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Project Summary

Selection Criteria for Mathematical Models Used in Exposure Assessments: Ground-Water Models

Prior to the issuance of the Guidelines for Estimating Exposures in 1986, The U.S. Environmental Protection Agency (EPA) published proposed guidelines in the *Federal Register* for public review and comment. The purpose of the guidelines is to provide a general approach and framework for carrying out human and nonhuman exposure assessments for specific pollutants. As a result of the review process, four areas were identified that required further research. One of these was the area of selection criteria for mathematical models used in exposure assessments.

The purpose of this document is to present criteria which provide a means for selecting the most appropriate mathematical model(s) for conducting an exposure assessment related to ground-water contamination.

General guidelines and principles for model selection criteria are presented followed by a step-by-step approach to identifying the appropriate model(s) for use in a specific application. Several of the currently-available models are grouped into categories and a framework is provided for selecting the appropriate model(s) based on the response to the technical criteria. Brief summaries of all the currently available models discussed in this report are contained in the appendix.

Two site-specific example problems are provided to demonstrate the procedure for selecting the appropriate mathematical model for a particular application.

This Project Summary was developed by EPA's Office of Health and Environmental Assessment, Washington, DC, to announce key findings of the research project that is fully documented in a separate report of the same title (See Project Report ordering information at back).

Introduction

This document presents a set of criteria which provide a means of selecting the most appropriate mathematical model for conducting an exposure assessment related to ground-water contamination. These criteria were developed in recognition of the growing use of exposure assessments across the U.S. Environmental Protection Agency's regulatory programs. Use of the criteria will expedite the regulatory process by eliminating the use of unacceptable or inappropriate models. Their use will also improve the quality of data used in the decision-making processes and promote consistency in exposure assessments.

When performing a predictive exposure assessment, a major task is to predict the transport of contaminants. Since ground-water flow is an integral part of contaminant transport, it is equally important, if not more so, to accurately predict the ground-water flow. Therefore, both ground-water flow and contaminant transport mathematical models, and criteria for selecting these models, are discussed in this document.

Background Information

Some of the general background information necessary to understand the selection of a ground-water flow and/or contaminant transport model is discussed in this section. This chapter is intended for the exposure assessor or the non-modeler who is not completely familiar with hydrogeologic and modeling terms.

The first section provides a primer on ground-water flow. The intent of this section is to provide a brief summary of the background information necessary to understand ground-water problems. The chapter discusses the general terms used to describe and define ground-water flow and presents the basic equation for flow in a ground-water system.

The second section provides background information on contaminant transport in ground-water. The chapter presents the basic equation for advective-dispersive transport and discusses the important terms in detail.

The last section provides definitions for terms used throughout the report.

General Guidelines and Principles of Model Selection Criteria

In order to enhance understanding and facilitate implementation of the mathematical model selection criteria, the following terms are defined: mathematical model, process equation, analytical solution, analytical models, numerical models, objectives criteria, technical criteria, and implementaiton criteria. The relationship between these terms may be thought of as follows. A mathematical model consists of two aspects: a process equation and a solution technique to solve the process equation. An analytical solution solves a very simple process equation analytically by hand calculations. An analytical model solves a more complex, but still relatively simple, process equation analytically with a computer program. A numerical model solves a simple or complex process equation numerically with a computer program. In the context of this document, mathematical model refers to all three solution techniques of a process equation. The more detailed the specific application, the more complex the process equation. The complexity of the process equation dictates the solution technique required.

There are three factors which dictate the level of complexity of the mathematical model chosen in the selection process:

1. objectives criteria;
2. technical criteria; and
3. implementation criteria.

The objectives criteria refer to the level of modeling detail required to meet the objectives of the study. There are many different objectives of modeling studies, however, in the context of model selection, all objectives are classified in two broad categories: 1) to perform a screening study or 2) to perform a detailed study.

A screening study is one where the purpose is to make a preliminary screening of a site or to make a general comparison between several sites. A detailed study, on the other hand, is one where the objective is to make an assessment of the environmental impact, performance, or safety of a specific site.

Based on the objectives of the study (screening or detailed levels), the analyst or modeler will select either a screening or detailed model. The specific model to be used will be selected based on the technical selection criteria discussed below.

Technical Criteria

The second level of consideration when selecting a mathematical model is the technical criteria. Technical criteria are those criteria related to the mathematical model's ability to simulate the site-specific contaminant transport and fate phenomena of importance.

With regard to model selection, the technical criteria can be divided into three categories:

1. transport and transformation processes;
2. domain configuration; and
3. fluid(s) and media properties.

Transport and transformation process criteria relate to those significant processes or phenomena known to occur on site that must be modeled in order to properly represent the site. Domain configuration relates to the ability of the model to accurately represent the geohydrologic system. When high levels of resolution are required to predict contaminant concentrations for comparison to health or design standards, it is generally necessary to simulate site-specific geometry and dimensionality for which numerical models are most appropriate. If simplifying the site geometry can be defended on a geologic and hydrologic basis, then the use of a simpler analytical model solution may be justified. The third category of technical criteria corresponds to the ability of the mathematical model to represent the spatial variability of *fluid(s) and media properties* of the geohydrologic site.

Once the level of model has been decided, the technical criteria will direct the analyst to the specific type of model needed to properly simulate the transport and transformation aspects of the environmental setting.

Implementation Criteria

The third level of consideration when selecting a mathematical model is related to the implementation criteria. Implementation criteria are those criteria dependent on the ease with which a model can be obtained and its acceptability demonstrated. Whereas the technical criteria identify the models capable of simulating the relevant phenomena within the specified environmental setting, the implementation criteria identify documentation, verification, validation requirements, and ease of use so that the model selected provides accurate, meaningful results.

