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Revision 0

Regulatory Criteria for the Selection of Vadose Zone Modeling in Support of the 200-UW-1 Operable Unit

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

United States Department of Energy
P.O. Box 550
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EXECUTIVE SUMMARY

The evaluation of potential impacts to groundwater from contaminants in the vadose zone soils at the Hanford Site is important for making final remedial action decisions at the Hanford Site. Federal and state regulations, requirements, and guidelines concerning environmental remediation form the basis for the methods used to conduct these evaluations. Although many methods and/or models may be used to evaluate the potential impacts to groundwater, the use of environmental regulatory models (ERMs) is appropriate for applications to evaluate pathways involving vadose zone and/or groundwater systems.

This document identifies and addresses the items needed for appropriate and consistent regulatory methods/models for the assessment and characterization of the impacts/risk to groundwater from vadose zone contamination at the Hanford Site for the 200-UW-1 Operable Unit waste sites. This documentation may also be used to support other assessments of vadose zone contamination at the Hanford Site. It also describes the manner in which Federal and state requirements and guidelines concerning the selection and use of ERMs can be employed to address these issues.

The primary aspects of these issues addressed in this document include the following:

- Identifying and comparing the technical and Federal and state regulatory requirements and expectations associated with the selection and use of ERMs in general, and specifically for vadose zone modeling
- Applying these requirements and guidelines that result in the determination that fate and transport modeling is the most appropriate model type for most vadose zone modeling risk characterization applications at the Hanford Site
- Demonstrating the acceptability of the Subsurface Transport Over Multiple Phases (STOMP) code for implementing the fate and transport model type
- Demonstrating and documenting consistency with Federal and state requirements and guidelines concerning method/model selection for most vadose zone modeling applications
- Documenting the correspondence of the pertinent Federal and state requirements and guidelines, as well as consistency with the Federal guidelines that can satisfies all pertinent regulatory requirements.

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TERMS

AFT	Alternative Fate and Transport
ARAR	applicable or relevant and appropriate requirement
ATFERM	Agency Task Force on Environmental Regulatory Modeling
BCB	Brooks and Corey-Burdine
BCM	Brooks and Corey-Mualem
bgs	below ground surface
CERCLA	*Comprehensive Environmental Response, Compensation, and Liability Act of 1980*
CFR	*Code of Federal Regulations*
COC	contaminant of concern
CREM	Committee on Regulatory Environmental Modeling
CVS	concurrent version system
DF	dilution factor
DOE	U.S. Department of Energy
Ecology	Washington State Department of Ecology
EPA	U.S. Environmental Protection Agency
ERM	environmental regulatory model
FEPs	features, events, and processes
GOSPL	Geographic and Operational Site Parameters List
Kd	instantaneous equilibrium distribution coefficient
MCL	maximum contaminant level
N/A	not applicable
NAPL	nonaqueous phase liquid
NCP	National Contingency Plan
NEA	Nuclear Energy Agency
NPL	National Priorities List
NRC	U.S. Nuclear Regulatory Commission
OU	operable unit
PNNL	Pacific Northwest National Laboratory
QA	quality assurance
QC	quality control
RAG	remedial action goal
RCRA	*Resource Conservation and Recovery Act of 1976*
RCW	*Revised Code of Washington*
STOMP	Subsurface Transport Over Multiple Phases
Tri-Party Agreement	*Hanford Federal Facility Agreement and Consent Order*
TVD	total variation diminishing
VGB	van Genuchten-Burdine
VGM	van Genuchten-Mualem
WAC	*Washington Administrative Code*
WIDS	Waste Information Data System

METRIC CONVERSION CHART

Into metric units			Out of metric units		
If you know	Multiply by	To get	If you know	Multiply by	To get
Length			**Length**		
inches	25.40	millimeters	millimeters	0.03937	inches
inches	2.54	centimeters	centimeters	0.393701	inches
feet	0.3048	meters	meters	3.28084	feet
yards	0.9144	meters	meters	1.0936	yards
miles (statute)	1.60934	kilometers	kilometers	0.62137	miles (statute)
Area			**Area**		
square inches	6.4516	square centimeters	square centimeters	0.155	square inches
square feet	0.09290304	square meters	square meters	10.7639	square feet
square yards	0.8361274	square meters	square meters	1.19599	square yards
square miles	2.59	square kilometers	square kilometers	0.386102	square miles
acres	0.404687	hectares	hectares	2.47104	acres
Mass (weight)			**Mass (weight)**		
ounces (avoir)	28.34952	grams	grams	0.035274	ounces (avoir)
pounds	0.45359237	kilograms	kilograms	2.204623	pounds (avoir)
tons (short)	0.9071847	tons (metric)	tons (metric)	1.1023	tons (short)
Volume			**Volume**		
ounces (U.S., liquid)	29.57353	milliliters	milliliters	0.033814	ounces (U.S., liquid)
quarts (U.S., liquid)	0.9463529	liters	liters	1.0567	quarts (U.S., liquid)
gallons (U.S., liquid)	3.7854	liters	liters	0.26417	gallons (U.S., liquid)
cubic feet	0.02831685	cubic meters	cubic meters	35.3147	cubic feet
cubic yards	0.7645549	cubic meters	cubic meters	1.308	cubic yards
Temperature			**Temperature**		
Fahrenheit	subtract 32 then multiply by 5/9ths	Celsius	Celsius	multiply by 9/5ths, then add 32	Fahrenheit
Energy			**Energy**		
kilowatt hour	3,412	British thermal unit	British thermal unit	0.000293	kilowatt hour
kilowatt	0.94782	British thermal unit per second	British thermal unit per second	1.055	kilowatt
Force/Pressure			**Force/Pressure**		
pounds (force) per square inch	6.894757	kilopascals	kilopascals	0.14504	pounds per square inch

06/2001

Source: *Engineering Unit Conversions*, M. R. Lindeburg, PE., Third Ed., 1993, Professional Publications, Inc., Belmont, California.

