

## ***Bibliography of Guidance and Information Sources on Subsurface Modeling to Support Site Remediation***

At the May 22, 2019 Federal Remediation and Technology Roundtable (FRTR) meeting on ***Modeling in Support of Site Remediation***, an *Ad Hoc* subcommittee of the FRTR Steering Committee was formed to organize a search of guidance documents by FRTR agencies and industry on subsurface modeling in support of site remediation. The following list of guidance documents and information sources were identified to assist practitioners involved in their site remediation, contaminant source characterization, and remediation activities.

To assist the reader, each guidance document and information source cited has two brackets, (e.g., **[GG]** **[RIG]**) identifying first the **topical area**, followed by the **cross-cutting category**. Listed below are definitions for the **topical areas**. The acronym in the first bracket corresponds to those **topical areas**.

### ***Topical Area Definitions and Acronyms:***

- **General Guidance [GG]:** General guidance documents are governmental and academic sources that the committee considers to be guiding information for practitioners on model construction, calibration, and implementation. These documents are not endorsed by this committee; however, they may act as a starting place for practitioners interested in model recommendations and construction information.
- **Characterization to Support Development of Conceptual Site Models [CCSM]:** Documents included in this topical area include available standards and governmental guidelines for the development of conceptual site models. This topical area also includes information on calibration, validation, and construction for the purposes of fate and transport modeling within the context of the conceptual site model. Each document in this category includes a section and/or emphasis on preliminary conceptual site modeling, as well as its importance in the development of the final modeling product(s).
- **Numerical Models, their Manuals and Output Portrayals [NMMO]:** Documents included in this category discuss the creation of numerical models, with an emphasis on finite difference and element construction methodologies. This topical area includes selected modeling code manuals, guidelines for the evaluation of models, and applied model instructions.
- **QA/QC of Data and Model Inputs [QAQC]:** This topical area includes documents related to the selection of calibration information as well as its use in the calibration of fate and transport modeling.
- **Calibration, Verification and Validation of Models [CVVM]:** Documents included in this topical area include available standards and governmental guidelines for the calibration, verification, and validation of numerical models. While some sources focus on groundwater flow models, information for the calibration of fate and transport modeling (even if not a document's emphasis) was included. Additionally, documents including best practices in the fields of calibration, verification, and validation were also included in this category if they were deemed to provide useful guidelines for fate and transport modeling.

- **Uncertainty Analysis of Models [UAM]:** Documents included in this topical area focus on the evaluation of uncertainty within a fate and transport model. Different than the Calibration, Verification and Validation of Models [CVVM] category, these documents include uncertainty as it applies to all stages of the model development process, including the conceptual site model, model selection, construction, calibration, and final scenario implementations.
- **Case Studies of Modeling which Supports Remediation Decisions [CSMRD]:** The final topical area category assessed by this committee focuses on a selection of documents containing examples and case studies of fate and transport numerical models. Primarily it includes textbook examples, as well as peer-reviewed journals, which include both specific examples, as well as potential sources for case studies. In places where individual sites are highlighted, we designate examples, (e.g., **Hanford 300-Area**). The committee does not endorse the design, construction, or results of any particular case study within this topical area. Instead, the documents and sources may prove useful for practitioners looking for ideas and insights in their own fate and transport modeling solutions.

**Cross-Cutting Definitions and Acronyms categories:**

- A. Regulatory and/or Industry Guidance [RIG]
- B. Modeling Tools, Manuals and Output Portrayals [MTMO]
- C. Lessons Learned from Modeling Case Studies focused on Remediation Successes [LLMR]
- D. Subsurface Flow Modeling [SFM]
- E. Contaminant Transport Modeling [CTM]

American Nuclear Society, ***Evaluation of Subsurface Radionuclide Transport at Commercial Nuclear Power Plants***, ANSI/ANS-2.17-2010 (R-2016), La Grange Park, IL, 2010 (endorsed by: U.S.NRC in Regulatory Guide 4.25).

[https://webstore.ansi.org/preview-pages/ANSI/preview\\_ANSI+ANS-2.17-2010+\(R2016\).pdf](https://webstore.ansi.org/preview-pages/ANSI/preview_ANSI+ANS-2.17-2010+(R2016).pdf).

**[GG][CCSM] [RIG][SFM][CTM]**

**Abstract/Scope:** This standard establishes the requirements for evaluating the occurrence and movement of radionuclides in the subsurface resulting from abnormal radionuclide releases at commercial nuclear power plants. This standard applies to abnormal radionuclide releases that affect groundwater, water supplies derived from groundwater, and surface waters affected by subsurface transport, including exposure pathways across the groundwater-surface-water transition zone.

This standard constitutes a major revision of the original standard, ANSI/ANS-2.17-1980, which was adopted on April 9, 1980, reaffirmed on October 3, 1989, and withdrawn on July 28, 2000. A new working group, Working Group ANS-2.17 of ANS-25 Subcommittee on Siting: Environmental & Emergency Preparedness of the American Nuclear Standards Committee, was constituted November 2005 to revise the original standard.

This standard might reference documents and other standards that have been superseded or withdrawn at the time the standard is applied. A statement has been included in the references section that provides guidance on the use of references.

This standard mentions, but does not exhaustively describe, the concepts of generating risk-informed insights, performance-based requirements, and a graded approach to quality assurance. The user is advised that one or more of these techniques could enhance the application of this standard.

Two appendices are provided to assist practitioners who would implement the guidance in this standard. Appendix A provides information on relevant U.S. Nuclear Regulatory Commission regulatory criteria and guidance, and its Table A provides a listing of standard documents for conducting subsurface radionuclide transport characterization, monitoring, and modeling programs. Appendix B provides tables that summarize information and parameters identified in the guidance.

Anderson, M.P., Woessner, W. and Hunt, R. ***Applied Groundwater Modeling, Simulation of Flow and Advective Transport***, Elsevier Academic Press, San Diego, CA, 2015, ISBN:978-0-12-058103. <https://www.elsevier.com/books/applied-groundwater-modeling/anderson/978-0-08-091638-5>.

**[GG][CCSM][NMMO][QA/QC][UAM] [MTMO][SFM][CTM]**

**Abstract/Scope:** This edition is extensively revised throughout with expanded discussion of modeling fundamentals and coverage of advances in model calibration and uncertainty analysis that have revolutionized the science of groundwater modeling. The text is intended for undergraduate and graduate level courses in applied groundwater modeling and as a comprehensive reference for environmental consultants and scientists/engineers in industry and governmental agencies.

- Explains how to formulate a conceptual model of a groundwater system and translate it into a numerical model.
- Demonstrates how modeling concepts, including boundary conditions, are implemented in two groundwater flow codes—MODFLOW (for finite differences); and FEFLOW (for finite elements).
- Discusses particle tracking methods and codes for flowpath analysis and advective transport of contaminants.
- Summarizes parameter estimation and uncertainty analysis approaches using the code PEST to illustrate how concepts are implemented.
- Discusses modeling ethics and preparation of the modeling report.
- Includes “Breakout Boxes” that amplify and supplement topics covered in the text.
- Each chapter presents lists of common modeling errors and problem sets that illustrate concepts.

Argonne National Laboratory, **RESRAD Family of Codes: RESRAD, RESRAD Offsite.**  
<http://resrad.evs.anl.gov/>.

**[NMMO] [RIG][CTM]**

**Abstract/Scope:** The RESRAD family of codes is developed at Argonne National Laboratory to analyze potential human and biota radiation exposures from the environmental contamination of RESidual RADioactive materials. The codes use pathway analysis to evaluate radiation exposure and associated risks, and to derive cleanup criteria or authorized limits for radionuclide concentrations in the contaminated source medium. The RESRAD family of codes is widely used by regulatory agencies, the risk assessment community, and universities in more than 100 countries around the world.

- RESRAD-ONSITE—For assessing radiation exposures of a human receptor located on top of soils contaminated with radioactive materials.
- RESRAD-OFFSITE—For assessing radiation exposures of a human receptor located on top of or at some distance from soils contaminated with radioactive materials.
- RESRAD-BUILD—For assessing radiation exposures of a human receptor in a contaminated building or a building housing contaminated furniture or equipment.
- RESRAD-RDD—For evaluating human radiation exposures during the early, intermediate, or late phase of response after a radiological dispersal device (RDD) incident.
- RESRAD-BIOTA—For evaluating radiation exposures of nonhuman biota, including flora and fauna, in a terrestrial or aquatic ecosystem.

ASTM, ***RBCA (Risk-Based Corrective Action) Fate and Transport Models: Compendium and Selection Guidance***, West Conshohocken, PA, 1999. [EPA National Service Center for Environmental Publications](#).

**[GG] [RIG][SFM][CTM]**

**Abstract/Scope:** This guidance document catalogs and describes non-proprietary fate and transport models that are readily available and in common use for risk-based corrective action (as of the publishing date 1999). It is intended as a compendium and resource guide assisting the user in their model selection process. It is not intended to be a comprehensive review or implementation-guidance of all available fate and transport models. Listed models are neither endorsed or ranked, and their accuracy and performance is not evaluated. Models not listed in this guidance may be appropriate choices for fate and transport modeling at any site. This guidance is not applicable for complex multi-phase and/or multi-component models. This guidance does not cover movement of nonaqueous phase liquids or movement through fractured media. Proprietary models are not listed in the guidance.

*Document disclaimer: This document is not a standard and has not been approved by the ASTM consensus system.*

ASTM, ***Standard Guide for Application of a Numerical Groundwater Flow Model to a Site-Specific Problem***, D5447-17, West Conshohocken, PA, January 2018. <https://www.astm.org/Standards/D5447.htm>.