Other Factors Affecting Model Selection

Other general factors related to model selection which are secondary to the technical or implementation criteria include data availability, schedule, budget, staff and equipment resource, and level of complexity of system(s) under study. Schedule and budget constraints refer to the amount of time and money available for the assessment. If both analytical and numerical models meet the selection criteria, time and cost may be considered factors for electing to use an analytical approach.

Model Selection Decision Process

The decisions to be made when selecting a ground-water flow model are discussed in detail in this section. Some guidance is provided for making the decision and some discussion is provided regarding the errors associated with using the incorrect model or feature(s) of a model. The criteria for ground-water flow are presented followed by those for contaminant transport.

- Are you simulating a water table (i.e., unconfined) or a confined aquifer, or a combination of both (i.e., conditions change spatially)?
- Does the ground water flow through porous media, fractures, or a combination of both?
- Is it necessary to simulate three-dimensional flow or can the dimensionality be reduced without losing a significant amount of accuracy?
- Are you simulating a single-phase (i.e., water) or a multi-phase (i.e., water and oil) flow system?
- Can the system be simulated with a uniform value (homogeneous) or spatially variable values (heterogeneous) of hydraulic conductivity, porosity, recharge, and/or specific storage?
- Is there a single or are there multiple hydrogeologic layers to be simulated?
- Is (are) the hydrogeologic layer(s) of constant or variable thickness spatially?
- Is the hydrologic system in a steady-state condition or do water levels fluctuate with time (transient condition)?

After all these criteria have been satisfied, in most cases there will be several ground-water flow models which would be appropriate. At this point the analyst can either select a ground-water flow model and then continue with the selection process to select a compatible (but separate) contaminant transport model, or the user can continue the process to select a combined flow and transport model. It is quite common to develop a fairly sophisticated flow model to predict ground-water travel paths and velocities and link it with a simpler transport model.

The decisions to be made when selecting a contaminant transport model are discussed in detail in this section. Some guidance is provided to help in making the decision and some discussion is provided regarding the errors associated with using the incorrect model or feature(s) of the model.

- Does the contaminant enter the ground-water flow system at a point or is it distributed along a line or over an area or a volume?
- Does the source consist of an initial slug of contaminant or is it constant over time?
- Is it necessary to simulate three-dimensional transport or can the dimensionality be reduced without losing a significant amount of accuracy?
- Does the model simulate dispersion?
- Does the model simulate adsorption (i.e., distribution or partitioning coefficient) and, if so, does it simulate temporally and/or spatially variable adsorption? Temporally or spatially variable adsorption is important where the soil conditions and/or concentrations change with time and space.
- Does the model simulate first or second-order decay and/or radionuclide decay?
- Does the model simulate density effects related to changes in temperature and concentration? A truly coupled model is one where the ground-water flow is influenced by the density and viscosity of the water, which are influenced by the temperature of the water and the concentration of the solute. In some cases (i.e., large heat source or large fluctuations in solute concentration) it may be important to consider temperature and contaminant concentration effects or ground-water flow.

After sequencing through the decision tree, there will, in most cases, be several models which meet the desired criteria. Since several models could meet the desired criteria, it is difficult to list a single model as a standard model. At this point the analyst can either select a transport model which is compatible with the flow model selection above, or select a combined ground-water flow/contaminant transport model.

Regardless of the approach selected, separate or combined flow and transport model, it is likely that there will be several models which meet the techical criteria. The selection of the final model(s) should be based on the implementation criteria, i.e., the model has been through a rigorous quality assurance program so that it is thoroughly verified and the model is well documented with user's manuals and test cases.

If several models pass the quality assurance and documentation criteria, the final selection of a model should be based on familiarity with and availability of the model, schedule, budget, and staff and equipment resources.

A model selection worksheet is included in this section which facilitates a selection of the actual model or suite of models to be used based on the response to the technical criteria. Separate worksheets are provided for both analytical solutions and for analytical and numerical models (coded for the computer). A summary of each of the *models* contained in the worksheets is contained in Appendix A.

A discussion of waste management models has been included in this section. Waste management models are defined as models which trace contaminant movement through the three primary environmental pathways: air, surface water, and/or ground water. It is not the objective of this document to cover waste management models in any detail. Rather, a few such models are described briefly to make the reader aware of them. The models discussed are:

1. risk assessment methodology for regulatory sludge disposal through land application;
2. risk assessment methodology for regulating landfill disposal of sludge;
3. RCRA risk/cost policy model (WET model);
4. the liner location risk and cost analysis model; and
5. landfill ban model.

Model Selection Eample Problems

Two site-specific example problems are provided in this section to demonstrate the procedure for selecting the appropriate mathematical model for a particular application. The first example is an application where the objective is to perform a screening study, while the objective of the second example is to perform a detailed study. The discussions of the example problems are presented in the order that should be followed when conducting a ground-water flow and contaminant transport model study, with model selecting being one element of the process.

Appendix A

The appendix of the document contains a summary page for each of the analytical and numerical mathematical models discussed in Table 5-3 of the full report. The models are divided into seven categories:

1. analytical flow models;
2. analytical transport models;
3. numerical flow models which can be applied to both saturated and unsaturated systems;
4. numerical flow models which can only be applied to saturated systems;
5. numerical contaminant transport models which can be applied to both saturated and unsaturated systems;
6. numerical contaminant transport models which can only be applied to saturated systems; and
7. numerical contaminant and heat transport models which couple the solutions for pressure, temperature, and concentration (coupled models).

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The complete report, entitled "Selection Criteria for Mathematical Models Used in Exposure Assessments: Ground-Water Models," (Order No. PB 88-248 752/AS; Cost: $25.95, subject to change) will be available only from:

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