) has probably made the most significant contribution to practical application of analytical ground-water models for both flow and transport. In his numerous publications, he has collected and described a large number of flow and solute transport models. These are presented in a systematic manner and for many of them he has developed simplistic computer codes.

Hunt (1973; 1978) provided one-, two-, and three-dimensional solutions for instantaneous, continuous, and steady-state pollution sources in uniform ground-water flow. The solutions have been used to determine how long a continuous source must be in place before steady-state conditions are approached, as well as to examine the effect of a finite aquifer depth upon solutions for an aquifer of infinite depth.

Prakash (1977; 1982; 1984) described analytical models for prediction of effluents released in a two- or three-dimensional ground-water flow field from a point, line, and plane source. The effects of the upper and lower boundaries in the models are accounted for by the method of images.

Yeh (1981) presented a generalized analytical transient, one-, two-, and three-dimensional model (AT123D) with a computer code to compute the spatial and temporal distribution of a contaminant plume in an aquifer system. The closed-form solutions are based on the application of Green's functions (Yeh and Tsai, 1976). Due to the versatility of these functions, the source configuration can be: a point source, a line source parallel to the x-axis, a line source parallel to the y-axis, an area source perpendicular to the x-axis, an area source perpendicular to the y-axis, an area source perpendicular to the z-axis, and a volume source. Three kinds of releases are included: instantaneous, continuous, and finite duration releases. Four variations of the aquifer dimensions are: finite depth and finite width, finite depth and infinite width, infinite depth and finite width, and infinite depth and infinite width. Combining all these options, the user can select 288 options for the three-dimensional case. AT123D was tested against numerical models by EPRI (1984). A pre- and post-processor have been developed to accommodate handling of input data and model results (U.S. EPA, 1984).

Sagar (1982) obtained approximate solutions to the three-dimensional solute transport equation by integrating the appropriate Green's functions. This method offers an advantage because Green's function in three-dimensions is simply a product of three Green's functions, one for each direction. Two approximations are used during the integration. First, error function differences are approximated by exponential functions through Taylor's expansion series; second, the time integral is approximated by the Laplace method. The pollution sources are considered to be of finite size in space, and a function of time. The boundary conditions considered are of a stream in a horizontal flow field and a water table in a vertical flow field.

Domenico and Palciauskas (1982) developed for compliance and regulatory purposes a simple model for maximum concentration predictions (U.S. EPA VHS Model). The source configuration is a vertical plane. The model assumptions are that the flow is one-dimensional with lateral spreading of contaminant in two dimensions and with vertical spreading downward, perpendicular to the flow path. The model does not include chemical reaction or longitudinal dispersion. The maximum concentrations encountered in the steady-state model occur in the plane of symmetry ($y = z = 0$). Robbins and Domenico (1984) and Domenico and Robbins (1985) developed a three-dimensional advection-dispersion model under transient conditions. The model includes dispersion and advection only. Domenico (1987) extended the model to include first-order reactions.

Goltz (1986) and Goltz and Roberts (1986) presented analytical solutions for the solute transport in a three-dimensional infinite medium with (1) first-order and (2) diffusion rate limitations. Sorption is assumed to be governed by a linear isotherm. The porous medium was divided into regions of mobile and immobile water and the advective-dispersive solute transport equation was coupled either with (1) expressions for the first-order rate solute transfer between the mobile and immobile regions (first-order rate models), or with (2) expressions for diffusional transfer between the two regions (diffusion models). Solutions are given for point sources. The principle of superposition can be used to integrate the point source response to obtain responses for other initial conditions. The first-order rate model solution was also obtained by Carnaham and Remer (1984); they provide solutions for various initial condition geometries.

Huyakorn et al. (1986; 1987) presented an analytical model for predicting contaminant transport from a Gaussian vertical strip source in a one-dimensional uniform ground-water flow field. The model takes account of dispersion, adsorption, and decay. In addition, the effects of partial penetration of the contaminant source and finite aquifer thickness are accounted for. Type curve procedures were developed for evaluating steady-state concentration along the plume center line. The model has been compared with other analytical models and two examples are presented.

El-Kadi et al. (1987) have applied the U.S. EPA Screening Level Ground Water Model or SLM (U.S. EPA, 1985), which is based on the Huyakorn model (Huyakorn et al., 1987), to site-specific settings. SLM employs a three-dimensional analytical solution for contaminant transport under steady-state conditions. It is interesting to note that the model is the only one that includes the scale-dependent dispersivity parameters (e.g., $a_L = 0.1x$; $a_T = 0.03x$; and $a_Z = 0.0025x$ to $0.01x$). SLM has been tested against a well-validated numerical model CFEST (Gupta et al., 1987) and an alternative analytical model AT123D (Yeh, 1981).

Wexler (1989) compiled a list of analytical solutions from existing literature and derived his own solutions for a variety of boundary condition types and solute source configurations in one-, two-, and three-dimensional systems. Regarding three-dimensional problems, a solution modified from Cleary and Ungs (1978, pp. 24-25) and two new solutions were presented in Wexler's report. In the first solution, the aquifer is assumed to be of infinite extent along all three coordinate axes. Fluid is injected into the aquifer through a point source at a constant rate. The remaining solutions are based on the assumptions that the aquifer system is semi-infinite in length with a solute source located along the inflow boundary. The semi-infinite aquifer can be either finite in both width and height, or infinite in width and height. The solute source is referred to as a "patch" source with a finite width and height. The concentration within the patch is uniform. First-order solute decay, adsorption, and ion exchange are included. Three computer program listings for models POINT3, PATCHF, and PATCHI are given in the report.

Transport of Radionuclides

The disposal of radioactive waste in deep geological formations is being considered by many countries. Mathematical models have been used to simulate physical and chemical processes that would occur if the waste escapes from the sites into ground water (Codell and Schreiber, 1979; Simmons and Cole, 1985).

Codell et al. (1982) developed ground-water models for evaluating the transport of radionuclides. The models were used for estimating the migration of radionuclides from low-level waste facilities. Two computer programs were developed: the first program, GROUND, calculates concentration and flux from a variety of sources for a single radioactive component released from a vertical plane; the second program, GRDFLX, calculates concentration and flux from sources typical of low-level waste burial grounds (horizontal areal sources). The programs consist of two parts: Part 1 is the point concentration model (used for calculating the concentration in the aquifer at some point downgradient of a release), and Part 2 is the flux model (used to calculate the discharge rate of radionuclide entering a surface-water body). The point concentration model has been developed for a variety of boundary and source configurations: (1) a point source, (2) a vertical line source, (3) a horizontal line source, (4) a vertical plane source, and (5) a horizontal plane source. Galya (1987) presented a solution to a horizontal plane source model that is identical to the solution given by Codell et al. (1982) without referring to the latter.

The verification and testing of numerical accuracy of ground-water models for the transport of radionuclides in a three-dimensional permeable medium is of great concern (Herbert, 1984). Verification of one- and two-dimensional transport codes was carried out in the international INTRACOIN study (INTRACOIN, 1984; Cole et al., 1987). However, three-dimensional codes have not yet been tested in a similar way. Chambre et al. (1982) discussed equilibrium and nonequilibrium transport of radionuclides in porous media. They also developed mathematical analysis for transport of radionuclides in fractured media, wherein radionuclides are advected by ground water flowing through planar fissures. Molecular diffusion into and out of micropores penetrating the rock surfaces of the fissures plays an important role in retarding the migration of radionuclides through the fissures. Solutions were given for an impulse release, stop release, band release, and solubility-limited dissolution.

INTERA (1983) developed a package of analytical solutions, VERTPAK-1, covering fluid flow, rock deformation, and solute transport in fractured and unfractured media. The package contains two analytical solute transport models: one for one-dimensional dispersive-advective transport of a simple chain of three radionuclide components in a semi-infinite porous medium (LESTER model), and the other for transport of a solute along a planar fracture (TANG model). The solute diffuses into the rock mass adjacent to the fracture and may be subject to first-order decay, adsorption and the fracture-rock mass interface, and adsorption within the rock mass.

Herbert (1984) presented analytical solutions to the three-dimensional transport equation of a single radionuclide in a steady-state flow field. The solutions were obtained by the method of separation of variables. Two cases were considered: the first represents a model with the dispersion term as a constant diffusion type; the second case is more realistic by including dispersion as a velocity-dependent term. The sorption is accounted for by a constant retardation factor (the nuclide is assumed to be retarded by equilibrium sorption onto the soil). The solutions and parameter values are given for both cases, which may be used to test any numerical radionuclide transport model. The solutions were used to verify the three-dimensional finite-element transport code NAMSOL (Dolman and Robinson, 1983).

Chambre et al. (1982; 1985) prepared a number of analytical performance models for geologic repositories. They provide the most complete and comprehensive available mathematical treatment of radionuclide transport in fractured media. However, these models are one-dimensional and are not included in this review.

3 Theory

This section gives a quick review of the theory of solute transport through porous media. Interested reader can find a number of excellent textbooks covering the topic in much more depth (e.g., Bear, 1979; Hunt, 1983; Bear and Bachmat, 1990).

3.1 Advective-Dispersive Equation

Three-dimensional solute transport through a porous medium with a uniform ground water flow in x-direction can be expressed mathematically by the following partial differential equation (Anderson, 1979; Freeze and Cherry, 1979):

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}, \tag{1}$$

where

$$\begin{aligned}
C &= \text{concentration of the solute} \\
D_{xx} &= \text{dispersion coefficient in } x\text{-direction,} \\
&= a_L V \\
D_{yy} &= \text{dispersion coefficient in } y\text{-direction,} \\
&= a_T V \\
D_{zz} &= \text{dispersion coefficient in } z\text{-direction,} \\
&= a_T V \\
a_L &= \text{longitudinal dispersivity} \\
a_T &= \text{transverse dispersivity} \\
V &= \text{ground-water velocity (in } x\text{-direction)}
\end{aligned}$$

The relationship between the concentration of adsorbed, S, and dissolved constituent, C, is defined by an isotherm. For analytical models, assumptions have been made that the solid and liquid phases are in equilibrium, and that their concentrations are related by a linear formula

$$S = K_d C, \tag{2}$$

where K_d is the distribution coefficient.

The ground-water velocity V is the same as the velocity of contaminant for a nonreactive (conservative) solute. For a reactive (nonconservative) solute, as the result of sorption, the solute transport is retarded relative to the transport caused by advection and dispersion only. The retardation factor (or retardation coefficient), R_d, is defined as

$$R_d = 1 + \frac{\rho_b}{n} K_d, \tag{3}$$

where ρ_b is the bulk density of the porous medium and n is the porosity.

Solute may undergo radioactive or biological decay as it is transported through the porous medium. The decay is expressed by the following equation:

$$\frac{\partial C}{\partial t} = -\lambda C, \tag{4}$$

where λ is the first-order decay constant of the solute and can be calculated if the half-life of the solute, $t_{1/2}$, is known

$$\lambda = ln(2)/t_{1/2}. \tag{5}$$

Equation 1 with both adsorption and radioactive decay processes included becomes

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda R_d C = R_d\frac{\partial C}{\partial t}. \tag{6}$$

Depending on initial and boundary conditions associated with equations 1 and 6, a number of closed-form analytical solutions are published in the ground-water literature. The solutions are listed and grouped in this report according to the geometry (configuration) of contaminant sources.