**[GG] [RIG][SFM]**

**Abstract/Scope:** This guide covers the application and subsequent documentation of a groundwater flow model to a particular site or problem. In this context, “groundwater flow model” refers to the application of a mathematical model to the solution of a site-specific groundwater flow problem. This document provides the following:

- Illustrates the major steps to take in developing a groundwater flow model that reproduces or simulates an aquifer system that has been studied in the field. This guide does not identify particular computer codes, software, or algorithms used in the modeling investigation.
- Specifically written for saturated, isothermal, groundwater flow models. The concepts are applicable to a wide range of models designed to simulate subsurface processes, such as variably saturated flow, flow in fractured media, density-dependent flow, solute transport, and multiphase transport phenomena; however, the details of these other processes are not described in this guide.
- Not intended to be all inclusive. Each groundwater model is unique and may require additional procedures in its development and application. All such additional analyses should be documented, however, in the model report.
- Offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience, and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace

the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.

- Is one in a series of standards on groundwater model applications. Other standards include D5981, D5490, D5609, D5610, D5611, and D6033.

*Document disclaimer: This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

ASTM, **Standard Guide for Calibrating a Groundwater Flow Model Application**, D5981/D5981M - 18, West Conshohocken, PA, February 2018. <https://www.astm.org/Standards/D5981.htm>.

**[CVVM] [RIG][SFM]**

**Abstract/Scope:** This guide covers techniques that can be used to calibrate a groundwater flow model. Most site-specific groundwater flow models must be calibrated prior to use in predictions. In these cases, calibration is a necessary, but not sufficient, condition which must be obtained to have confidence in the model's predictions. Often, during calibration, it becomes apparent that there are no realistic values of the hydraulic properties of the soil or rock which will allow the model to reproduce the calibration targets. In these cases, the conceptual model of the site may need to be revisited or the construction of the model may need to be revised. In addition, the source and quality of the data used to establish the calibration targets may need to be reexamined. For example, the modeling process can sometimes identify a previously undetected surveying error, which would result in inaccurate hydraulic head targets. Flow models are usually calibrated using either the manual (trial-and-error) method or an automated (inverse) method. This guide presents some techniques for calibrating a flow model using either method.

This guide is written for calibrating saturated porous medium (continuum) groundwater flow models. However, these techniques, suitably modified, could be applied to other types of related groundwater models, such as multi-phase models, non-continuum (karst or fracture flow) models, or mass transport models.

ASTM, **Standard Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information**, D5490-93 (Reapproved 2014), West Conshohocken, PA, October 2014. <https://www.astm.org/Standards/D5490.htm>.

**[GG] [RIG][SFM]**

**Abstract/Scope:** This guide covers techniques that should be used to compare the results of groundwater flow model simulations to measured field data as a part of the process of calibrating a groundwater model. This comparison produces quantitative and qualitative measures of the degree of correspondence between the simulation and site-specific information related to the physical hydrogeologic system.

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This guide does not establish criteria for successful calibration, nor does it describe techniques for establishing such criteria, nor does it describe techniques for achieving successful calibration.

This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances.

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ASTM, **Standard Guide for Defining Boundary Conditions in Groundwater Flow Modeling**, D5609-16, West Conshohocken, PA, March 2016. <https://www.astm.org/Standards/D5609.htm>.

**[CCSM] [RIG][SFM]**

**Abstract/Scope:** Accurate definition of boundary conditions is an important part of conceptualizing and modeling groundwater flow systems. This guide describes the properties of the most common boundary conditions encountered in groundwater systems and discusses major aspects of their definition and application in groundwater models. It also discusses the significance and specification of boundary conditions for some field situations and some common errors in specifying boundary conditions in groundwater models. This guide covers the specification of appropriate boundary conditions that are to be considered part of conceptualizing and modeling groundwater systems. This guide describes techniques that can be used in defining boundary conditions and their appropriate application for modeling saturated groundwater flow model simulations.

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ASTM, **Standard Guide for Defining Initial Conditions in Groundwater Flow Modeling**, D5610-94 (Reapproved 2014), West Conshohocken, PA, January 2015. <https://www.astm.org/Standards/D5610.htm>.

**[CCSM] [RIG][SFM]**

**Abstract/Scope:** This guide covers techniques and procedures used to set initial conditions for modeling saturated groundwater flow. The assignment of initial conditions is a critical step for modeling transient groundwater flow. Any errors made in setting the initial conditions are propagated throughout the model and may prevent convergence to a solution.

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ASTM, **Standard Guide for Developing Conceptual Site Models for Contaminated Sites**, E1689-95 (Reapproved 2014), West Conshohocken, PA, May 2014. <https://www.astm.org/Standards/E1689.htm>.

**[CCSM] [RIG][CTM]**

**Abstract/Scope:** This guide is intended to assist in the development of conceptual site models to be used for the following:

1. Integration of technical information from various sources;
2. Support of the selection of sample locations for establishing background concentrations of substances;
3. Identification of data needs and guide data collection activities; and
4. Evaluation of the risk to human health and the environment posed by a contaminated site.

This guide generally describes the major components of conceptual site models, provides an outline for developing models, and presents an example of the parts of a model. This guide does not provide a detailed description of a site-specific conceptual site model because conditions at contaminated sites can vary greatly from one site to another.

Uncertainties associated with the conceptual site model need to be identified clearly so that efforts can be taken to reduce these uncertainties to acceptable levels. Early versions of the model, which are usually based on limited or incomplete information, will identify and emphasize the uncertainties that should be addressed.

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Barnett, B. and Townley, L.R., **Australian Groundwater Modelling Guidelines**, Waterlines Report, National Water Commission, Canberra, Australia, 2012. ISBN: 978-1-921853-91-3. <https://www.researchgate.net/publication/258245391> Australian Groundwater Modelling Guidelines.

**[GG][CVVM][UAM] [RIG][SFM][CTM]**

**Abstract/Scope:** The objective of the Australian groundwater modelling guidelines is to promote a consistent and sound approach to the development of groundwater flow and solute transport models in Australia. It builds on existing guidelines (Murray-Darling Basin Commission 2001) that have been adopted throughout Australia in recent years. While it is acknowledged that the term



groundwater modelling refers to a variety of methods, the guidelines focus on computer-based numerical simulation models. The guidelines should be seen as a point of reference and not as a rigid standard. They seek to provide direction on the scope and approaches common to modelling projects. The continual evolution of modelling techniques through adaptation and innovation is not only acknowledged but encouraged. It is recognized there are other approaches to modelling not covered in these guidelines and that such approaches may well be appropriate and justified in certain circumstances.

California Department of Water Resources, **Modeling BMP—Best Management Practices for the Sustainable Management of Groundwater**, Sacramento, CA, December 2016. [https://water.ca.gov/-/media/DWR-Website/Web-Pages/Programs/Groundwater-Management/Sustainable-Groundwater-Management/Best-Management-Practices-and-Guidance-Documents/Files/BMP-5-Modeling\\_ay\\_19.pdf](https://water.ca.gov/-/media/DWR-Website/Web-Pages/Programs/Groundwater-Management/Sustainable-Groundwater-Management/Best-Management-Practices-and-Guidance-Documents/Files/BMP-5-Modeling_ay_19.pdf).

[GG] [RIG]

**Abstract/Scope:** The objective of this Best Management Practice (BMP) is to assist with the use and development of groundwater and surface water models. The California Department of Water Resources has developed this document as part of the obligation in the Technical Assistance chapter (Chapter 7) of the Sustainable Groundwater Management Act to support the long-term sustainability of California’s groundwater basins. Information in this BMP provides technical assistance to Groundwater Sustainability Agencies and other stakeholders on how to address modeling requirements outlined in the Groundwater Sustainability Plan Emergency Regulations. This BMP identifies available resources to support the development of groundwater and surface water models.

Davis, J.A., **Surface Complexation Modeling of Uranium (VI) Adsorption on Natural Mineral Assemblages**, NUREG/CR-6708, U.S.NRC, Washington, D.C., March 2001. <https://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6708/>.

[GG] [RIG][CTM]

**Abstract/Scope:** The value of surface complexation modeling of radionuclide adsorption in supporting the selection of distribution coefficient ( $K_d$ ) values should be given wider recognition within the performance assessment modeling process. Studies of uranium(VI) adsorption by a weathered schist and specimen mineral phases that comprise the schist were conducted as a function of aqueous chemical conditions in laboratory experiments. The schist was collected from weathered, subsurface soil in the vicinity of the Koongarra uranium deposit (Northern Territory, Australia). The variable aqueous chemical conditions in the experiments caused significant variations in the speciation of dissolved uranium(VI) and the distribution coefficient,  $K_d$ , that describes the partitioning of uranium(VI) between the aqueous and solid phases.  $K_d$  values determined in the laboratory experiments compared favorably with *in-situ* partitioning constants derived from analyses of dissolved uranium(VI) in groundwater and in the subsurface soils. Mineral coatings were more important than bulk mineralogy in controlling uranium(VI) adsorption by the schist. Various surface complexation modeling approaches were developed to describe adsorption of uranium(VI) on the schist and its reference mineral phases. One of the modeling

approaches, the Generalized Composite approach, can reduce the uncertainty in  $K_d$  values chosen for performance assessment modeling. Surface complexation modeling offers a scientifically defensible means of linking the selection of  $K_d$  values for performance assessment modeling to existing knowledge of thermodynamic data for radionuclides and radionuclide speciation in aqueous systems.

Eisenberg, N.A., *et al.*, **Regulatory Perspectives on Model Validation in High-Level Radioactive Waste Management Programs: A Joint NRC/SKI White Paper**, NUREG-1636, U.S.NRC, Washington, D.C., March 1999. <http://www.nrc.gov/docs/ML0122/ML012260054.pdf>.