General Assumptions

The following assumptions are associated with equations (1) and (6) and are common to all models in the report:

- the aquifer is homogeneous and isotropic
- one-dimensional steady-state ground-water flow (a constant velocity)

- the direction of the ground water flow coincides with the positive x-axis
- the model coefficients V, D_{ij}, R_d, and λ are constants
- the density and viscosity of the solute are same as those of native ground water

In addition, solute injection rates are often assumed to be negligible relative to the regional ground-water flow rate (in order to satisfy the constant ground-water velocity assumption). In some of the models presented, lateral dispersion is assumed to dominate mixing conditions. Any additional assumptions made in the model development are given along with the model description.

3.2 Initial and Boundary Conditions

To obtain a particular solution of equation (1), it is necessary to provide additional information about the system. The additional information include initial and boundary conditions. Assigning correct boundary conditions is a particularly important step in ground-water modeling.

Initial conditions describe the distribution of concentration in the studied domain at some initial time ($t = 0$). The general initial condition of the advection-dispersion equation (1) is written as (Javandel et al., 1984)

$$C = f(x, y, z, t = 0) \tag{7}$$

where $f(x, y, z, t = 0)$ can be a constant or some other known function.

Boundary conditions provide information on interaction between the considered domain and the rest of the universe. Different boundary conditions result in different solutions. Three types of boundary conditions are:

1. *Dirichlet or first-type boundary condition.*

$$C = C_0(x, y, z, t) \tag{8}$$

where $C_0(x, y, z, t)$ is a given function for the particular portion of the boundary.

Examples of this type of boundary condition are specified concentration on the boundary, zero concentration, or specified concentration at injection wells.

2. *Neumann or second-type boundary condition.*

$$(D_{ij}\frac{\partial C}{\partial x_j})n_i = q(x,y,z,t) \tag{9}$$

where q is a known function and n_i are components of the unit vector normal to the boundary.

Typical examples are zero concentration gradient on impervious boundaries, and concentration gradient on outflow boundary.

3. *Cauchy or third-type boundary condition.*

$$(D_{ij}\frac{\partial C}{\partial x_j} - CV_i)n_i = g(x,y,z,t) \tag{10}$$

where g is some known function. The first term represents flux by dispersion and diffusion, and the second term represents the advection effect.

Examples include specified mass flux of contaminant at injection wells, specified mass flux of contaminant from landfills, streams, and so forth.

One of the common assumptions associated with analytical models is that the domain is infinite. The boundary conditions are then prescribed at infinity without any need to define their character (de Marsily, 1986).

4 Mathematical Models

All analytical models in this section are classified according to the geometry of the contaminant source (point, line, areal, or volumetric source). In addition, they are divided according to the type of contaminant release: instantaneous or continuous.

4.1 Point Source

This section includes models with a point source. In practice this source may be an underground storage tank, an injection well, or a small spill. If the size of the source is small compared to the model area, the source can be treated as a point source (e.g., a lagoon or a small landfill). Another way of modeling such a plane (or volumetric) source is by dividing the source into smaller areas (volumes) and by representing each area (volume) as a point source. Based on the principle of superposition, the resulting plume from the point sources will be equivalent to the plume from the areal (or volumetric) source.

Regarding time of activity of a source, the source can be continuous (a constant release of contaminant into the aquifer system) or instantaneous (a spill or a contaminant source that is active for a short time relative to the total elapsed time). Again, using the principle of superposition in time, one can simulate a variable source rate of contaminant as the sum of a finite number of constant source rates distributed in time (Wagner et al., 1985).

4.1.1 Case A1-i

Let the governing equation for the solute transport take the following form:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}. \tag{11}$$

The solution to the equation 11 for an instantaneous point source (Figure 1) can be obtained by applying the following initial and boundary conditions:

$$C(x,y,z,0) = \frac{M}{n}\delta(x,y,z), \tag{12}$$

in which n is the porosity, $\delta(x, y, z)$ is the Dirac delta function, and M is the total mass of pollutant released at the coordinate origin at time $t = 0$:

$$M = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} C(x, y, z) n dx dy dz. \tag{13}$$

The mass of the contaminant introduced at the source equals $C_0 V_0$, where C_0 is the initial concentration and V_0 is the initial volume (Freeze and Cherry, 1979, p. 395). In the mathematical formulation of the initial conditions, the contaminant input occurs at a point and therefore has mass but no volume. In practice, this is expressed by the quantity $C_0 V_0$.

The aquifer is assumed to be infinite and the boundary conditions can be specified as follows:

$$C(\infty, y, z, t) = 0; \quad C(x, \infty, z, t) = 0; \quad C(x, y, \infty, t) = 0. \tag{14}$$

In a case of the instantaneous point source at the coordinate origin, the solution is given by Hunt (1978, p. 76, equation 10)

$$C(x, y, z, t) = \frac{M}{8n\sqrt{\pi^3 t^3 D_{xx} D_{yy} D_{zz}}} \exp\left(\frac{(x - Vt)^2}{4D_{xx}t} - \frac{y^2}{4D_{yy}t} - \frac{z^2}{4D_{zz}t}\right). \tag{15}$$

The spreading from a point source occurs in the direction of flow, and the peak concentration, C_{max}, is where $y = z = 0$ and $x = Vt$:

$$C_{max} = \frac{M}{8n\sqrt{\pi^3 t^3 D_{xx} D_{yy} D_{zz}}}. \tag{16}$$

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Case A1-i*

- *instantaneous point source*
- *aquifer is of infinite depth*
- *transient state (for solute transport)*

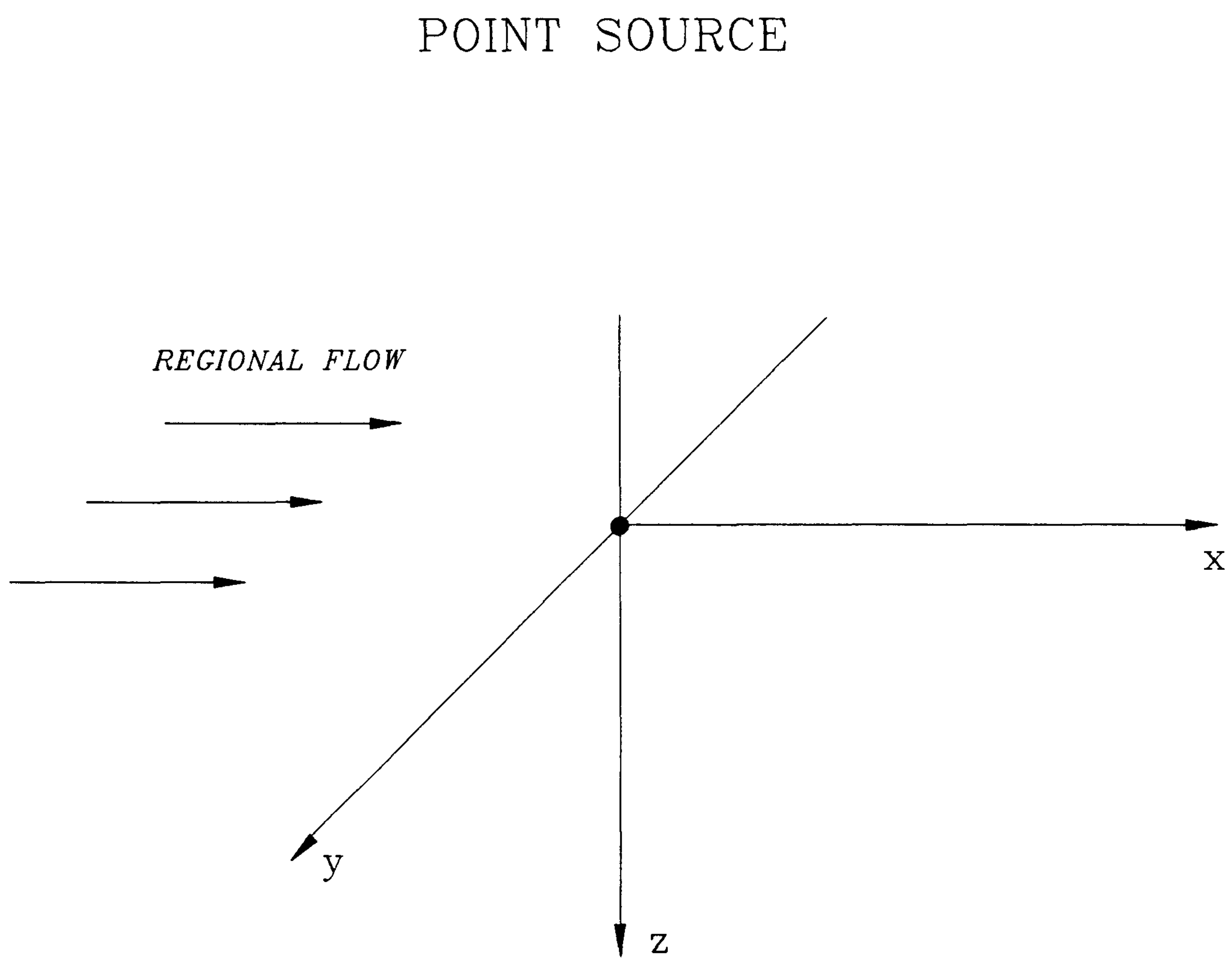

Figure 1: Point source in an infinite aquifer.

4.1.2 Case B1-i

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda C = \frac{\partial C}{\partial t}. \tag{17}$$

The solution to the above equation for an instantaneous point source at the origin with radioactive decay was first developed by Baetsle (1969) and later included with the other analytical solutions in a text by Hunt (1983, p. 133, equation 6.47)

$$C(x,y,z,t) = \frac{M}{8n\sqrt{\pi^3 t^3 D_{xx} D_{yy} D_{zz}}} \exp\left(-\lambda t - \frac{(x-Vt)^2}{4D_{xx}t} - \frac{y^2}{4D_{yy}t} - \frac{z^2}{4D_{zz}t}\right). \tag{18}$$

The initial and boundary conditions are identical to those in the model *Case A1-i*.

A small spill can be modeled as a point source if the considered domain is relatively large compared to the size of the spill. In that case, the given solution can be used to predict the concentration distribution caused by the spill.