**[CVVM] [RIG][CTM]**

**Abstract/Scope:** Validation (or confidence building) should be an important aspect of the regulatory uses of mathematical models in the safety assessments of geologic repositories for the disposal of spent nuclear fuel and other high-level radioactive wastes (HLW). A substantial body of literature exists indicating the manner in which scientific validation of models is usually pursued. Because models for a geologic repository performance assessment cannot be tested over the spatial scales of interest and long time periods for which the models will make estimates of performance, the usual avenue for model validation—that is, comparison of model estimates with actual data at the space-time scales of interest—is precluded. Further complicating the model validation process in HLW programs are the uncertainties inherent in describing the geologic complexities of potential disposal sites, and their interactions with the engineered system, with a limited set of generally imprecise data, making it difficult to discriminate between model discrepancy and inadequacy of input data. A successful strategy for model validation, therefore, should attempt to recognize these difficulties, address their resolution, and document the resolution in a careful manner. The end result of validation efforts should be a documented enhancement of confidence in the model to an extent that the model's results can aid in regulatory decision-making. The level of validation needed should be determined by the intended uses of these models, rather than by the ideal of validation of a scientific theory. This White Paper presents a model validation strategy that can be implemented in a regulatory environment. It was prepared jointly by staff members of the U.S. Nuclear Regulatory Commission and the Swedish Nuclear Power Inspectorate. This document should not be viewed as, and is not intended to be, formal guidance or as a staff position on this matter. Rather, based on a review of the literature and previous experience in this area, this White Paper presents the views of members of the two organizations regarding how, and to what degree, validation might be accomplished in the models used to estimate the performance of HLW repositories.

Electric Power Research Institute, **Groundwater and Soil Remediation Guidelines for Nuclear Power Plants: Public Edition**, Technical Report 1023464, EPRI, Palo Alto, CA, July 2011. <https://www.epri.com/#/pages/product/1023464/?lang=en-US>.

**[CCSM][CSMRD] [RIG][SFM][CTM]**

**Abstract/Scope:** The Electric Power Research Institute (EPRI) Groundwater and Soil Remediation Guidelines provide the nuclear power industry with technical guidance for evaluating the need for and timing of remediation of soil and/or groundwater contamination from onsite leaks,

spills, or inadvertent releases to a) prevent migration of licensed material off-site; and b) minimize decommissioning impacts. EPRI case studies are published in separate documents; examples are listed below:

*US Energy Systems and Climate Analysis*—In 2007, EPRI released its first Prism and MERGE analyses. These analyses outlined technically and economically feasible scenarios for the electricity sector to reduce its greenhouse gas emissions over the next few decades. The Prism analysis provided a comprehensive assessment of potential CO<sub>2</sub> reductions in eight key technology areas of the electricity sector. The MERGE analysis identified cost-effective technology portfolios over time in response to a given CO<sub>2</sub> emissions constraint. Both analyses have been cited in numerous national and international publications and provided thought leadership for the electric power industry. <https://eea.epri.com/research.html>.

*EPRI's research and development portfolio*—EPRI sees clearly the pivotal changes and progress across the electricity sector. EPRI's research offerings are shaped by its comprehensive view of multiple studies at various locations, based on almost a half-century of research and development. Its R&D portfolio addresses the technology, systems, operations, and workforce as they are today and drives the innovations to shape them for the decades ahead. <https://www.epri.com/portfolio/programs>.

**EPA, *A Technical Guide to Ground-Water Model Selection at Sites Contaminated with Radioactive Substances***, EPA 402-R-94-012, EPA Offices of Radiation and Indoor Air and Solid Waste and Emergency Response, Washington, D.C., June 1994. <https://www.epa.gov/sites/production/files/2015-05/documents/402-r-94-012.pdf>.

**[GG] [RIG][SFM][CTM]**

**Abstract/Scope:** A joint program is underway between the EPA Offices of Radiation and Indoor Air and Solid Waste and Emergency Response, the DOE Office of Environmental Restoration and Waste Management, and the U.S.NRC Office of Nuclear Material Safety and Safeguards. The purpose of the program is to promote the appropriate and consistent use of mathematical models in the remediation and restoration process at sites containing, or contaminated with, radioactive materials. This report is one of a series of reports designed to accomplish this objective. Other reports completed under this program have identified the models in actual use at National Priorities List sites and facilities licensed under the Resource Conservation and Recovery Act, and at DOE sites and U.S.NRC sites undergoing decontamination and decommissioning, as well as the role of modeling and modeling needs in each phase of the remedial investigation. This report specifically addresses the selection of ground-water flow and contaminant transport models and is intended to be used by hydrogeologists and geoscientists responsible for identifying and selecting ground-water flow and contaminant transport models for use at sites containing radioactive materials.

**EPA, *Environmental Cleanup Best Management Practices: Effective Use of the Project Life Cycle Conceptual Site Model***, EPA 542-F-11-011, Office of Solid Waste and Emergency Response (5102G), Office of Superfund Remediation and Technology Innovation, Washington,

D.C., July 2011. <https://www.epa.gov/sites/production/files/2015-04/documents/csm-life-cycle-fact-sheet-final.pdf>.

[CCSM][CSMRD] [RIG][SFM]

**Abstract/Scope:** EPA supports the use of best management practices (BMPs) as a mechanism for maximizing technical effectiveness and resource efficiency in the execution of site assessment and cleanup projects. This fact sheet is the first in a series of documents that address conceptual site models (CSMs). This fact sheet summarizes how environmental practitioners can use CSMs to achieve, communicate, and maintain stakeholder consensus on site understanding, while satisfying the technical and quality objectives required for each stage of a cleanup project's life cycle. The focus is on defining stages and products of CSMs along with potential applications of CSMs at various stages of a project life cycle. Content herein is presented in a Superfund Program context; however, to the extent practical, text has been written to maximize applicability in other programs and regulatory frameworks. Other agencies and programs may find these concepts useful and environmental cleanup practitioners are encouraged to explore the utility and integration of a project life cycle CSM within their own program requirements and deliverable schedules. This document also includes case studies from **NASA Ames Research Center** and **Naval Air Station Moffett Field**.

EPA, **EPA On-line Tools for Site Assessment Calculation**, [https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/JnE\\_lite.html](https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/JnE_lite.html), for the following models, tools and databases relevant to remediation activities with links:

On-Line Calculator: Johnson Ettinger Vapor Intrusion Model.  
[https://cfpub.epa.gov/si/si\\_public\\_record\\_report.cfm?Lab=NERL&TIMSType=&count=10000&dirEntryId=152524&searchAll=&showCriteria=2&simpleSearch=0&startIndex=40001](https://cfpub.epa.gov/si/si_public_record_report.cfm?Lab=NERL&TIMSType=&count=10000&dirEntryId=152524&searchAll=&showCriteria=2&simpleSearch=0&startIndex=40001).

[NMMO] [RIG][MTMO][SFM][CTM]

**Abstract/Scope:** Migration of volatile chemicals from the subsurface into overlying buildings is called vapor intrusion (VI). Volatile organic chemicals in contaminated soils or groundwater can emit vapors, which may migrate through subsurface soils and may enter the indoor air of overlying buildings. Building depressurization may cause these vapors to enter the home through cracks in the foundation. Depressurization can be caused by a combination of wind effects and stack effects, which are the result of heating within the building and/or mechanical ventilation. In extreme cases, the vapors may accumulate in dwellings to levels that may pose near-term safety hazards, such as explosion. Typically, however, vapor concentrations are present at low levels, to which long-term exposure may pose increased risk for chronic health effects.

This on-line calculator implements the Johnson and Ettinger (J&E) (Johnson and Ettinger, 1991) simplified model to evaluate the vapor intrusion pathway into buildings. This J&E model replicates the implementation that the EPA's Office of Solid Waste and Emergency Response (OSWER) used in developing its draft vapor intrusion guidance, but includes a number of enhancements that are facilitated by web implementation: temperature dependence of Henry's Law Constants, automatic sensitivity analysis of certain parameters, and others described on the background page.

The results you obtain from this OnSite implementation of the J&E model may differ from other versions of the J&E model. In addition to the OSWER implementation that was used for the draft vapor intrusion guidance, EPA's Office of Emergency Response and Remediation (OERR) distributes a set of spreadsheet implementations of the model. The differences among these implementations is described in detail on the results page. Beyond these differences, the on-line version includes a simplified uncertainty analysis the other implementations lack.

EPA, *EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP), Technical Background Document*, EPA530-R-03-006, Office of Solid Waste, Washington, D.C., April 2003. <https://www.epa.gov/smm/epas-composite-model-leachate-migration-transformation-products-epacmtp>.

**[GG][NMMO][UAM] [LLMR][SFM][CTM]**

**Abstract/Scope:** EPACMTP is a fate and transport model developed by EPA to simulate the release constituents from waste managed in land disposal units, and the subsequent impacts of these constituents to the subsurface environment. The model combines two modules to simulate one-dimensional downward flow and transport of constituents in the unsaturated zone beneath a waste disposal unit, as well as ground water flow and three-dimensional constituent transport in the underlying saturated zone. The model is designed to run in a probabilistic or deterministic mode and comes with built-in distributions of national and regional modeling parameters. The output of the model includes predicted concentrations of constituents arriving at a downgradient well under steady-state conditions or as a function of time.

EPA, *Ground Water Issue: Fundamentals of Ground-Water Modeling*, EPA/540/S-92/005, Office of Research and Development, and Office of Solid Waste and Emergency Response, Washington, D.C., April 1992. [https://www.epa.gov/sites/production/files/2015-06/documents/fund\\_gw\\_modeling.pdf](https://www.epa.gov/sites/production/files/2015-06/documents/fund_gw_modeling.pdf).