The spreading from the point (spill) occurs in the direction of flow, and the peak concentration, C_{max}, is where $y = z = 0$ and $x = Vt$:

$$C_{max} = \frac{M}{8n\sqrt{\pi^3 t^3 D_{xx} D_{yy} D_{zz}}} \exp(-\lambda t). \tag{19}$$

Assumptions:

The following assumptions are associated with *Case B1-i*:

- *instantaneous point source*
- *first-order radioactive decay*
- *aquifer is of infinite depth*
- *transient state*

4.1.3 Case A1-c

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}. \tag{20}$$

The solution to the equation for an instantaneous point source was obtained (Case A1-i) by using the following initial condition (Hunt, 1978):

$$C(x,y,z,0) = \frac{M}{n}\delta(x,y,z), \tag{21}$$

where M is the total mass of pollutant released at the coordinate origin at time $t = 0$:

$$M = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} C(x,y,z)n\,dx\,dy\,dz. \tag{22}$$

The aquifer is again assumed to be infinite and boundary conditions for this model are the same as for *Case A1-i*, e.g., the concentration is zero at infinity:

$$C(\infty,y,z,t) = 0; \quad C(x,\infty,z,t) = 0; \quad C(x,y,\infty,t) = 0. \tag{23}$$

A solution of the governing equation with the initial and boundary conditions is given by Hunt (1978, p. 77, equation 11) as

$$\begin{aligned} C(x,y,z,t) &= \frac{\dot{M}\exp\left(\frac{xV}{2D_{xx}}\right)}{8\pi n r\sqrt{D_{yy}D_{zz}}}\left[\exp\left(-\frac{rV}{2D_{xx}}\right) erfc\left(\frac{r - Vt}{2\sqrt{D_{xx}t}}\right)\right] \\ &\quad + \left[\exp\left(\frac{rV}{2D_{xx}}\right) erfc\left(\frac{r + Vt}{2\sqrt{D_{xx}t}}\right)\right] \end{aligned} \tag{24}$$

where $\dot{M} = dM/dt$ is the mass flux; *erfc* = complementary error function; and r is defined as

$$r = \sqrt{x^2 + y^2\frac{D_{xx}}{D_{yy}} + z^2\frac{D_{xx}}{D_{zz}}}. \tag{25}$$

Assumptions:

In addition to the general assumptions associated with the solute transport governing equation, this model assumes the following assumptions:

- *continuous point source*
- *aquifer is of infinite depth*
- *transient state*

4.1.4 Case A2-c

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = 0. \tag{26}$$

The steady state solution of the model *Case A1-c* follows from equation 24 by taking the limit as $t \to \infty$ (Hunt, 1978, p. 77, equation 12).

$$C(x, y, z, \infty) = \frac{\dot{M}}{4\pi n r\sqrt{D_{yy}D_{zz}}} \exp\left[\frac{(x-r)V}{2D_{xx}}\right]. \tag{27}$$

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Case A2-c*

- *continuous point source*
- *aquifer is of infinite depth*
- *steady state*

4.1.5 Case A3-c

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = 0. \tag{28}$$

When the source is located at the coordinate origin either upon the free surface of an unconfined aquifer with the depth B (Figure 2), or midway between two parallel, impermeable planes spaced a distance $2B$ apart in z-direction, the steady-state solution, $C'(x, y, z, \infty)$, can be obtained from the method of images (Hunt, 1978, p. 80, equation 23)

$$\begin{aligned} C'(x,y,z,\infty) &= C(x,y,z,\infty) + \sum_{i=1}^{\infty}[C(x,y,z-2iB,\infty) \\ &\quad + C(x,y,z+2iB,\infty)] \end{aligned} \tag{29}$$

in which $C(x, y, z, \infty)$ is given by equation 27 *(Case A2-c)*.

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Case A3-c*

- *continuous point source*
- *aquifer is of finite depth*
- *steady state*

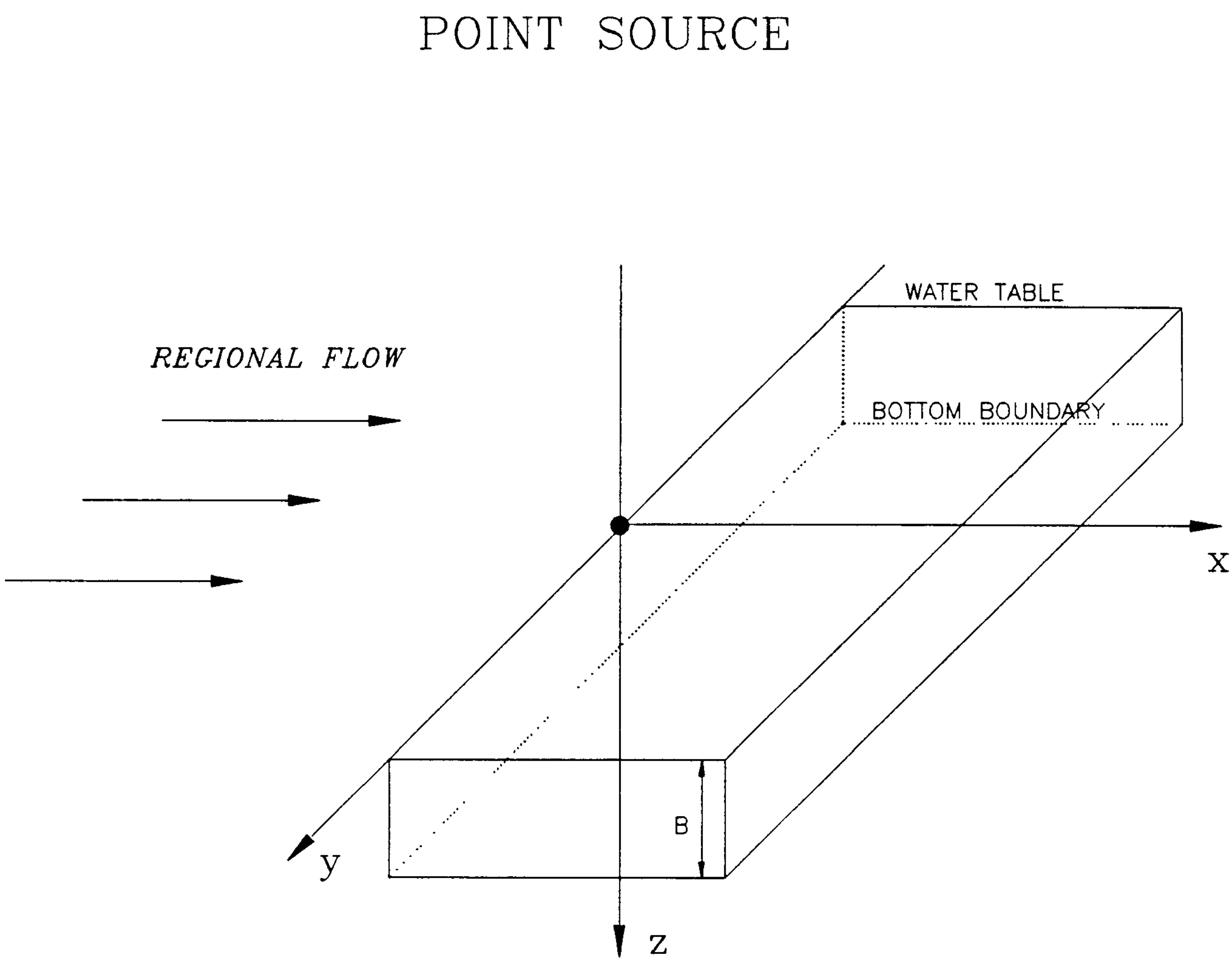

Figure 2: Point source in a finite-thickness aquifer.

4.1.6 Case B1-c

The governing equation for this model includes radioactive decay and has the following form:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda C = \frac{\partial C}{\partial t}, \tag{30}$$

The solution to equation 30 is given by Hunt (1983, p. 135, equation 6.53) as

$$\begin{aligned} C(x,y,z,t) &= \frac{\dot{M}\exp\left(\frac{xV}{2D_{xx}}\right)}{8\pi n r\sqrt{D_{yy}D_{zz}}}\left[\exp\left(-\frac{ar}{\sqrt{D_{xx}}}\right) erfc\left(\frac{r}{2\sqrt{D_{xx}t}} - a\sqrt{t}\right)\right] \\ &+ \left[\exp\left(\frac{ar}{\sqrt{D_{xx}}}\right) erfc\left(\frac{r}{2\sqrt{D_{xx}t}} + a\sqrt{t}\right)\right], \end{aligned} \tag{31}$$

in which r and a are defined as

$$r = \sqrt{x^2 + y^2\frac{D_{xx}}{D_{yy}} + z^2\frac{D_{xx}}{D_{zz}}}, \tag{32}$$

$$a = \sqrt{\lambda + \frac{V^2}{4D_{xx}}}. \tag{33}$$

All other symbols were defined previously.

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Case B1-c*:

- *continuous point source*
- *first-order radioactive decay*
- *aquifer is of infinite depth*
- *transient state*

4.1.7 Case B2-c

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda C = \frac{\partial C}{\partial t}. \tag{34}$$

The steady-state solution for a continuous point source can be obtained simply by letting $t \to \infty$ in equation 31 (Hunt, 1983, p. 136, equation 6.62):

$$C(x,y,z,\infty) = \frac{\dot{M}}{4\pi n r\sqrt{D_{yy}D_{zz}}}\exp\left[\frac{xV}{2D_{xx}} - \frac{ar}{\sqrt{D_{xx}}}\right], \tag{35}$$

where r and a are defined again as

$$r = \sqrt{x^2 + y^2\frac{D_{xx}}{D_{yy}} + z^2\frac{D_{xx}}{D_{zz}}}, \tag{36}$$

$$a = \sqrt{\lambda + \frac{V^2}{4D_{xx}}}. \tag{37}$$

Assumptions:

The following assumptions are associated with *Case B2-c*:

- *continuous point source,*
- *first-order radioactive decay*
- *aquifer is of infinite depth*
- *steady state*

4.2 Line Source

Analytical solutions for two-dimensional dispersion model with a horizontal line source are well known and have been described by Cleary and Ungs (1978). The solutions are available for two different cases: (a) the line source orthogonal to the ground-water flow, and (b) the direction of flow forming an angle with the x-axis (Javandel et al., 1984). The three-dimensional dispersion models described below include cases of vertical and horizontal line source. The line source is assumed to be perpendicular to the ground-water flow.

4.2.1 Vertical Line Source

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda R_d C = R_d\frac{\partial C}{\partial t}. \quad (38)$$

Green's functions are powerful tools in deriving solutions to the above three-dimensional advection-dispersion equation for various geometry of sources (Yeh, 1981; Codell et al., 1982; Sagar, 1982; Galya, 1987). Codell et al. (1982, p. 3.6, equation 3.13) developed a solution for a vertical line source of length B (the thickness of the aquifer) as

$$C(x,y,z,t) = \frac{1}{nR_d}X_1(x,t)Y_1(y,t)Z_2(z,t)T(t), \quad (39)$$

where

$$X_1 = \frac{1}{2\sqrt{\pi D_x t/R_d}}\exp\left[-\frac{\left(x-\frac{Vt}{R_d}\right)^2}{4D_x t/R_d}\right], \quad (40)$$

$$Y_1 = \frac{1}{2\sqrt{\pi D_y t/R_d}}\exp\left[-\frac{y^2}{4D_y t/R_d}\right], \quad (41)$$

$$Z_2 = \frac{1}{B}, \quad (42)$$

$$T(t) = \exp(-\lambda t). \quad (43)$$

The terms in the above equation are defined as

X_1	=	Green's function in x-direction
Y_1	=	Green's function in y-direction
Z_2	=	Green's function in z-direction
T	=	degradation function (due to decay of contaminants biodegradation, hydrolysis, etc.)
D_{ij}	=	dispersion coefficient tensor
R_d	=	retardation factor
λ	=	decay constant

Assumptions:

In addition to the general assumptions, the following assumptions are associated with the line model:

- *a unit mass released,*
- *instantaneous vertical line source*
- *first-order radioactive decay*
- *aquifer is of finite depth*
- *transient state*

4.2.2 Horizontal Line Source

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda R_d C = R_d\frac{\partial C}{\partial t}. \quad (44)$$

Codell et al. (1982, p. 3.6, equation 3.16) obtained a solution for the horizontal line source of length L centered at $(0, y_s, z_s)$ (Figure 3) as

$$C(x,y,z,t) = \frac{1}{nR_d}X_1(x,t)Y_2(y,t)Z_1(z,t)T(t), \quad (45)$$

where

$$X_1 = \frac{1}{2\sqrt{\pi D_x t/R_d}}\exp\left[-\frac{\left(x-\frac{Vt}{R_d}\right)^2}{4D_x t/R_d}\right], \quad (46)$$

$$Y_2 = \frac{1}{2L}\left[erf\left(\frac{\frac{L}{2}+y-y_s}{2\sqrt{D_y t/R_d}}\right) + erf\left(\frac{\frac{L}{2}-y+y_s}{2\sqrt{D_y t/R_d}}\right)\right], \quad (47)$$

$$Z_1 = \frac{1}{B}\left[1 + 2\sum_{i=1}^{\infty}\exp(-\frac{i^2\pi^2 D_z t}{B^2 R_d})\cos(i\pi z/B)cos(i\pi z_s/B)\right], \quad (48)$$

$$T(t) = \exp(-\lambda t). \quad (49)$$

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Horizontal Line Source Model*

- *a unit mass released*
- *instantaneous horizontal line source*
- *first-order radioactive decay*
- *aquifer is of finite depth, B*
- *transient state*

HORIZONTAL LINE SOURCE

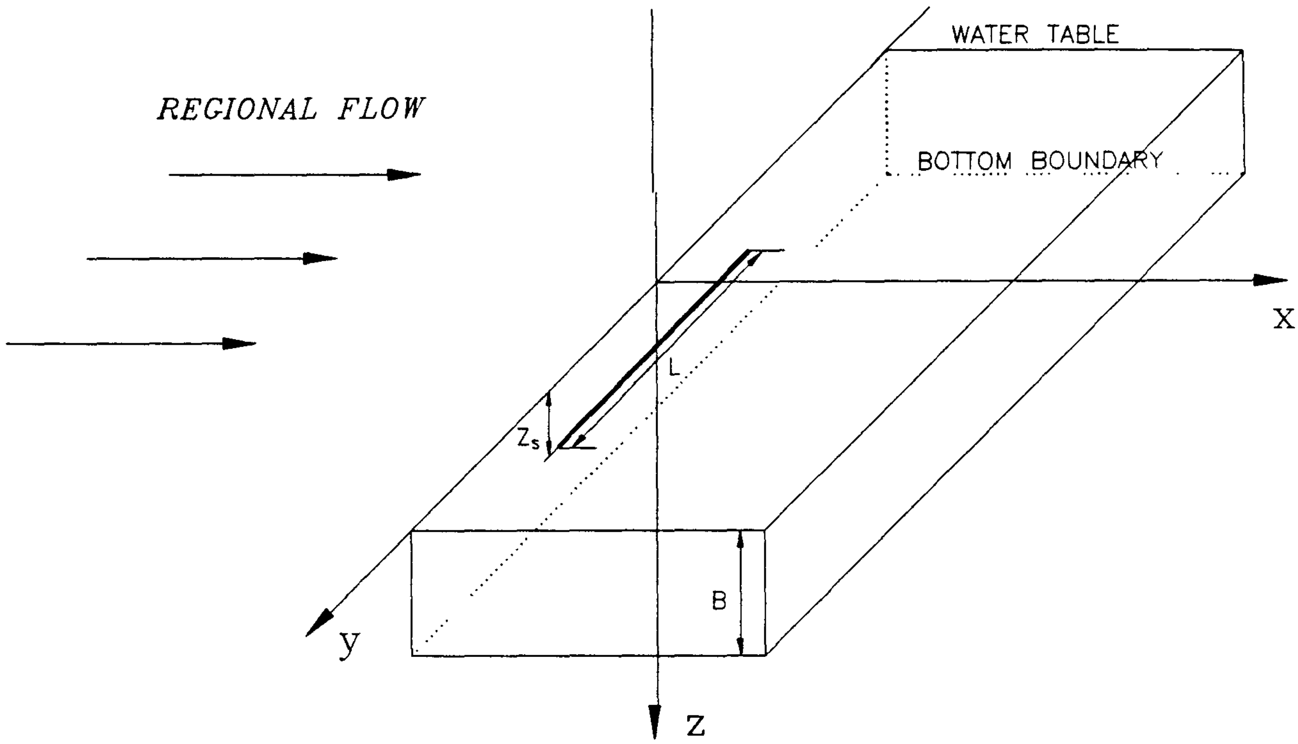

Figure 3: Horizontal line source in a finite-depth aquifer.

4.3 Plane Source

The finite plane source is more realistic than a point source in many "real-world" problems. Whether the solution is given in a closed-form or not, two types of models are available. Cleary (1978), Cleary and Ungs (1978), Codell et al. (1982), Huyakorn et al. (1987), and others developed solutions that require numerical integration. Domenico and Palciauskas (1982, Domenico and Robbins (1984), and Domenico (1987) presented analytical solutions in closed-forms with no numerical integration required. The porous medium is assumed to be infinite, semi-infinite, or finite.

4.3.1 Vertical Plane Source of Width L and Depth B

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda R_d C = R_d\frac{\partial C}{\partial t}. \qquad (50)$$

Codell et al. (1982, p. 3.7, equation 3.17) give the solution for the vertically averaged concentration of a horizontal line source of length L centered at $(0, y_s, z_s)$ (equivalent to an area source of width L and depth B) as

$$C(x,y,z,t) = \frac{1}{nR_d}X_1(x,t)Y_2(y,t)Z_2(z,t)T(t), \qquad (51)$$

where

$$X_1 = \frac{1}{2\sqrt{\pi D_x t/R_d}}\exp\left[-\frac{\left(x-\frac{Vt}{R_d}\right)^2}{4D_x t/R_d}\right], \qquad (52)$$

$$Y_2 = \frac{1}{2L}\left[erf\left(\frac{\frac{L}{2}+y-y_s}{2\sqrt{D_y t/R_d}}\right) + erf\left(\frac{\frac{L}{2}-y+y_s}{2\sqrt{D_y t/R_d}}\right)\right], \qquad (53)$$

$$Z_2 = \frac{1}{B}, \qquad (54)$$

$$T(t) = \exp(-\lambda t). \qquad (55)$$

Assumptions:

In addition to the general assumptions, the following assumptions are associated with the plane model:

- *a unit mass released*
- *instantaneous vertical plane source*
- *first-order radioactive decay*
- *aquifer is of finite depth, B*
- *transient state*

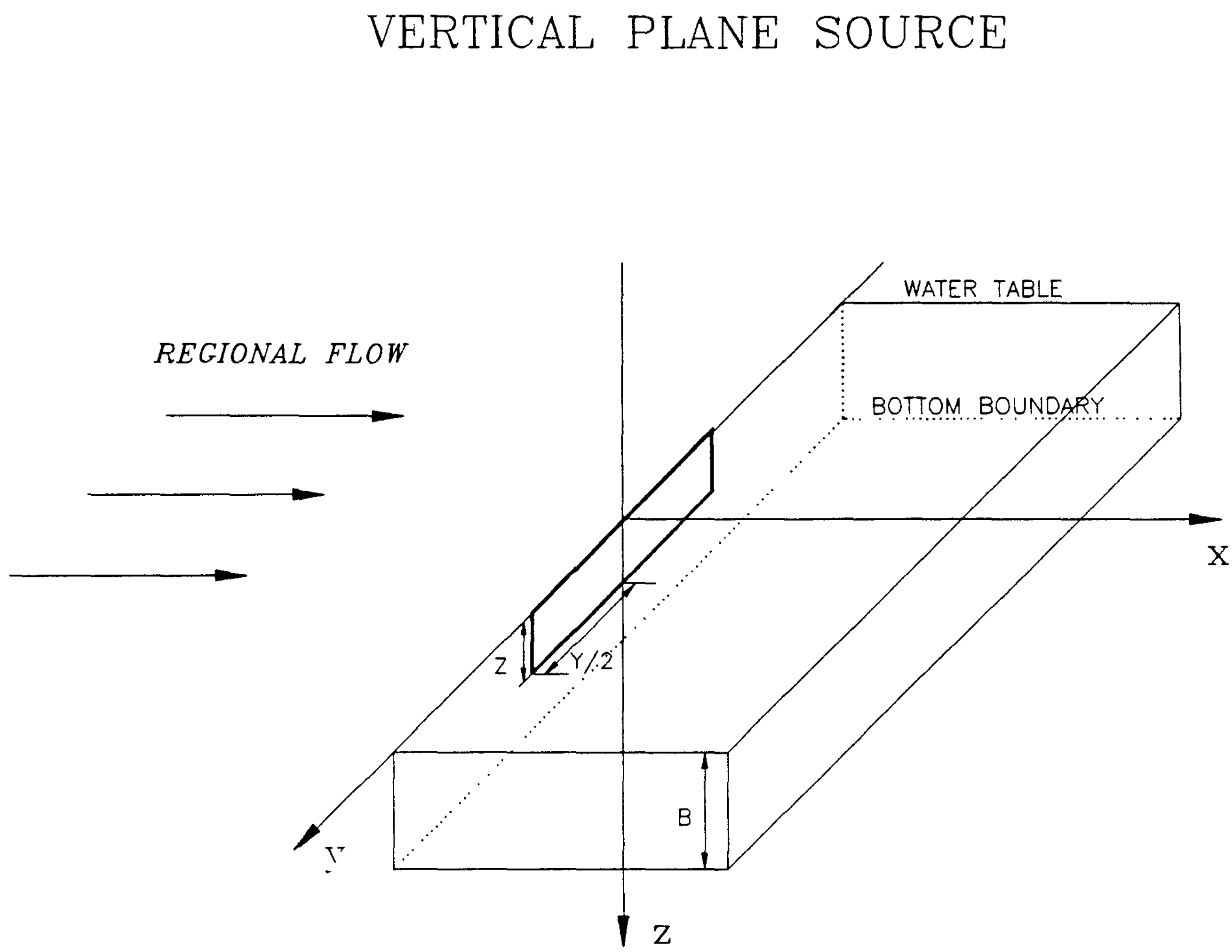

Figure 4: Vertical plane source in a finite-depth aquifer.