**[GG][NMMO][CVVM][UAM] [RIG][SFM]**

**Abstract/Scope:** Ground-water flow and contaminant transport modeling has been used at many hazardous waste sites with varying degrees of success. Models may be used throughout all phases of the site investigation and remediation processes. The ability to reliably predict the rate and direction of groundwater flow and contaminant transport is critical in planning and implementing groundwater remediations. This paper presents an overview of the essential components of ground-water flow and contaminant transport modeling in saturated porous media. While fractured rocks and fractured porous rocks may behave like porous media with respect to many flow and contaminant transport phenomena, they require a separate discussion and are not included in this paper. Similarly, the special features of flow and contaminant transport in the unsaturated zone are also not included. This paper was prepared for an audience with some technical background and a basic working knowledge of ground-water flow and contaminant transport processes.

EPA, **Guidance on Systematic Planning Using the Data Quality Objectives Process**, EPA QA/G-4, EPA/240/B-06/001, Office of Environmental Information, Washington, D.C., February 2006. <https://www.epa.gov/sites/production/files/2015-06/documents/g4-final.pdf>.

**[CCSM][QAQC] [RIG]**

**Abstract/Scope:** Systematic Planning Using the Data Quality Objectives Process provides information on how to apply systematic planning to generate performance and acceptance criteria for collecting environmental data. The type of systematic planning described is known as the Data Quality Objectives (DQO) Process. This process fully meets all aspects of EPA Order 5360.1 A2, 2000, that establishes a Quality System for the Agency and organizations funded by EPA.

The DQO Process is a series of logical steps that guides managers or staff through a plan for the resource-effective acquisition of environmental data. It is both flexible and iterative, and applies to both decision-making (e.g., compliance/non-compliance with a standard) and estimation (e.g., ascertaining the mean concentration level of a contaminant). The DQO Process is used to establish performance and acceptance criteria, which serve as the basis for designing a plan for collecting data of sufficient quality and quantity to support the goals of the study. Use of the DQO Process leads to efficient and effective expenditure of resources; consensus on the type, quality, and quantity of data needed to meet the project goal; and the full documentation of actions taken during the development of the project.

This guidance document is intended for use by technical managers and Quality Assurance (QA) staff responsible for collecting data by: (1) providing basic guidance on applicable practices; (2) outlining systematic planning and developing performance or acceptance criteria; and (3) identifying resources and references that may be utilized by environmental professionals during the application of systematic planning.

The guidance discussed is non-mandatory and is intended to be a QA guide for project managers and QA staff in environmental programs to help them better understand when and how quality assurance practices should be applied to the collection of environmental data.

*Please note: The document addresses data quality objectives as they relate to planning data requirements to solve a specific problem. This document contains almost no reference to groundwater, but exhorts development of a strategic plan to identify: the problem, the project goal, input requirement, boundaries, parameters of interest, and acceptable performance for the purpose of developing the plan for procuring the applicable data to complete the project.*

EPA, **Guidance on the Development, Evaluation, and Application of Environmental Models**, EPA/100/K-09/003, Council for Regulatory Environmental Modeling, Washington, D.C. 20460, March 2009.

[https://www.epa.gov/sites/production/files/2015-04/documents/cred\\_guidance\\_0309.pdf](https://www.epa.gov/sites/production/files/2015-04/documents/cred_guidance_0309.pdf).

**[GG][CCSM][QAQC][CVVM][UAM] [RIG]**

**Abstract/Scope:** This guidance developed in 2009 provides recommendations for the effective development, evaluation, and use of models in environmental decision making once an environmental issue has been identified. These recommendations are drawn from Agency white papers, EPA Science Advisory Board reports, the National Research Council's Models in

Environmental Regulatory Decision Making, and peer-reviewed literature. This guidance recommends best practices to help determine when a model, despite its uncertainties, can be appropriately used to inform a decision. Specifically, it recommends that model developers and users: (a) subject their model to credible, objective peer review; (b) assess the quality of the data they use; (c) corroborate their model by evaluating the degree to which it corresponds to the system being modeled; and (d) perform sensitivity and uncertainty analyses. Sensitivity analysis evaluates the effect of changes in input values or assumptions on a model's results. Uncertainty analysis investigates the effects of lack of knowledge and other potential sources of error in the model (e.g., the “uncertainty” associated with model parameter values). When conducted in combination, sensitivity and uncertainty analysis allow model users to be more informed about the confidence that can be placed in model results. A model's quality to support a decision becomes better known when information is available to assess these factors.

EPA, **Implementation Guidance for Radionuclides (with Appendices A-J)**, Office of Ground Water and Drinking Water (4606M), EPA 816-F-00-002, Washington, D.C., March 2002. [https://www.epa.gov/sites/production/files/2015-09/documents/2009\\_04\\_16\\_radionuclides\\_guide\\_radionuclides\\_stateimplementation.pdf](https://www.epa.gov/sites/production/files/2015-09/documents/2009_04_16_radionuclides_guide_radionuclides_stateimplementation.pdf). [https://www.epa.gov/sites/production/files/2015-09/documents/2009\\_04\\_16\\_radionuclides\\_guide\\_radionuclides\\_stateimplementation\\_appendie s.pdf](https://www.epa.gov/sites/production/files/2015-09/documents/2009_04_16_radionuclides_guide_radionuclides_stateimplementation_appendie s.pdf).

**[GG] [RIG][CTM]**

**Abstract/Scope:** The purpose of this guidance manual is to provide assistance to EPA, the States, and community water systems during the implementation of The Radionuclides Rule published in the *Federal Register* on December 7, 2000 (65 Fed. Reg. 76708). EPA and State decision-makers retain the discretion to adopt approaches on a case-by-case basis that differ from this guidance where appropriate. Any decisions regarding a particular facility will be based on the applicable statutes and regulations. Therefore, interested parties are free to raise questions and objections about the appropriateness of the application of this guidance to a particular situation, and EPA will consider whether the recommendations or interpretations in the guidance are appropriate in that situation. EPA may change this guidance in the future.

EPA, **Models, Tools, and Databases for Land and Waste Management Research**, <https://www.epa.gov/land-research/models-tools-and-databases-land-and-waste-management-research>, for the following models, tools and databases relevant to remediation activities with links:

BIOCHLOR, BIOSCREEN, BIOPLUME, REMChlor, REMFuel, Natural Attenuation Decision Support System, Version 1.4, July 1997. <https://nepis.epa.gov/Adobe/PDF/P1007K50.pdf>.

**[NMMO] [RIG][SFM][CTM]**

**Abstract/Scope:**

BIOCHLOR Version 2.2 models a decaying chlorinated solvent source, which allows the simulation of both plume expansion and contraction. Lastly, an animation feature has

been incorporated, which permits the visualization of plume behavior. <https://www.epa.gov/water-research/biochlor-natural-attenuation-decision-support-system>.

BIOPLUME III is based on the USGS solute transport code MOC and solves the solute transport equation six times to determine the fate and transport of the hydrocarbons and the electron acceptors ( $O_2$ ,  $NO_3^-$ ,  $Fe_3^+$ ,  $SO_4^{2-}$ , and  $CO_2$ ) and the reaction by-products ( $Fe_2^+$ ). A number of aerobic and anaerobic electron acceptors, such as oxygen, nitrate, sulfate, iron(III) and carbon dioxide, have been considered in this model to simulate the biodegradation of organic contaminants. Three different kinetic expressions can be used to simulate the aerobic and anaerobic biodegradation reactions. The model has been integrated with a sophisticated groundwater modeling platform known as EIS. The input parameters of the model are discretization of time and space, hydrogeologic characteristics of the aquifer, initial and boundary conditions, sources and sinks, sorption, source decay, radioactive decay, ion-exchange and biodegradation variables. <https://www.epa.gov/water-research/bioplume-iii>.

BIOPLUME IV has been rewritten to allow an evaluation of sustainability in those cases where the limiting substrate is an integral component of the aquifer matrix. Chlorinated solvents such as perchloroethylene or trichloroethylene can be destroyed by abiotic reactions with magnetite in the aquifer matrix. Fuel-derived contaminants such as benzene, methyl tert-butyl ether, and tert-butyl alcohol can be degraded by iron-reducing bacteria that consume iron (III) minerals in the aquifer matrix in the process of degrading the contaminant and associated organic materials. When the limiting substrate is consumed in one portion of the aquifer, the contaminant can be expected to move with the flow of ground water until it enters a portion of the aquifer where the limiting substrate is still available. Over time, the region of the aquifer where the limiting substrate has been totally consumed will expand, and the footprint of the contaminant in the plume will expand with it. Sustainability can be evaluated by comparing the total loading of contaminant (and associated materials that will also consume the limiting substrate) to the supply of the limiting substrate that is available to be consumed before a plume reaches a receptor.

[https://cfpub.epa.gov/si/si\\_public\\_record\\_report.cfm?Lab=NRMRL&dirEntryId=155947](https://cfpub.epa.gov/si/si_public_record_report.cfm?Lab=NRMRL&dirEntryId=155947).

BIOSCREEN is an easy-to-use screening model which simulates remediation through natural attenuation (RNA) of dissolved hydrocarbons at petroleum fuel release sites. The software, programmed in the Microsoft® Excel spreadsheet environment and based on the Domenico analytical solute transport model, has the ability to simulate advection, dispersion, adsorption, and aerobic decay as well as anaerobic reactions that have been shown to be the dominant biodegradation processes at many petroleum release sites. The model is designed to simulate biodegradation by both aerobic and anaerobic reactions. It was developed for the Air Force Center for Environmental Excellence Technology Transfer Division at Brooks Air Force Base by Groundwater Services, Inc., Houston, Texas. <https://www.epa.gov/water-research/bioscreen-natural-attenuation-decision-support-system>.