4.3.2 U.S. EPA VHS Model

This steady-state model describes the spreading of a contaminant plume in the vertical and lateral directions perpendicular to the flow direction. The following governing equation is given (Domenico and Palciauskas, 1982, p. 309, equation 17)

$$D_T\left(\frac{\partial^2 C}{\partial y^2}+\frac{\partial^2 C}{\partial z^2}\right)-V\frac{\partial C}{\partial x}=0, \qquad (56)$$

where

$$D_T = D_{yy} = D_{zz} = a_T V.$$

The problem is viewed as a two-dimensional problem in a semi-infinite medium bounded at the top by a zero flux boundary. The maximum concentration of the contaminant C_0 is assigned over a specified area:

$$\begin{aligned} C(0,y,z) &= C_0 \qquad & 0 < z < Z \\ &= C_0 \qquad & -Y/2 < z < Y/2 \\ &= 0 \qquad & otherwise. \end{aligned}$$

where Y and Z are the source dimensions in y- and z-direction, respectively (Figure 5). The solution to equation 56 for the given boundary conditions is (Domenico and Palciauskas, 1982, p. 309, equation 18)

$$\begin{aligned} C(x,y,z) &= \frac{C_0}{4}\left[erf\left(\frac{y+Y/2}{2\sqrt{a_T x}}\right)-erf\left(\frac{y-Y/2}{2\sqrt{a_T x}}\right)\right] \\ & \left[erf\left(\frac{z+Z}{2\sqrt{a_T x}}\right)-erf\left(\frac{z-Z}{2\sqrt{a_T x}}\right)\right] \qquad (57) \end{aligned}$$

in which *erf* is the error function.

The maximum concentration occurs along the centerline ($y = z = 0$) and is given as

$$C(x,0,0)=C_0 erf\left[\frac{Y}{2\sqrt{a_T x}}\right] erf\left[\frac{Z}{2\sqrt{a_T x}}\right]. \qquad (58)$$

Equation 58 was used by the U.S. EPA to evaluate delisting petitions to exclude certain waste from the hazardous waste list (Domenico and Palciauskas, 1982; van der Heijde, 1989).

Assumptions:

In addition to the list of general assumptions, the following assumptions are associated with the model:

- *continuous vertical plane source*
- *semi-infinite domain*
- *no longitudinal spreading*
- *steady state*

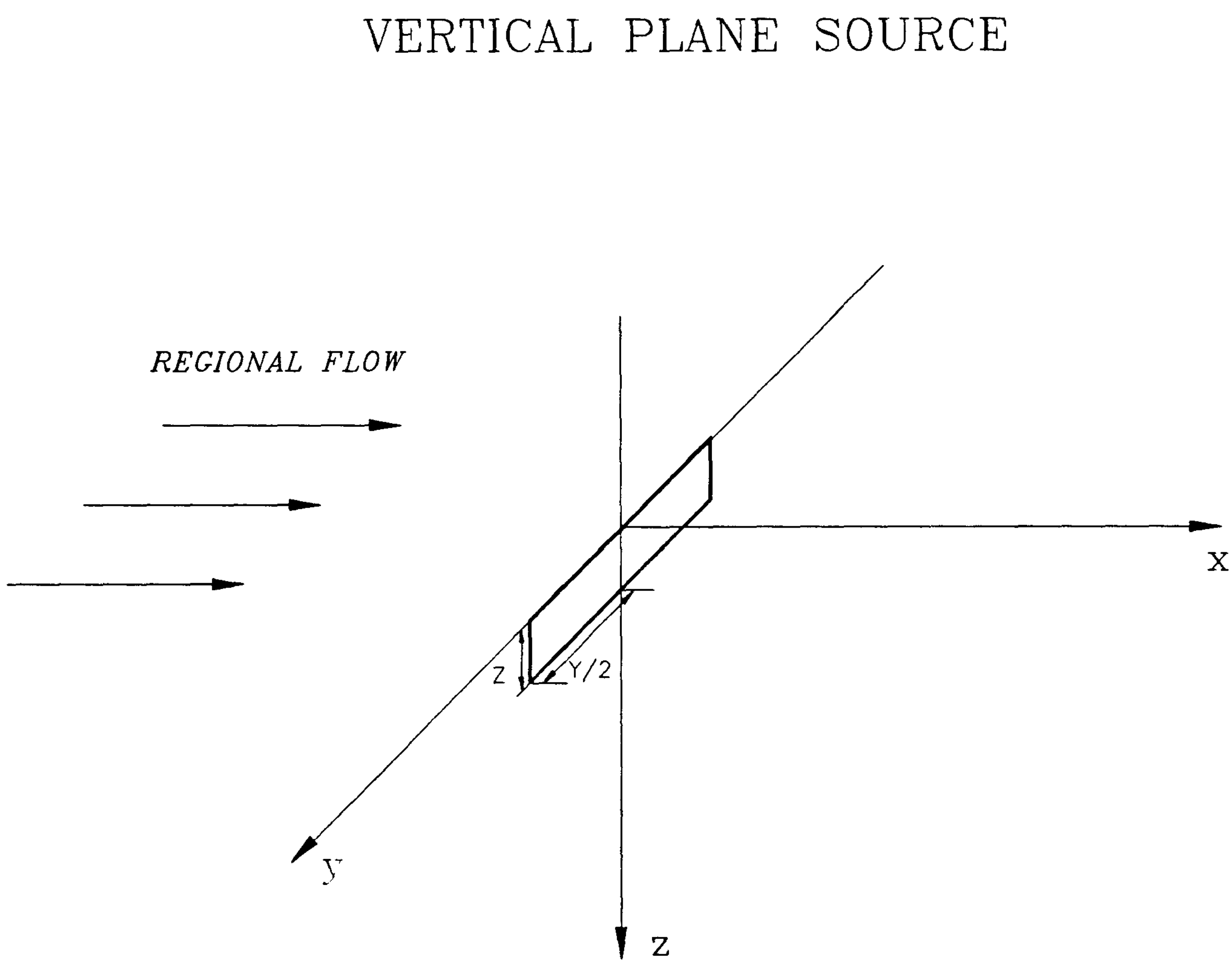

Figure 5: Vertical plane source in a semi-infinite aquifer.

4.3.3 Domenico's Model

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}. \tag{59}$$

Domenico and Robbins (1985) and Domenico and Schwartz (1990, p. 646, equation 17.18) presented a solution to the problem of a vertical plane source in a semi-infinite aquifer. The domain is bounded at the top by a zero flux boundary. The maximum concentration of the contaminant C_0 is assigned over the areal source:

$$\begin{aligned} C(0,y,z) &= C_0 \qquad 0 < z < Z \\ &= C_0 \qquad -Y/2 < z < Y/2 \\ &= 0 \qquad \textit{otherwise.} \end{aligned}$$

where Y and Z are the source dimensions in y- and z-direction, respectively (Figure 5). The solution to the problem for the given boundary conditions is

$$\begin{aligned} C(x,y,z,t) &= \frac{C_0}{8} erfc\left(\frac{x - Vt}{2\sqrt{a_x Vt}}\right) \\ &\left[erf\left(\frac{y + Y/2}{2\sqrt{a_T x}}\right) - erf\left(\frac{y - Y/2}{2\sqrt{a_T x}}\right)\right] \\ &\left[erf\left(\frac{z + Z}{2\sqrt{a_T x}}\right) - erf\left(\frac{z - Z}{2\sqrt{a_T x}}\right)\right] \end{aligned} \tag{60}$$

The maximum concentration occurs along the centerline ($y = z = 0$) and is given as

$$C(x,0,0,t) = \frac{C_0}{2} erfc\left(\frac{x - Vt}{2\sqrt{a_x Vt}}\right) erf\left[\frac{Y}{2\sqrt{a_T x}}\right] erf\left[\frac{Z}{2\sqrt{a_T x}}\right]. \tag{61}$$

Assumptions:

In addition to the general assumptions, the following assumptions are associated with *Domenico's Model*

- *continuous vertical plane source,*
- *semi-infinite domain,*
- *transient state.*

Special Cases:

Case 1:

For $x << Vt$ the argument of *erfc* approaches -2, and the above solution collapses to the U.S. EPA VHS steady-state model.

Case 2:

If the vertical plane source is located in an infinite aquifer (with two spreading directions in z), the source dimension Z should be replaced with $Z/2$.

Case 3:

If dispersion in z-direction is eliminated, the error function terms are ignored and $C_0/8$ is replaced with $C_0/4$ (Domenico and Schwartz, 1990).

4.3.4 Horizontal Plane Source

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} - \lambda R_d C = R_d\frac{\partial C}{\partial t}. \tag{62}$$

The initial and boundary conditions to be applied for the horizontal plane source are given as (Galya, 1987, p. 734, equations 2 - 5)

$$\begin{aligned} C(x,y,z,0) &= 0 \\ C(x,\infty,z,t) &= 0 \\ D_z\frac{\partial C}{\partial z} &= 0 \qquad z=0 \\ D_z\frac{\partial C}{\partial z} &= 0 \qquad z=B \\ C(x,y,\infty,t) &= 0 \end{aligned}$$

where B the saturated thickness of the aquifer. The plane source has length X in the x-direction and width Y in the y-direction (Figure 5).

The solution for an instantaneous unit release of mass over the area has the following form (Codell et al., 1982, p. 3.8, equation 3.21; Galya, 1987, p. 734, equation 6):

$$C(x,y,z,t) = \frac{1}{nR_d}X_0(x,t)Y_0(y,t)Z_1(z,t)T(t). \tag{63}$$

Application of a convolution integral with respect to time provides the concentration C due to a continuous or transient release at a rate M_s for any time t (Galya, 1987, p. 735, equation 14):

$$C(x,y,z,t) = \frac{1}{nR_d}\int_0^t M_s(\tau)X_0(x,t-\tau)Y_0(y,t-\tau)Z_0(z,t-\tau)T(t-\tau)d\tau, \tag{64}$$

where

$$X_0 = \frac{1}{2X}\left[erf\left(\frac{\frac{X}{2}+x-x_s-\frac{Vt}{R_d}}{2\sqrt{D_x t/R_d}}\right) + erf\left(\frac{\frac{X}{2}-x+x_s+\frac{Vt}{R_d}}{2\sqrt{D_x t/R_d}}\right)\right] \tag{65}$$

$$Y_0 = \frac{1}{2Y}\left[erf\left(\frac{\frac{Y}{2}+y-y_s}{2\sqrt{D_y t/R_d}}\right) + erf\left(\frac{\frac{Y}{2}-y+y_s}{2\sqrt{D_y t/R_d}}\right)\right] \tag{66}$$

$$Z_1 = \frac{1}{B}\left[1+2\sum_{i=1}^{\infty}\exp(-\frac{i^2\pi^2 D_z t}{B^2 R_d})\cos(i\pi z/B)cos(i\pi z_s/B)\right] \tag{67}$$

$$T(t) = \exp(-\lambda t) \tag{68}$$

where

M_s	=	mass release rate
X_0	=	Green's functions in x-direction
Y_0	=	Green's functions in y-direction
Z_1	=	Green's functions in z-direction
T	=	degradation function (due to decay of contaminants biodegradation, hydrolysis, etc.)
x_s	=	distance to center of line source in x-direction
y_s	=	distance to center of line source in y-direction
z_s	=	depth to the source in z-direction
D_{ij}	=	dispersion coefficient
R_d	=	retardation factor
λ	=	decay constant

Assumptions:

In addition to the general assumptions, the following assumptions are associated with the model:

- *instantaneous or continuous horizontal plane source*
- *first order decay*
- *linear adsorption*
- *finite-depth aquifer*
- *transient state*

HORIZONTAL PLANE SOURCE

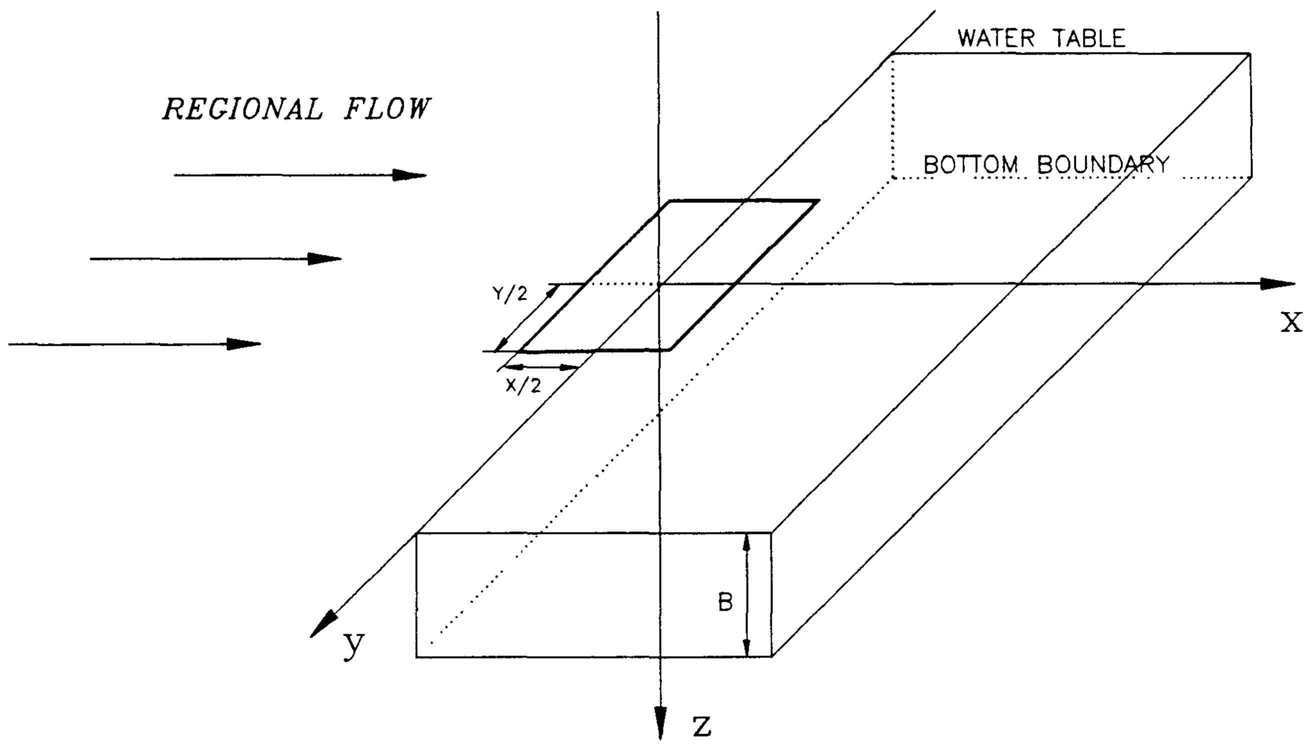

Figure 6: Horizontal plane source in a finite-depth aquifer.

4.4 Volume Source

This section describes solutions to the solute transport equation when the source of contamination is three-dimensional (volumetric). With respect to the geometry of the source, it can be represented as a cube or a parallelepiped. The source activity can be instantaneous or continuous.

4.4.1 Cubical Volumetric Source

The governing equation for the model takes the following form:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}. \tag{69}$$

An instantaneous contaminant source of finite size has its center located at the coordinate origin (Figure 6). The following initial conditions are given

$$\begin{aligned} C(x,y,z,0) &= \frac{M}{n}L^3; \qquad 0 \le |x|, |y|, |z| < \frac{L}{2} \\ &= 0; \qquad \frac{L}{2} < |x|, |y|, |z| < \infty, \end{aligned} \tag{70}$$

in which L is the side length of the cubical source at $t = 0$.

The solution of the problem is given as (Hunt, 1978, p. 82, equation 33)

$$\begin{aligned} C(x,y,z,t) = &\frac{M}{8nL^3}\left[erf\left(\frac{\frac{L}{2}+x-Vt}{2\sqrt{D_{xx}t}}\right) + erf\left(\frac{\frac{L}{2}-x+Vt}{2\sqrt{D_{xx}t}}\right)\right] \\ &\left[erf\left(\frac{\frac{L}{2}+y}{2\sqrt{D_{yy}t}}\right) + erf\left(\frac{\frac{L}{2}-y}{2\sqrt{D_{yy}t}}\right)\right] \\ &\left[erf\left(\frac{\frac{L}{2}+z}{2\sqrt{D_{zz}t}}\right) + erf\left(\frac{\frac{L}{2}-z}{2\sqrt{D_{zz}t}}\right)\right] \end{aligned} \tag{71}$$

The peak concentrations calculated for a point source (at distance $x = Vt$ and $y = z = 0$) and a source of finite size will be within 1% of each other when (Hunt, 1978, p. 83, equation 36)

$$\frac{L^2}{t}\left(\frac{1}{D_{xx}} + \frac{1}{D_{yy}} + \frac{1}{D_{zz}}\right) \le 0.48. \tag{72}$$

The above equation can be used to predict how long it would take for the solution of the cubical source to approach the solution of a point source.

Assumptions:

In addition to the general assumptions, the following assumptions are associated with the model:

- *instantaneous cubical source*
- *aquifer is of infinite depth*
- *transient state*

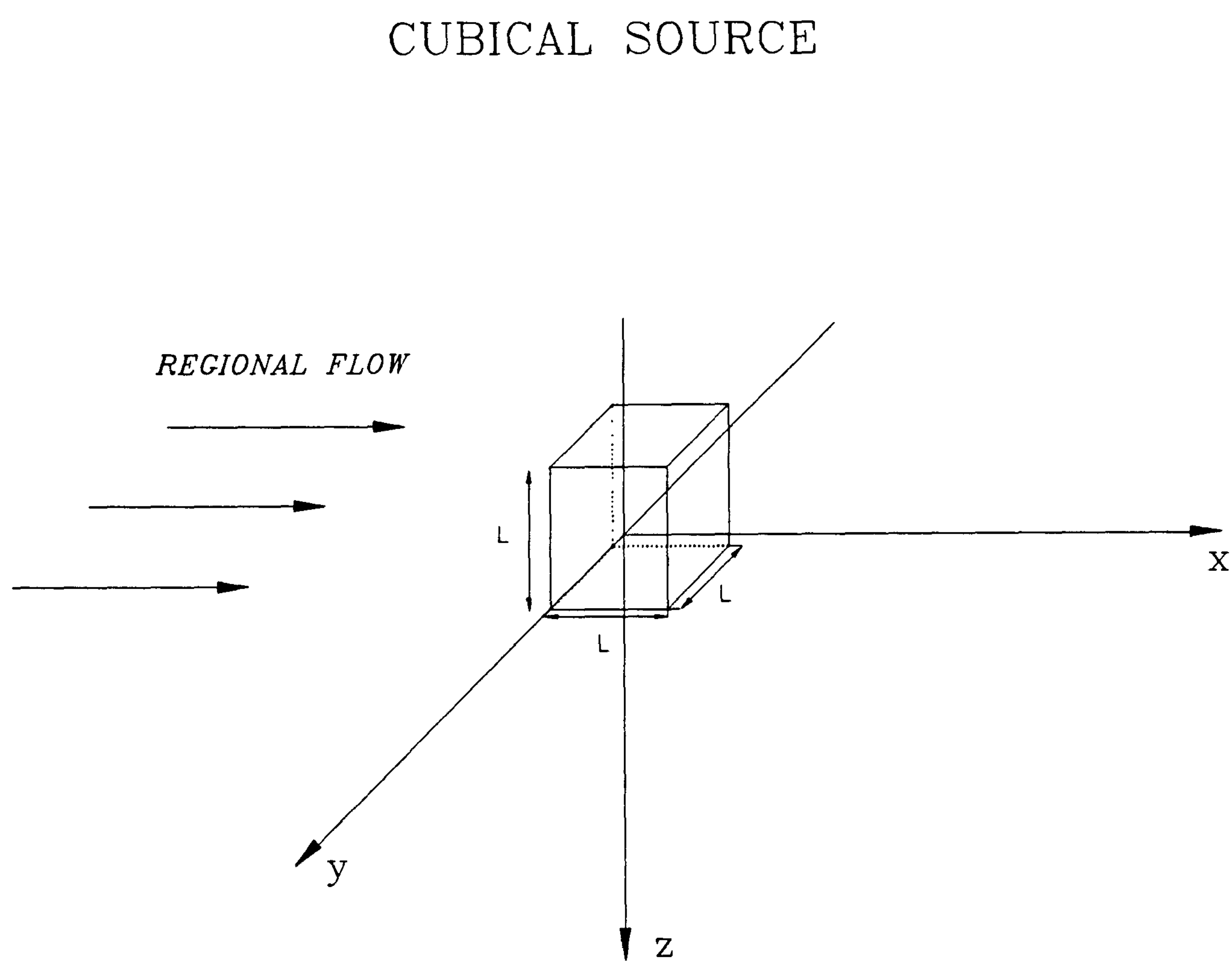

Figure 7: Cubical source in an infinite aquifer.