Remediation Evaluation Model for Chlorinated Solvents (REMChlor) is an analytical model that simulates the transient remediation effects of groundwater from chlorinated solvent contamination source to the toe of the contaminated plume. In the analytical method, the contaminant source model is based on a power-function relationship between source mass and source discharge, and it can consider partial source remediation at any time after the initial release. The source model serves as a time-dependent, mass-flux boundary condition to the analytical plume model, where flow is assumed to be one dimensional. <https://www.epa.gov/water-research/remediation-evaluation-model-chlorinated-solvents-remchlor>.



Remediation Evaluation Model for Fuel hydrocarbons (REMFuel) is an analytical model that simulates the transient remediation effects of groundwater from contamination source to the toe of the contaminated plume. The analytical approach is the same as that of REMChlor, but the target contaminants are fuel components. REMFuel can also simulate zero order or Monod's kinetics for decay of fuel components in the plume. The decay rates and other reaction coefficients are variable functions of time and distance in the plume. This approach allows for flexible simulation of enhanced plume remediation that may be temporary in time, limited in space, and which may have different effects on different contaminant species in the plume. <https://www.epa.gov/water-research/remediation-evaluation-model-fuel-hydrocarbons-remfuel>.

EPA, **Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites**, OSWER 9355.4-24, Office of Solid Waste and Emergency Response, Washington, D.C., December 2002. <https://semspub.epa.gov/work/HQ/175878.pdf>.

[GG] [RIG]

**Abstract/Scope:** This document is intended as companion guidance to the 1996 Soil Screening Guidance (SSG) for residential use scenarios at National Priorities List sites. It builds upon the soil screening framework established in the original guidance, adding new scenarios for soil screening evaluations. It also updates the residential scenario in the 1996 SSG, adding exposure pathways and incorporating new modeling data. The following specific changes included in this document supersede the 1996 SSG: This document presents new methods for developing SSLs based on non-residential land use and construction activities; new residential Soil Screening Level (SSL) equations for combined exposures via ingestion and dermal absorption; updated dispersion modeling data for the soil screening guidance air exposure model; and presents new methods to develop residential and non-residential SSLs for the migration of volatiles from subsurface sources into indoor air.

Falta, R.W., Farhat, S.K., Newell, C.J., and Lynch, K., **A Practical Approach for Modeling Matrix Diffusion Effects in REMChlor**, Clemson University, ER-201426. <https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-201426>.

[NMMO] [RIG][MTMO][SFM][CTM]

**Abstract/Scope:** The objective of this project is to develop practical and efficient mathematical methods for simulating the effects of matrix diffusion in groundwater transport and remediation models. These methods will apply to various types of heterogeneous settings, including fractured porous media and sites with extensive low permeability layers and lenses. The new mathematical methods will then be implemented in EPA groundwater remediation screening model REMChlor to develop a new generation model that considers matrix diffusion in the plume: REMChlor-MD.

The problem of matrix diffusion of chlorinated volatile organic compounds (CVOCs) in groundwater plumes is mathematically analogous to heat conduction in fractured rocks and heterogeneous reservoirs. Elegant numerical and semi-analytical methods for modeling the heat conduction processes that occur during fluid injection or extraction were developed in the 1980s by geothermal reservoir engineers. With some modifications, these methods are directly

applicable to the problem of CVOC matrix diffusion. They offer accurate solutions that do not require explicit discretization of the low permeability zones. Instead, the low permeability zones that occur at scales smaller than a normal numerical gridblock are represented with sub-gridblock scale analytical or numerical approximations. In most cases of interest, these approximations are expected to offer a level of simulation accuracy comparable to the fine-grid numerical simulations, but at a tiny fraction of the computational and user effort.

Finsterle, S., ***Multiphase Inverse Modeling: Review and iTOUGH2 Applications***, Vadose Zone Journal 3:747-762, 2004.

<https://www.osti.gov/biblio/842556-multiphase-inverse-modeling-review-itough2-applications>.

**[NMMO][QAQC][UAM]**

**Abstract/Scope:** Calibration of a numerical process model against laboratory or field data is often referred to as “inverse modeling.” As the numerical simulation models become more complex, the number of parameters to be estimated generally increases, requiring new testing, modeling, and inversion strategies. The purpose of this survey is to review inverse modeling approaches for unsaturated and multiphase flow models. The discussion focuses on applications rather than theoretical considerations, which have been previously reviewed in the context of saturated flow and transport modeling. We also examine model parameterization issues, specifically the representation of heterogeneity through a limited number of variables that can be subjected to parameter estimation and uncertainty propagation analyses. Different parameterization strategies are illustrated using the multiphase flow simulation-optimization code iTOUGH2. A comprehensive inverse modeling package (such as iTOUGH2, which includes automatic model calibration followed by an extensive residual, error, and uncertainty propagation analysis) is an essential tool to improve test design and data analysis of complex multiphase flow systems.

Finsterle, S., Sonnenthal, E.L., and Spycher, N., ***Advances in Subsurface Modeling Using the TOUGH Suite of Simulators***. Computers & Geosciences, 65, 2-12, 2014.

<https://pubag.nal.usda.gov/catalog/5996023>.

**[CCSM][NMMO] [MTMO][SFM][CTM]**

**Abstract/Scope:** The TOUGH suite of non-isothermal multiphase flow and transport simulators is continually updated to improve the analysis of complex subsurface processes through numerical modeling. Driven by research questions in the Earth sciences and by application needs in industry and government organizations, the codes are extended to include the coupling of relevant processes and subsystems, to improve computational performance, to support model development and analysis tasks, and to provide more convenient pre- and post-processing capabilities. This review paper briefly describes the history of the simulator, discusses recent advances, and comments on potential future developments and applications.

Georgia Department of Natural Resources, Environmental Protection Division, Land Protection Branch, **Guidance: Groundwater Contaminant Fate and Transport Modeling**, Revision 1, Atlanta, GA, October 2016.

[https://epd.georgia.gov/sites/epd.georgia.gov/files/LPB\\_Fate\\_and\\_Transport\\_Guidance.pdf](https://epd.georgia.gov/sites/epd.georgia.gov/files/LPB_Fate_and_Transport_Guidance.pdf).

[GG][QAQC][CVVM] [RIG][SFM][CTM]

**Abstract/Scope:** The purpose of this guidance is to provide general guidelines for the application of groundwater contaminant fate and transport models, including the planning and evaluation of models for use at sites with groundwater contamination that are subject to regulation by the Georgia Department of Natural Resources Environmental Protection Division (EPD).

This document describes the process of preparing a fate and transport model for consideration. Each section provides a brief discussion of each step and the rationale for its use. Additional steps may be necessary to meet modeling objectives. For example, a site investigation may provide additional data that can be used in the modeling process. The development of a Modeling Work Plan may assist EPD in determining if the proposed modeling is appropriate.

This guidance outlines recommended practices and explains their rationale. However, EPD may not require an entity to follow methods recommended by this or any other guidance document. The entity may, however, need to demonstrate that an alternate method produces data and information that meet the pertinent requirements. This guidance is not a substitute for professional judgment, which must be applied in the selection and application of fate and transport modeling, nor does it advocate modeling over the collection and interpretation of quality media-specific site data.

Hammond, G.E., Lichtner, P.C., Lu, C., and Mills, R.T., **PFLOTRAN: Reactive Flow and Transport Code for Use on Laptops to Leadership-Class Supercomputers**. Groundwater Reactive Transport Models, 141-159, 2012.

[https://www.researchgate.net/publication/255001950\\_PFLOTRAN\\_Reactive\\_Flow\\_and\\_Transport\\_Code\\_for\\_Use\\_on\\_Laptops\\_to\\_Leadership-Class\\_Supercomputers](https://www.researchgate.net/publication/255001950_PFLOTRAN_Reactive_Flow_and_Transport_Code_for_Use_on_Laptops_to_Leadership-Class_Supercomputers).

[CCSM][NMMO] [CTM]

**Abstract/Scope:** PFLOTRAN, a next-generation reactive flow and transport code for modeling subsurface processes, has been designed from the ground up to run efficiently on machines ranging from leadership-class supercomputers to laptops. Based on an object-oriented design, the code is easily extensible to incorporate additional processes. It can interface seamlessly with Fortran 9X, C, and C++ codes. Domain decomposition parallelism is employed, with the Portable, Extensible Toolkit for Scientific Computation (PETSc) parallel framework used to manage parallel solvers, data structures, and communication. Features of the code include a modular input file, implementation of high-performance I/O using parallel Hierarchical Data Format version 5, ability to perform multiple realization simulations with multiple processors per realization in a seamless manner, and multiple modes for multiphase flow and multicomponent geochemical transport. Chemical reactions currently implemented in the code include homogeneous aqueous complexing reactions and heterogeneous mineral precipitation/dissolution, ion exchange, surface complexation and a multi-rate kinetic sorption model. PFLOTRAN has demonstrated petascale performance using 217 processor cores on problems composed of over 2 billion degrees of

freedom. The code is currently being applied to simulate uranium transport at the Hanford-300 Area and CO<sub>2</sub> sequestration in deep geologic formations.

Hill, M.C., *The Practical Use of Simplicity in Developing Ground Water Models*, *Groundwater* 44.6: 775-781, 2006.

<https://ngwa.onlinelibrary.wiley.com/doi/10.1111/j.1745-6584.2006.00227.x>.

[GG][CVVM] [SFM][CTM]

**Abstract/Scope:** The advantages of starting with simple models and building complexity slowly can be significant in the development of ground water models. In many circumstances, simpler models are characterized by fewer defined parameters and shorter execution times. In this work, the number of parameters is used as the primary measure of simplicity and complexity; the advantages of shorter execution times also are considered. The ideas are presented in the context of constructing ground water models but are applicable to many fields. Simplicity first is put in perspective as part of the entire modeling process using 14 guidelines for effective model calibration. It is noted that neither very simple nor very complex models generally produce the most accurate predictions and that determining the appropriate level of complexity is an ill-defined process. It is suggested that a thorough evaluation of observation errors is essential to model development. Finally, specific ways are discussed to design useful ground water models that have fewer parameters and shorter execution times.

Lebrón, C.A., Wiedemeier, T.H., Wilson, J.T., Löffler, F.E., Hincbee, R.E., and Singletary, M.A., *Development and Validation of a Quantitative Framework and Management Expectation Tool for the Selection of Bioremediation Approaches at Chlorinated Solvent Sites*, Naval Facilities Engineering Command, Expeditionary Warfare Center, Port Hueneme, CA, ER-201129. <https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Persistent-Contamination/ER-201129/ER-201129>.

[NMMO] [RIG][MTMO][SFM][CTM]

**Abstract/Scope:** The quantitative framework developed is a systematic approach that uses the relationships between specific biogeochemical parameters and degradation rates to deduce major degradation pathways and determine the best bioremediation approach at sites impacted with chlorinated ethenes. The major element of this demonstration was to quantify the relationship(s) between selected, measurable biogeochemical screening parameters and both biotic and abiotic degradation rates. Evaluating these relationships enabled the development of the quantitative framework. In turn, the quantitative framework enabled the development of BioPIC, a software tool that guides users (e.g., remedial project managers [RPMs]) through a hierarchical set of questions to ultimately identify the optimal pathway for remediating chlorinated ethenes at a particular site. BioPIC is an easy-to-use decision tool that informs RPMs about relevant biogeochemical parameters and their impacts on degradation pathways and rates at a given site.

A number of measurable parameters, such as the concentrations of volatile organic compounds (VOCs); alternate electron acceptors (e.g., oxygen, sulfate); reduced products (e.g., ferrous iron {Fe[II]}, methane [CH<sub>4</sub>]); Dehalococoides(Dhc) 16S rRNA gene and reductive dehalogenase

(RDase) gene abundances; and magnetic susceptibility, affect the detoxification of chlorinated ethenes. The relationships between each parameter and the degradation rates were determined and used to develop the decision matrix and BioPIC.

*Document disclaimer: The decision framework and the management expectation tool (BioPIC) are based on the current scientific understanding of the processes contributing to the detoxification of chlorinated ethenes. Although process understanding has significantly improved over the past decade, knowledge gaps remain.*

*Please note: This tool does not address chlorinated ethanes or methanes.*

Meyer, P.D., and Gee, G.W., **Information on Hydrologic Conceptual Models, Parameters, Uncertainty Analysis, and Data Sources for Dose Assessments at Decommissioning Sites**, NUREG/CR-6656, PNNL-13091, U.S.NRC, Washington, D.C., December 1999. <https://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6656/>.

**[CCSM][UAM] [RIG][SFM][CTM]**

**Abstract/Scope:** This report addresses issues related to the analysis of uncertainty in dose assessments conducted as part of decommissioning analyses. The analysis is limited to the hydrologic aspects of the exposure pathway involving infiltration of water at the ground surface, leaching of contaminants, and transport of contaminants through the groundwater to a point of exposure. The basic conceptual models and mathematical implementations of three dose assessment codes are outlined along with the site-specific conditions under which the codes may provide inaccurate, potentially nonconservative results. In addition, the hydrologic parameters of the codes are identified and compared. A methodology for parameter uncertainty assessment is outlined that considers the potential data limitations and modeling needs of decommissioning analyses. This methodology uses generic parameter distributions based on national or regional databases, sensitivity analysis, probabilistic modeling, and Bayesian updating to incorporate site-specific information. Data sources for best-estimate parameter values and parameter uncertainty information are also reviewed. A follow-on report will illustrate the uncertainty assessment methodology using decommissioning test cases.

Meyer, P.D. and S. Orr, **Evaluation of Hydrologic Uncertainty Assessments for Decommissioning Sites Using Complex and Simplified Models**, NUREG/CR-6767, PNNL-13832, U.S.NRC, Washington, D.C., April 2002. <https://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6767/>.

**[CCSM][UAM] [RIG][SFM][CTM]**

**Abstract/Scope:** This report addresses issues related to hydrologic uncertainty assessment at decommissioning sites. Simplified models are particularly attractive when the impact of uncertainty in flow and transport needs to be evaluated. These same simplifications, however, have the potential to provide unrepresentative estimates of dose and its uncertainty. Such misrepresentation may have important consequences for decisions based on the dose assessments. The significance of this concern was evaluated by comparing results from

uncertainty assessments conducted on a test case using a simplified modeling approach and a more complex/realistic modeling approach.

Meyer, P.D., Ye, M. (DRI), Rockhold, M.L., Neuman (UA), S.P., and Cantrell, K.J., **Combined Estimation of Hydrogeologic Conceptual Model, Parameter, and Scenario Uncertainty with Application to Uranium Transport at the Hanford Site 300 Area**, NUREG/CR-6940, U.S.NRC, Washington, D.C., July 2007.

<https://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6940/>.

**[CCSM][UAM][CSMRD] [RIG][SFM][CTM]**

**Abstract/Scope:** This document describes the development and application of a methodology to systematically and quantitatively assess predictive uncertainty in groundwater flow and transport modeling. The methodology considers the combined impact of hydrogeologic uncertainties associated with the conceptual-mathematical basis of a model, model parameters, and the scenario to which the model is applied. The methodology is based on an extension of a Maximum Likelihood implementation of Bayesian Model Averaging. Model uncertainty is represented by postulating a discrete set of alternative conceptual models for a site with associated prior model probabilities. The prior model probabilities reflect a subjective belief about the relative plausibility of each model based on its apparent consistency with available knowledge and data. Posterior model probabilities are computed, and parameter uncertainty is estimated by calibrating each model to observed system behavior. Posterior model probabilities are modifications of the subjective prior values based on an objective evaluation of each model's consistency with available data. Prior parameter estimates are optionally included. Scenario uncertainty is represented as a discrete set of alternative future conditions affecting boundary conditions, source/sink terms, or other aspects of the models. The associated prior scenario probabilities reflect a subjective belief about the relative plausibility of the alternative scenarios. A joint assessment of uncertainty results from combining model predictions computed under each scenario using as weights the posterior model and prior scenario probabilities. The computed model predictions incorporate parameter uncertainties using, for example, Monte Carlo simulation. The uncertainty methodology was applied to modeling of groundwater flow and uranium transport at the Hanford Site 300 Area. Eight alternative models representing uncertainty in the hydrogeologic and geochemical properties as well as the temporal variability were considered. Two scenarios representing alternative future behavior of the Columbia River adjacent to the site were considered. The scenario alternatives were implemented in the models through the boundary conditions. Alternative models were calibrated using hydraulic head and uranium concentration observations over a seven-year period. Uranium concentrations under each scenario were predicted over a 20-year period. Results demonstrate the feasibility of applying a comprehensive uncertainty assessment to large-scale, detailed groundwater flow and transport modeling. Results also illustrate the ability of the methodology to provide better estimates of predictive uncertainty, quantitative results for use in assessing risk, and an improved understanding of the system behavior and the limitations of the models.

This document contains a case study from **Hanford Site 300 Area**. U.S.NRC published multiple case study documents covering a broad spectrum of situations and topics. <https://www.nrc.gov/site->

[help/search.html?q=case+studies&site=allSites#qsc.tab=0&qsc.q=case%20studies&qsc.page=1](http://help/search.html?q=case+studies&site=allSites#qsc.tab=0&qsc.q=case%20studies&qsc.page=1).

National Academies of Sciences, ***Natural Attenuation for Groundwater Remediation***, National Academy Press, Washington, D.C., 2000. ISBN: 0-309-06932-7. <https://www.nap.edu/read/9792/chapter/1>.

[CSMRD] [LLMR][SFM][CTM]

**Abstract/Scope:** The National Research Council formed the committee that prepared this report—the Committee on Intrinsic Remediation—in 1997 in order to establish a proper basis for selecting remedies that rely on natural attenuation processes. The committee was charged with the following tasks: assess current knowledge about the natural subsurface processes that play critical roles in intrinsic remediation; outline what intrinsic remediation can and cannot achieve; assess risks associated with leaving contaminants in place; identify the measurements, observations, and monitoring needed when intrinsic remediation is chosen instead of engineered remediation; and evaluate the adequacy of existing protocols for determining whether intrinsic remediation is an appropriate strategy for contaminant management.

This report summarizes the findings of the committee, which was made up of 14 experts in the technical and decision-making aspects of natural attenuation. Committee members brought to the table state-of-the-art expertise in environmental microbiology, geochemistry, environmental engineering, hydrogeology, soil science, and risk assessment. Academia, industry, government, and community-based institutions were represented. The committee also interviewed a wide range of community activists, researchers, regulators, practitioners, and protocol developers.

The findings presented in this report represent the unanimous consensus of the committee. Despite coming from disparate backgrounds and interest groups, all of the committee members agreed with the message that this report delivers. Clearly, the concept that natural attenuation processes can, under the proper conditions, cause the destruction or transformation of contaminants in the environment is valid. However, natural attenuation should never be a default choice. The cause-and-effect link between a decrease in contaminant concentration and the process or processes causing it must be documented before natural attenuation is accepted as a remedy. These processes must continue to occur for as long as is necessary to protect human health and the environment. Furthermore, affected communities need to be part of the decision to accept natural attenuation.