4.4.2 Parallelepiped Source

Governing Equation:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} + D_{zz}\frac{\partial^2 C}{\partial z^2} - V\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}. \tag{73}$$

A contaminant source shaped as a parallelepiped with dimensions X, Y, Z (in x-, y-, z-directions, respectively) is instantaneously injected into a uniform flow field. The concentration within the parallelepiped is at a constant value C_0, with its center of mass at $x = y = z = 0$. The solution to this problem is of the same form as for the cubical source (Domenico and Robbins, 1984, p. 125, equation 1)

$$\begin{aligned} C(x,y,z,t) &= \frac{C_0}{8}\left[erf\left(\frac{\frac{X}{2}+x-Vt}{2\sqrt{D_{xx}t}}\right) + erf\left(\frac{\frac{X}{2}-x+Vt}{2\sqrt{D_{xx}t}}\right)\right] \\ &\quad \left[erf\left(\frac{\frac{Y}{2}+y}{2\sqrt{D_{yy}t}}\right) + erf\left(\frac{\frac{Y}{2}-y}{2\sqrt{D_{yy}t}}\right)\right] \\ &\quad \left[erf\left(\frac{\frac{Z}{2}+z}{2\sqrt{D_{zz}t}}\right) + erf\left(\frac{\frac{Z}{2}-z}{2\sqrt{D_{zz}t}}\right)\right] \end{aligned} \tag{74}$$

The concentration along the centerline of spreading where $y = z = 0$, where the maximum concentrations will occur, is given as

$$\begin{aligned} C(x,0,0,t) &= \frac{C_0}{2}\left[erf\left(\frac{\frac{X}{2}+x-Vt}{2\sqrt{D_{xx}t}}\right) + erf\left(\frac{\frac{X}{2}-x+Vt}{2\sqrt{D_{xx}t}}\right)\right] \\ &\quad \left[erf\left(\frac{Y}{4\sqrt{D_{yy}t}}\right)\right]\left[erf\left(\frac{Z}{4\sqrt{D_{zz}t}}\right)\right] \end{aligned} \tag{75}$$

Assumptions:

- *instantaneous parallelepiped source*
- *aquifer is of infinite depth*
- *transient state*

5 Conclusions

Because analytical models give an exact solution of the governing equation, they are useful for development and for designing and verifying numerical models. A large portion of the literature on solute transport modeling is devoted to one- and two-dimensional models. The increasing development and use of three-dimensional numerical models will require more effort in verifying the models with three-dimensional analytical models. Within the past ten years, a number of three-dimensional solutions were obtained and presented in ground-water literature. However, many of the solutions are expressed as a complex series and are not easy to evaluate numerically. These research models are often buried in literature that is not easily accessible, particularly for models developed in nuclear engineering. It seems that some of the same solutions are being introduced over and over again, simply because the authors were not aware of other researchers' work.

This report attempts to gather available three-dimensional analytical models and catalog them in a systematic manner according to the geometry of the contaminant source and the type of release.

6 Recommendations

Future application and use of three-dimensional analytical solute transport models depends on the complexity of the mathematical solutions and on the difficulties in evaluating the solutions either by hand or using computers. For numerical models, in addition to the overall model development, future application and use depend how well they are verified and tested.

In developing a computer code of an analytical model, the following criteria should be observed:

- the code should be easy to use ("user-friendly")
- the code is well-documented
- the code does not require excessive data input
- the code does not require excessive computer time
- the code gives reasonable (or conservative) estimates (often adequate for regulatory purposes)

For complete testing of numerical three-dimensional models, future needs include:

- development of a library of subroutines (functions) for solving a selected number of models given in this and other reports
- careful testing of the library (with single and double precision, on various machines, etc.)
- development of hypothetical three-dimensional problems and solving them using the library
- development of a database for real-life cases (note: the IGWMC has started such a database)
- make results available in the form of tables and software to model developers and users

One has to keep in mind that analytical models must be tested and verified as well. The carefully checked results of the above-mentioned hypothetical cases can be used for such a verification.

There is also a need for better model documentation and user's guides. A good example is the model AT123 (Yeh, 1981). Although, it is a very good model (mathematically speaking), because of its poor documentation and "user-unfriendliness" it has never been used widely in practice. This chronic problem of poor or incomplete documentation is of even greater concern when working with numerical models.

The problems related to independent testing of the models and the mathematical correctness of the solutions are still unresolved. However, these problems will be resolved eventually. IGWMC, among others, is well qualified to perform this role.

For both analytical and numerical models, parameter uncertainty is another area in need of future reasearch. So far, all the comments and discussion have focused on deterministic values of the coefficients. However, it is recognized that subsurface phenomena are too complex to be described with certainty. A future study should test the analytical models against field measurements of contaminant concentrations. Such a test should reveal uncertainty caused by inaccurate or incomplete input data. Evaluating and quantifying the uncertainties will be a particularly critical task and will pose a future challenge.

References

Anderson, M.P. 1979. Using models to simulate the movement of contaminants through ground water flow systems. CRC Critical Review in *Environmental Control*, November 1979.

Baetsle, L.H. 1969. Migration of radionuclides in porous media. Progress in Nuclear Energy Series XII, Health Physics, ed. A. Duhamel, Elmsford, New York, Pergamon Press.

Bear, J. 1979. *Hydraulics of Groundwater*. McGraw-Hill, New York, N.Y.

Bear, J. and A. Verruijt. 1987. *Modeling Groundwater Flow and Pollution*. D. Reidel Publishing Company, Dordrecht, Holland.

Bear, J. and A. Bachmat. 1990. *Introduction to Transport Phenomena in Porous Media*. D. Reidel Publishing Company, Dordrecht, Holland.

Beljin, M. 1985. *SOLUTE: Analytical Models for Solute Transport in Porous Media*. IGWMC, Indianapolis, Indiana.

Carnaham, C.L. and J.S. Remer. 1984. Nonequilibrium and equilibrium sorption with a linear sorption isotherm during mass transport through an infinite porous medium: Some analytical solutions. *J. of Hydrology*, vol. 73, pp. 227-258.

Chambre, P.L., T.H. Pigford, A. Fujitsa, T. Kanki, A. Kobayashi, H. Lung, D. Ting, Y. Sato, and S.J. Zavoshy. 1982. *Analytical performance models for geological repositories*. LBL-14842, Lawrence Berkeley Laboratory, Berkeley, California.

Chambre, P.L., T.H. Pigford, W.W. Lee, J. Ahn, and S. Kajivara. 1985. *Mass transfer and transport in a geologic environment*. LBL-19430, Lawrence Berkeley Laboratory, Berkeley, California.

Cleary, R.W., and D.D. Adrian. 1973. New analytical solutions for dye diffusion equations. *J. of the Environmental Eng. Div.*, ASCE, vol. 99, no. EE3, pp. 213-227.

Cleary, R.W. 1978. Final report 208 project. Nassau-Suffolk Regional Planning Board, Hauppauge, New York.

Cleary, R.W. and M.J. Ungs. 1978. *Groundwater pollution and hydrology, mathematical models and computer programs.* Report 78-WR-15, Princeton University, Princeton, New Jersey.

Codell, R.B. and D.W. Shreiber. 1979. NRC models for evaluating the transport of radionuclides in groundwater. In *Management of Low Level Radioactive Waste*, M.W. Carter, A.A. Moghissi, and B. Kahn editors, Pergamon Press.

Codell, R.B., K.T. Key, and G. Whelan. 1982. *A collection of mathematical models for dispersion in surface water and groundwater.* NUREG-0868, U.S. Nuclear Regulatory Commission, Washington, D.C.

Cole, C.R. et al. 1987. Lessons learned from the HYDROCOIN experience. Presented at GEOVAL-87, April 7-9, Stockholm, Sweden.

Collette, R. 1985. *A three dimensional model for simulating flow and mass transport in ground-water systems.* M.S. Thesis, Dep. Geol., Univ. of Alberta, Edmonton, Alberta, 106 pp.

de Marsily, G. 1986. *Quantitative Hydrogelogy: Groundwater Hydrology for Engineers.* Academic Press, Inc., San Diego, California.

Dolman, E.A. and P.C. Robinson. 1983. UKAEA Report AERE-R.10882, Harwell, Oxfordshire.

Domenico, P.A. and V.V. Palciauskas. 1982. Alternative boundaries in solid waste management. *Ground Water.* vol. 20, pp. 303-311.

Domenico, P.A. and G.A. Robbins. 1984. A dispersion scale effect in model calibrations and field tracer experiments. *J. of Hydrology.* vol. 70, pp. 123-132.

Domenico, P.A. and G.A. Robbins. 1985. A new method of contaminant plume analysis. *Ground Water.* vol. 23, no. 4, pp. 476-485.

Domenico, P.A. 1987. An analytical model for multidimensional transport of a decaying contaminant species. *J. of Hydrology.* vol. 91, pp. 49-58.

Domenico, P.A. and F.W. Schwartz. 1990. *Physical and chemical hydrogeology.* John Wiley and Sons, New York.

El-Kadi, A., S.A. Williams, and P.K.M. van der Heijde. 1987. *Applicability of the Screening Level Groundwater Model to Site-Specific Settings.* IGWMC, Holcomb Research Institute, Indianapolis, Indiana. 90 pp.

EPRI. 1984. *Geohydrochemical models for solute migration, Vol. 2: preliminary evaluation of selected computer codes.* EPRI EA-3417, Electric Power Research Institute, Palo Alto, California.

Freeze, R.A. and J.A. Cherry. 1979. *Groundwater.* Prentice-Hall, Englewood Cliffs, N.J. 604 pp.

Galya, D.P. 1987. A horizontal plane source model for ground-water transport. *Ground Water.* vol. 25, no. 6, pp. 733-739.

Goltz, M.N. 1986. *Three-Dimensional Analytical Modeling of Diffusion-Limited Solute Transport.* Ph.D. Thesis, Stanford University, Stanford, California. 171 pp.

Goltz, M. and P. Roberts. 1986. Three-dimensional solutions for solute transport in an infinite medium with mobile and immobile zones. *Water Resources Research.* vol. 22, no. 7, pp. 1139-1148.

Gupta, S.K. et al. 1987. *Coupled fluid, energy, and solute transport (CFEST) model: Formulation and user's manual.* BMI/ONWI-660, Battelle Memorial Institute, Columbus, Ohio.

Gureghian, A.B. 1987. *Analytical solutions for multidimensional transport of a four-member radionuclide decay chain in ground water.* Battelle Office of Crystalline Repository Development, Columbus, Ohio.

Gureghian, A.B. 1988. *MASCOT: Analytical solutions for multidimensional transport of a four-member radionuclide chain in ground water.* Battelle Memorial Institute, Columbus, Ohio.

Herbert, A.W. 1984. *Analytical solutions to the three-dimensional radionuclide transport equation for computer code verification.* AERE Harwell, Oxfordshire.

Hunt, B.W. 1973. Dispersion from pit in uniform seepage. *J. of the Hydraulics Div.,* ASCE. vol. 99, no. HY1, pp. 13-21.

Hunt, B.W. 1978. Dispersive sources in uniform groundwater flow. *J. of the Hydraulics Div.,* ASCE. vol. 104, pp. 75-85.

Hunt, B.W. 1983. *Mathematical Analysis of Groundwater Resources.* Butterworth & Co., London. 271 pp.

Huyakorn, P., B.G. Jones, and P.F. Andersen. 1986. Finite-element algorithms for simulating three-dimensional groundwater flow and solute transport in multilayer systems. *Water Resources Research,* vol. 22, no. 3, pp. 361-374.