This document also includes case studies from ***U.S. Coast Guard Air Station at Traverse City, Michigan; St. Joseph, Michigan, Superfund site; Vandenberg Air Force Base in California; Edwards Air Force Base, California; Dover Air Force Base, Delaware; Hanford 216-B-5*** and various other sites.

National Ground Water Association, ***A Decision Framework for Minimum Levels of Model Complexity; A Stepwise Approach to Groundwater Modeling; Uncertainty in Groundwater Modeling; Application of Groundwater Modeling for Decision-Making in Water Management and Engineering with Water Supply and Remediation Case Studies;***

**Integrated Surface Water—Groundwater Modeling;** NGWA White Paper, NGWA Press, Westerville, OH, October 4, 2017. [https://my.ngwa.org/NC\\_Product?id=a183800000uwvpaAAA](https://my.ngwa.org/NC_Product?id=a183800000uwvpaAAA).

[GG][CCSM][UAM] [RIG][SFM][CTM]

**Abstract/Scope:** This white paper is a compilation of five papers drafted by the National Ground Water Association (NGWA) Groundwater Modeling Advisory Panel over the span of a year. The panel addressed the following topics relating to groundwater modeling in their papers:

- How should decision-makers consider groundwater modeling in project development and solution?
- How should the complexity of the subsurface be considered in developing groundwater models?
- What considerations should be made in moving from simple to more complex model development?
- How can uncertainty be included in modeling to inform decisions for groundwater supply and remediation?
- What approaches can be followed to address interaction of groundwater/surface water decisions?

Each paper covers a specific topic of current interest in groundwater modeling in-depth and as a set of five papers provides a broad perspective on the practice of groundwater modeling today.

Ohio EPA, Division of Drinking and Ground Waters, **Technical Manual for Ground Water Investigations, Chapter 14, Ground Water Flow and Fate and Transport Modeling**, Rev. 1, Columbus, OH, November 2007. <https://www.epa.state.oh.us/portals/28/documents/TGM-14.pdf>.

[GG] [RIG][SFM][CTM]

**Abstract/Scope:** This document is part of a series of chapters incorporated in Ohio EPA's Technical Guidance Manual for Hydrogeologic Investigations and Ground Water Monitoring (TGM), which was originally published in 1995. Ohio's Division of Drinking and Ground Waters (DDAGW) now maintains this technical guidance as a series of chapters rather than as an individual manual. The TGM identifies technical considerations for performing hydrogeologic investigations and ground water monitoring at potential or known ground water pollution sources. The purpose of the guidance is to enhance consistency within the Agency and inform the regulated community of the Agency's technical recommendations and the basis for them. In Ohio, the authority over pollution sources is shared among various Ohio EPA divisions, including the Emergency and Remedial Response (DERR), Hazardous Waste Management (DHWM), Solid and Infectious Waste (DSIWM), and Surface Water (DSW), as well as other state and local agencies. DDAGW provides technical support to these divisions. Ohio EPA utilizes guidance to aid regulators and the regulated community in meeting laws, rules, regulations, and policy. Guidance outlines recommended practices and explains their rationale. The Agency may not require an entity to follow methods recommended by this or any other guidance document. It may, however, require an entity to demonstrate that an alternate method produces data and information that meet the pertinent requirements. The procedures used usually should be tailored to the specific needs and circumstances of the individual site, project, and applicable regulatory program, and should not comprise a rigid step-by-step approach that is utilized in all situations.



Refsgaard, J.C., van der Sluijs, J.P., Højberg, A.L., and Vanrolleghem, P.A., ***Uncertainty in the Environmental Modelling Process – A Framework and Guidance***. 2007. <https://dspace.library.uu.nl/bitstream/handle/1874/27087/NWS-E-2007-102.pdf?sequence=1>.

**[UAM] [RIG]**

**Abstract/Scope:** A terminology and typology of uncertainty is presented together with a framework for the modelling process, its interaction with the broader water management process and the role of uncertainty at different stages in the modelling processes. Brief reviews have been made of 14 different (partly complementary) methods commonly used in uncertainty assessment and characterization: data uncertainty engine, error propagation equations, expert elicitation, extended peer review, inverse modelling (parameter estimation), inverse modelling (predictive uncertainty), Monte Carlo analysis, multiple model simulation, NUSAP, quality assurance, scenario analysis, sensitivity analysis, stakeholder involvement and uncertainty matrix. The applicability of these methods has been mapped according to purpose of application, stage of the modelling process and source and type of uncertainty addressed. It is concluded that uncertainty assessment is not just something to be added after the completion of the modelling work. Instead uncertainty should be seen as a red thread throughout the modelling study starting from the very beginning, where the identification and characterization of all uncertainty sources should be performed jointly by the modeler, the water manager, and the stakeholders.

Reilly, T.E. and Harbaugh, A.W., ***Guidelines for Evaluating Ground-Water Flow Models***, Office of Ground Water Technical Memorandum No. 96.04, USGS, Reston, VA, April 24, 1996. [https://pubs.usgs.gov/sir/2004/5038/PDF/SIR20045038\\_ver1.01.pdf](https://pubs.usgs.gov/sir/2004/5038/PDF/SIR20045038_ver1.01.pdf).

**[NMMO] [RIG][SFM]**

**Abstract/Scope:** Ground-water flow modeling is an important tool frequently used in studies of ground-water systems. Reviewers and users of these studies have a need to evaluate the accuracy or reasonableness of the ground-water flow model. This report provides some guidelines and discussion on how to evaluate complex ground-water flow models used in the investigation of ground-water systems. A consistent thread throughout these guidelines is that the objectives of the study must be specified to allow the adequacy of the model to be evaluated.

Steeffel, C.I., Yabusaki, S.B., and Mayer, K.U., ***Reactive Transport Benchmarks for Subsurface Environmental Simulation***, Computational Geosciences, 19(3), 439, 2015. <https://link.springer.com/content/pdf/10.1007/s10596-015-9499-2.pdf>.

**[CCSM][NMMO] [SFM][CTM]**

**Abstract/Scope:** The primary audience for this special issue is the model developers who will benefit from the availability of a set of rigorous benchmarks for complex subsurface environmental problems. Anybody who has been involved in code development, whether specifically for reactive transport modeling (RTM) or for some other application(s) in the earth and environmental sciences, will appreciate the value of a reliable set of benchmarks to test their own code against. This can dramatically shorten the development time for complex environmental software. The

focus in this special issue has been on establishing the accuracy of complex simulations rather than on computational performance. This second objective could be pursued relatively easily by taking the codes summarized in this issue, or other codes as feasible, and comparing their performance on the benchmark problems using the same space and time discretization.

USGS, **MODFLOW 6 and Related Programs**: <https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model>. Documentation: Hughes, J.D., Langevin, C.D., and Banta, E.R., **Documentation for the MODFLOW 6 Framework, Techniques and Methods 6-A57**. <https://pubs.usgs.gov/tm/06/a57/tm6a57.pdf>.

**[NMMO] [RIG][SFM]**

**Abstract/Scope:** MODFLOW is a popular open-source groundwater flow model distributed by USGS. Growing interest in surface and groundwater interactions, local refinement with nested and unstructured grids, karst groundwater flow, solute transport, and saltwater intrusion, has led to the development of numerous MODFLOW versions. Often times, there are incompatibilities between these different MODFLOW versions. The report describes a new MODFLOW framework called MODFLOW 6 that is designed to support multiple models and multiple types of models. The framework is written in Fortran using a modular object-oriented design. The primary framework components include the simulation (or main program), Timing Module, Solutions, Models, Exchanges, and Utilities. The first version of the framework focuses on numerical solutions, numerical models, and numerical exchanges. This focus on numerical models allows multiple numerical models to be tightly coupled at the matrix level.

USGS, **MODPATH: A Particle-Tracking Model for MODFLOW/MODPATH**, Version 7.2.001, December 15, 2017. <https://www.usgs.gov/software/modpath-a-particle-tracking-model-modflow>. Documentation: Pollock, D.W., **User Guide for MODPATH Version 7 -- A Particle-Tracking Model for MODFLOW**, USGS Open-File Report 2016-1086, 35 p., 2016. <https://pubs.usgs.gov/of/2016/1086/ofr20161086.pdf>.

**[NMMO] [RIG][SFM][CTM]**

**Abstract/Scope:** MODPATH is a particle-tracking post-processing program designed to work with MODFLOW, the USGS finite-difference groundwater flow model. MODPATH version 7 is the fourth major release since its original publication. Previous versions were documented in USGS Open-File Reports 89-381 and 94-464 and in USGS Techniques and Methods 6-A41. MODPATH version 7 works with MODFLOW-2005 and MODFLOW-USG. Support for unstructured grids in MODFLOW-USG is limited to smoothed, rectangular-based quadtree and quadpatch grids.

USGS, **MT3D-USGS: Groundwater Solute Transport Simulator for MODFLOW**, Version 1.1.0, June 28, 2019. <https://www.usgs.gov/software/mt3d-usgs-groundwater-solute-transport-simulator-modflow>. Documentation: Bedekar, V., Morway, E.D., Langevin, C.D., and Tonkin, M., **MT3D-USGS version 1: A U.S. Geological Survey Release of MT3DMS Updated with New and Expanded Transport Capabilities for Use with MODFLOW: Techniques and Methods 6-A53**, 69 p., 2016. <https://pubs.usgs.gov/tm/06/a53/tm06a53.pdf>.

[NMMO] [RIG][SFM][CTM]

**Abstract/Scope:** MT3D-USGS, a USGS updated release of the groundwater solute transport code MT3DMS, includes new transport modeling capabilities to accommodate flow terms calculated by MODFLOW packages that were previously unsupported by MT3DMS and to provide greater flexibility in the simulation of solute transport and reactive solute transport. Unsaturated-zone transport and transport within streams and lakes, including solute exchange with connected groundwater, are among the new capabilities included in the MT3D-USGS code. MT3D-USGS also includes the capability to route a solute through dry cells that may occur in the Newton-Raphson formulation of MODFLOW (that is, MODFLOW-NWT). New chemical reaction Package options include the ability to simulate inter-species reactions and parent-daughter chain reactions. A new pump-and-treat recirculation package enables the simulation of dynamic recirculation with or without treatment for combinations of wells that are represented in the flow model, mimicking the above-ground treatment of extracted water. A reformulation of the treatment of transient mass storage improves conservation of mass and yields solutions for better agreement with analytical benchmarks. Several additional features of MT3D-USGS are (1) the separate specification of the partitioning coefficient ( $K_d$ ) within mobile and immobile domains; (2) the capability to assign prescribed concentrations to the top-most active layer; (3) the change in mass storage owing to the change in water volume now appears as its own budget item in the global mass balance summary; (4) the ability to ignore cross-dispersion terms; (5) the definition of Hydrocarbon Spill-Source Package (HSS) mass loading zones using regular and irregular polygons, in addition to the currently supported circular zones; and (6) the ability to specify an absolute minimum thickness rather than the default percent minimum thickness in dry-cell circumstances.

Benchmark problems that implement the new features and packages test the accuracy of new code through comparison to analytical benchmarks, as well as to solutions from other published codes. The input file structure for MT3D-USGS adheres to MT3DMS conventions for backward compatibility: the new capabilities and packages described herein are readily invoked by adding three-letter package name acronyms to the name file or by setting input flags as needed. Memory is managed in MT3D-USGS using FORTRAN modules in order to simplify code development and expansion.

U.S.NRC, *Regulatory Guide 4.25, Assessment of Abnormal Radionuclide Discharges in Ground Water to the Unrestricted Area at Nuclear Power Plant Sites*, Washington, D.C., March 2017. <https://www.nrc.gov/docs/ML1625/ML16253A333.pdf>.

[GG][CCSM] [RIG][SFM][CTM]

**Abstract/Scope:** This regulatory guide (RG) describes an approach that the U.S.NRC staff considers acceptable for use in assessing abnormal discharges of radionuclides in ground water from the subsurface to the unrestricted area at nuclear power plant sites. The U.S.NRC is issuing this RG to provide guidance on acceptable methods to determine the quantity of licensed material (i.e., radionuclides) in abnormal discharges into the unrestricted area through the ground water discharge pathway. The guide lists all applicable regulations and Standards for Protection against Radiation.

*Document disclaimer: This RG does not substitute regulations and compliance with the guide is not required. Methods and solutions that differ from those set forth in regulatory guides will be*

*deemed acceptable if they provide a basis for the findings required for the issuance or continuance of a permit or license by U.S.NRC.*

Wainwright, H., Arora, B., Hubbard, S., Lipnikov, K., Moulton, D., Flach, G., Eddy-Dilek, C. and Denham, M., ***Sustainable Remediation in Complex Geologic Systems, Encyclopedia of Inorganic and Bioinorganic Chemistry***, pp.1-12, 2011.

<https://onlinelibrary.wiley.com/doi/abs/10.1002/9781119951438.eibc2562>.

[GG][CCSM][NMMO][CSMRD] [SFM][CTM]

**Abstract/Scope:** Sustainable remediation has been increasingly regarded as a promising alternative in recent years. It considers *net environmental impacts* such as energy use, greenhouse gas emission, and waste reduction. Passive *in situ* remediation or natural attenuation are the key components of sustainable remediation often intended to minimize the net environmental impacts. However, leaving contaminants in the subsurface requires the increased burden of proof to show that plumes are stable and residual contaminants do not pose a significant health risk. Particularly in complex geological environments and for actinide species with complex geochemical behaviors, it is difficult to ensure the system stability as well as to predict the future plume conditions. This article presents recent scientific advances to support sustainable remediation in complex geological systems, including site characterization techniques, hydrological and geochemical model developments, and numerical simulations. In particular, we highlight the recent developments in non-invasive geophysical characterization as well as computationally efficient geochemical models for describing uranium and other reactive species. We demonstrate this approach using the extensive data and models from the Savannah River Site F-area, which has been contaminated by low-level radioactive waste solutions including uranium, tritium, and other radionuclides. This document examines the ***Savannah River Site F-area site*** in detail.

White, M.D. and Oostrom, M., ***STOMP - Subsurface Transport Over Multiple Phases, Version 4.0 User's Guide*** (No. PNNL-15782), Pacific Northwest National Laboratory, Richland, WA, 2006. [https://www.pnnl.gov/main/publications/external/technical\\_reports/PNNL-15782.pdf](https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-15782.pdf).

[CCSM][NMMO] [SFM][CTM]

**Abstract/Scope:** This guide describes the general use, input file formatting, compilation, and execution of the *Subsurface Transport Over Multiple Phases* (STOMP) simulator, a scientific tool for analyzing single and multiple phase subsurface flow and transport. A description of the simulator's governing equations, constitutive functions, and numerical solution algorithms are provided in a companion theory guide. In writing these guides for the STOMP simulator, the authors have assumed that the reader comprehends concepts and theories associated with multiple-phase hydrology, heat transfer, thermodynamics, radioactive chain decay, and relative permeability-saturation-capillary pressure constitutive relations.

*Please note: We recommend that the reader be familiar with the computing environment on which they plan to compile and execute the STOMP simulator.*

Widdowson, M., Chappelle, F., Casey, C., and Kram, M., ***Estimating Cleanup Times Associated with Combining Source-Area Remediation with Monitored Natural Attenuation***, Groundswell Technologies, Inc., ER-200436. [https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Monitoring/ER-200436/ER-200436/\(language\)/eng-US](https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/Contaminated-Groundwater/Monitoring/ER-200436/ER-200436/(language)/eng-US) or <https://www.nas.cee.vt.edu/index.php>.

[NMMO] [RIG][MTMO][SFM][CTM]

**Abstract/Scope:** The Natural Attenuation Software (NAS) screening tool was co-developed by the U.S. Navy, the U.S. Geological Survey (USGS), and Virginia Tech. NAS is designed to make complex analytical and numerical solutions of the time of remediation (TOR) problem accessible to remedial project managers (RPM) and their contractors. NAS consists of a combination of computational tools implemented in three main interactive modules to provide estimates for target source concentration required for a plume extent to contract to regulatory limits; time required for contaminants in the source area to attenuate to a predetermined target source concentration; and time required for a plume extent to contract to regulatory limits after source reduction. NAS estimates TOR through consideration of multiple natural attenuation processes, including advection, dispersion, sorption, nonaqueous phase liquid (NAPL) dissolution, and biodegradation of petroleum hydrocarbons, chlorinated solvents, or any user-specified contaminants or mixtures. Simulations also account for variable rates of biodegradation based on specific redox zone conditions.

Zheng, C. and Bennett, G.D., ***Applied Contaminant Transport Modeling: Theory and Practice***, 1997, John Wiley & Sons, ISBN: 0-471-28536-6; 2<sup>nd</sup> edition, 2002, John Wiley & Sons, ISBN: 978-0-471-38477-9. [https://www.amazon.com/Applied-Contaminant-Transport-Modeling-Chunmiao/dp/0471384771/ref=dp\\_ob\\_title\\_bk](https://www.amazon.com/Applied-Contaminant-Transport-Modeling-Chunmiao/dp/0471384771/ref=dp_ob_title_bk).

[GG][CSMRD] [LLMR][SFM][CTM]

**Abstract/Scope:** The challenges facing groundwater scientists and engineers today demand expertise in a wide variety of disciplines—geology, hydraulics, geochemistry, geophysics, and biology. As the number of the subdisciplines has increased and as each has become more complex and quantitative, the problem of integrating their concepts and contributions into a coherent overall interpretation has become progressively more difficult. To an increasing degree, transport simulation has emerged as an answer to this problem, and the transport model has become a vehicle for integrating the vast amount of field data from a variety of sources and for understanding the relationship of various physical, chemical, and biological processes.

*Applied Contaminant Transport Modeling: Theory and Practice* is the first resource designed to provide coverage of the discipline's basic principles, including the theories behind solute transport in groundwater, common numerical techniques for solving transport equations, and step-by-step guidance on the development and use of field-scale modeling. The Second Edition incorporates recent advances in contaminant transport theory and simulation techniques, adding the following to the original text:

- An expanded discussion of the role of aquifer heterogeneity in controlling solute transport;
- A new section on the dual-domain mass transfer approach as an alternative to the classical advection-dispersion model;

- Additional chemical processes and reactions in the discussion of reactive transport;
- A discussion of the TVD (total-variation-diminishing) approach to transport solution; and
- An entirely new Part III containing two chapters on simulation of flow and transport under variable water density and under variable saturation, respectively, and a third chapter on the use of the simulation-optimization approach in remediation system design.

*Applied Contaminant Transport Modeling, Second Edition* remains the premier reference for practicing hydrogeologists, environmental scientists, engineers, and graduate students in the field. In 1998, in recognition of their work on the first edition, the authors were honored with the John Hem Excellence in Science and Engineering Award of the National Ground Water Association. This book includes case studies for contaminant transport modeling.

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#### **Note to Reader regarding Disclaimer of Liability**

With respect to documents listed in the ***Bibliography of Guidance and Information Sources on Subsurface Modeling to Support Site Remediation***, the government publications cited are available and free to the public. Non-governmental publications listed may be copyrighted and may be subject to additional costs to obtain.

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