Huyakorn, P., M.J. Ungs, L.A. Mulkey, and E.A. Sudicky. 1987. A three-dimensional analytical method for predicting leachate migration. *Ground Water.* vol. 25, no. 5, pp. 588-598.

INTERA. 1983. *VERTPAK-1: Package of analytical solutions for code verification.* Technical Report, ONWI-451, Battelle Memorial Institute, Columbus, Ohio.

INTRACOIN. 1984. *International nuclide transport code intercomparison study.* Final Report Level 1. Swedish Nuclear Power Inspectorate.

Javandel, I., C. Doughty, and C.F. Tsang. 1984. *Groundwater transport: Handbook of mathematical models.* American Geophysical Union (AGU) Water Resources Monograph 10, Washington, D.C.

Marino, M.A. 1974. Longitudinal dispersion in saturated porous media. *J. of the Hydraulics Div.,* ASCE, vol. 100, no. HY1, pp. 151-157.

Prakash, A. 1977. Convective-dispersion in perennial streams. *J. of the Environmental Eng. Div.,* ASCE, vol. 103, no. EE2, pp. 321-340.

Prakash, A. 1982. Groundwater contamination due to vanishing and finite size continuous sources. *J. of the Hydraulics Div.,* ASCE. vol. 108, no. HY4, pp. 572-590.

Prakash, A. 1984. Ground-water contamination due to transient sources of pollution. *J. of the Hydraulics Div.,* ASCE, vol. 110, no. 11, pp. 1642-1658.

Robbins, G.A. and P.A. Domenico. 1984. Determining dispersion coefficients and sources of model-dependent scaling. *J. of Hydrology,* vol 75, pp. 195-211.

Sagar, B. 1982. Dispersion in three-dimensions: approximate analytical solutions. *J. of the Hydraulics Div.,* ASCE. vol. 108, no. HY1, pp. 47-62.

Shen, H.T. 1976. Transient dispersion in uniform porous media flow. *J. of the Hydraulics Div.,* ASCE. vol. 102, no. HY6, pp. 707-716.

Simmons, C.S. and C.R. Cole. 1985. *Guidelines for selecting codes for ground-water transport modeling of low-level waste burial sites.* Pacific Northwest Laboratory PNL-4980, Richland, Washington.

U.S. EPA. 1984. *AT123D execution using the data management supporting systems AT123DIN and AT123DOUT, User's Guide.* PB86-140634, U.S. EPA, OSW, Washington, D.C.

U.S. EPA. 1985. Background document for the ground water screening procedure to support 40 CFR part 268, Land Disposal Restrictions, U.S. EPA, OSW, Washington, D.C.

van der Heijde, P.K.M. 1989. *EPA-VHS: Analytical Solute Transport Model.* International Ground Water Modeling Center, Indianapolis, Indiana.

van der Heijde, P.K.M. 1990. *PLUME 2.0: A Three-dimensional Analytical Solute Transport Model.* International Ground Water Modeling Center, Indianapolis, Indiana.

van Genuchten, M.Th. and W.J. Alves. 1982. *Analytical solutions of one-dimensional convective-dispersive solute transport equation.* USDA Technical Bulletin No. 1661, Riverside, California.

Wagner, J., S. Watts, and D.C Kent. 1985. *PLUME3D: Three-dimensional plumes in uniform ground water flow.* EPA Report EPA/600/2-85/067, Robert S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

Walton, W. 1979. Progress in analytical groundwater modeling. In: W.Back and D.A. Stephenson (Editors), Contemporary Hydrogeology, *J. Hydrology,* vol. 4, pp. 149-159.

Walton, W. 1985. *WALTON35: Microcomputer programs.* International Ground Water Modeling Center, Indianapolis, Indiana.

Walton, W. 1988. *Practical Aspects of Ground Water Modeling.* National Water Well Association (NWWA), Columbus, Ohio.

Wexler, E.J. 1989. *Analytical solutions for one-, two-, and three-dimensional solute transport in ground-water systems with uniform flow.* U.S. Geological Survey, Open-File Report 89-56, Tallahassee, Florida.

Wolanski, E.J. 1973. Discussion of "Dispersion from pit in uniform seepage," by B.W. Hunt, *J. of the Hydraulics Div.,* ASCE, vol. 99. no. HY7, pp. 1198-199.

Yeh, G.T. and Y.J. Tsai. 1976. Analytical three-dimensional transient modeling of effluent discharges. *Water Resources Research.* v. 20, pp. 533-546.

Yeh, G.T. 1981. *AT123D: Analytical transient one-, two-, and three-dimensional simulation of waste transport in the aquifer system.* Oak Ridge National Lab., Report No. ORNL-5602. 83 pp.

Appendix A

Reference Table

MODEL 1.

Model Name:	A1-i (page 13)
Source:	Point
Release:	Instantaneous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Transient
References:	Hunt (1978)
Code:	SOLUTE (version 2.0)
Author:	Beljin (1985)
Contact Address:	IGWMC
Remarks:	
Code:	PLUME3D
Author:	Wagner et al. (1985)
Contact Address:	Oklahoma State University
Remarks:	
Code:	WALTON35D
Author:	Walton (1985)
Contact Address:	IGWMC
Remarks:	

MODEL 2.

Model Name:	B1-i (page 16)
Source:	Point
Release:	Instantaneous
Boundary:	Infinite
Processes:	Advection, Dispersion, Decay
Transport:	Transient
References:	Hunt (1983)
Code:	SOLUTE (version 2.0)
Author:	Beljin (1985)
Contact Address:	IGWMC
Remarks:	
Code:	WALTON35D
Author:	Walton (1985)
Contact Address:	IGWMC
Remarks:	

MODEL 3.

Model Name:	A1-c (page 17)
Source:	Point
Release:	Continuous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Transient
References:	Hunt (1978)
Code:	SOLUTE (version 2.0)
Author:	Beljin (1985)
Contact Address:	IGWMC
Remarks:	
Code:	WALTON35D
Author:	Walton (1985)
Contact Address:	IGWMC
Remarks:	

MODEL 4.

Model Name:	A2-c (page 19)
Source:	Point
Release:	Continuous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Steady
References:	Hunt (1978)
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 5.

Model Name:	A3-c (page 20)
Source:	Point
Release:	Continuous
Boundary:	Finite
Processes:	Advection, Dispersion
Transport:	Steady
References:	Hunt (1978)
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 6.

Model Name:	B1-c (page 22)
Source:	Point
Release:	Continuous
Boundary:	Infinite
Processes:	Advection, Dispersion, Decay
Transport:	Transient
References:	Hunt (1983)
Code:	SOLUTE (version 2.0)
Author:	Beljin (1985)
Contact Address:	IGWMC
Remarks:	
Code:	PLUME3D
Author:	Wagner, *et al.* (1985)
Contact Address:	Oklahoma State University
Remarks:	
Code:	WALTON35D
Author:	Walton (1985)
Contact Address:	IGWMC
Remarks:	

MODEL 7.

Model Name:	B2-c (page 23)
Source:	Point
Release:	Continuous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Steady
References:	Hunt (1983)
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 8.

Model Name:	Vertical Line Source Model (page 24)
Source:	Line
Release:	Instantaneous
Boundary:	Finite
Processes:	Advection, Dispersion, Adsorption, Decay
Transport:	Transient
References:	Codell et al. (1982); Galya (1987)
Code:	GROUND
Author:	Codell et al. (1982)
Contact Address:	
Remarks:	
Code:	PLUME (version 2.0)
Author:	van der Heijde (1990)
Contact Address:	IGWMC
Remarks:	

MODEL 9.

Model Name:	Horizontal Line Source (page 26)
Source:	Line
Release:	Instantaneous
Boundary:	Finite
Processes:	Advection, Dispersion
Transport:	Transient
References:	Codell et al. (1982)
Code:	GROUND
Author:	Codell et al. (1982)
Contact Address:	
Remarks:	
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 10.

Model Name:	Vertical Plane Source (page 28)
Source:	Vertical Plane
Release:	Instantaneous
Boundary:	Finite
Processes:	Advection, Dispersion, Adsorption, Decay
Transport:	Transient
References:	Codell et al. (1982)
Code:	GROUND
Author:	Codell et al. (1982)
Contact Address:	
Remarks:	
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 11.

Model Name:	US EPA VHS Model (page 30)
Source:	Vertical Plane
Release:	Continuous
Boundary:	Semi-Infinite
Processes:	Advection, Dispersion
Transport:	Steady
Remarks:	Spreading of contaminant only in vertical and lateral directions
References:	Domenico and Palciauskas (1982)
Code:	EPA-VHS (version 1.0)
Author:	van der Heijde (1989)
Contact Address:	IGWMC
Remarks:	

MODEL 12.

Model Name:	Domenico's Model (page 34)
Source:	Vertical Plane
Release:	Continuous
Boundary:	Semi-Infinite
Processes:	Advection, Dispersion
Transport:	Transient
Remarks:	Special cases on page 35
References:	Domenico and Robbins (1985)
Code:	No name
Author:	Domenico (1990)
Contact Address:	
Remarks:	FORTRAN listing of the code given in Domenico and Schwartz (1990)

MODEL 13.

Model Name:	Horizontal Plane Model (page 36)
Source:	Horizontal Plane
Release:	Instantaneous
Boundary:	Finite
Processes:	Advection, Dispersion, Adsorption, Decay
Transport:	Transient
References:	Galya (1987)
Code:	AT123D
Author:	Yeh (1981)
Contact Address:	IGWMC
Remarks:	
Code:	HPS
Author:	Galya (1987)
Contact Address:	
Remarks:	FORTRAN listing of the code given in *GROUND WATER*, vol.25, no.6.

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MODEL 14.

Model Name:	Horizontal Plane Model (page 37)
Source:	Horizontal Plane
Release:	Continuous
Boundary:	Finite
Processes:	Advection, Dispersion, Adsorption, Decay
Transport:	Transient
References:	Yeh (1981); Galya (1987)
Code:	AT123D
Author:	Yeh (1981)
Contact Address:	IGWMC
Remarks:	
Code:	HPS
Author:	Galya (1987)
Contact Address:	
Remarks:	FORTRAN listing of the code given in *GROUND WATER*, vol.25, no.6.

MODEL 15.

Model Name:	Cubical Model (page 39)
Source:	Volumetric Cubical
Release:	Instantaneous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Transient
References:	Hunt (1978)
Code:	AT123D
Author:	Yeh (1981)
Contact Address:	IGWMC
Remarks:	
Code:	
Author:	
Contact Address:	
Remarks:	

MODEL 16.

Model Name:	Parallelepiped Model (page 39)
Source:	Volumetric Parallelepiped
Release:	Instantaneous
Boundary:	Infinite
Processes:	Advection, Dispersion
Transport:	Transient
References:	Domenico and Robbins (1984)
Code:	AT123D
Author:	Yeh (1981)
Contact Address:	IGWMC
Remarks:	
Code:	
Author:	
Contact Address:	
Remarks:	