REGULATORY CRITERIA FOR THE SELECTION OF VADOSE ZONE MODELING IN SUPPORT OF THE 200-UW-1 OPERABLE UNIT

1.0 INTRODUCTION

This document provides regulatory and technical basis supporting the use of environmental regulatory models (ERMs) in the evaluations of potential impacts to groundwater from vadose zone contamination at the Hanford Site for 200-UW-1 Operable Unit (OU) waste sites. The document identifies the Federal and state regulations, requirements, and guidelines that provide the regulatory and technical basis pertaining to the selection, use, and required documentation of ERMs. Of particular importance are the requirements in the *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA) and *Resource Conservation and Recovery Act of 1976* (RCRA). The identification of these requirements and guidelines serve to establish the criteria and expectations necessary for the selection of a vadose zone model. This document may be also used to support the selection of other vadose zone models to assess risk from contamination.

The primary use of vadose zone modeling at the Hanford Site is to quantitatively assess potential impacts to groundwater from contaminants in the vadose zone. Federal and state regulations require the use of scientifically based method for assessing and demonstrating consistency with the primary objective of environmental cleanup regulations (i.e., protection of human health and the environment) (EPA 402-R-93-005, OSWER Directive 9200.4-18, EPA/100/B-04/001, *Washington Administrative Code* [WAC] 173-340-747). The primary guidelines state these computations involve methods appropriate for the objectives and conditions of the assessment (e.g., EPA 500-R-94-001, EPA 402-R-93-005, and OSWER Directive 9200.4-18).

The main issues associated with the assessment of groundwater impacts/risks from vadose zone contamination at Hanford, therefore, include the following:

- What methods/models are most appropriate for assessing impacts to groundwater from vadose zone contaminants at the Hanford Site?
- How are appropriate models determined?
- What regulatory requirements and technical rationale are associated with the selection of appropriate models?
- What regulatory requirements and technical rationale are associated with the use of an appropriate model for risk-based applications (e.g., risk characterization)?
- What is necessary to demonstrate consistency with these requirements and expectations, and the acceptability of a method?

This document addresses these issues and focuses on the selection and use of appropriate and acceptable ERMs for assessing potential impacts to groundwater from vadose zone contamination at Hanford in support of a final remedial action for the 200-UW-1 OU waste sites. The process for selection and use of ERMs discussed in this document may be useful in other applications at Hanford. U.S. Environmental Protection Agency (EPA) guidance on risk assessment (EPA/540/1-89/002) states that the evaluation of risks associated with all relevant pathways and the risk characterization methods be appropriate for the objectives and conditions of the assessment (e.g., EPA 500-R-94-001, EPA 402-R-93-005, and OSWER Directive 9200.4-18). Risk characterization associated with the vadose zone to groundwater pathway (also referred to here as the "protection of groundwater" pathway) involves a combination of the vadose zone and groundwater pathways and systems and is particularly important for environmental remediation efforts at Hanford for several reasons:

1. Risk characterization efforts associated with the protection of groundwater pathway are integral to the remediation efforts at the Hanford Site.

2. The "protection of groundwater" pathway can often dominate the risk and/or hazard posed by soil contamination and associated soil cleanup levels.

3. In the absence of a risk-based methods for assessing the levels of soil contaminants protective of groundwater, soil cleanup levels for this pathway are based soil background levels, detection limits, or predetermined values.

4. Federal environmental regulations (e.g., 40 *Code of Federal Regulations* [CFR] 300, CERCLA, and RCRA), and Federal risk assessment guidelines (EPA/540/1-89/002, EPA/540/R-92/003) require the use of technical methods that are risk-based, appropriate for the intended application, appropriate for the site conditions, and that use site-specific data.

5. Appropriate risk characterization methods provide a technically valid basis for defining the baseline risks, which are essential for the risk management and risk communication aspects (National Research Council 1983, 1994). The baseline risk for the protection of groundwater pathway is integral to evaluating the efficacy of remedies and to making decisions regarding the allocation of resources for effectively mitigating the risks at sites to levels/conditions protective of human health and the environment.

The selection and use of ERMs appropriate for the evaluation of groundwater impacts from contaminants in the Hanford vadose zone need to be selected in a manner that is technically justified and consistent with the purpose and requirements of the pertinent Federal and state regulations and guidelines.

This document addresses the issues associated with the need for technically appropriate and regulatory consistent methods/models for the assessment and characterization of the impacts/risk to groundwater from vadose zone contamination at Hanford. The following is an overview of the content and organization of this document, and the manner in which these issues are addressed.

- Section 1.0: Introduces the purpose of the document and the issues associated with vadose modeling at the Hanford. Describes why these issues are important to environmental remediation efforts, how and why modeling is used in the regulations, and provides an overview of the structure ant contents of this document.

- Section 2.0: Identifies Federal and state requirements, guidelines, and criteria pertaining to the selection and use of ERMs for assessing impacts/risk to groundwater from vadose zone contaminants at the Hanford Site.

- Section3.0: Provides documentation concerning the technical basis and rationale for using the processes identified in the Federal guidelines for selecting and using a model type appropriate for most vadose zone modeling risk characterization applications at the Hanford Site.

- Section 4.0: Describes the application of the Federal guidelines for the selection of a model type capable of meeting the objectives of most vadose modeling risk characterization applications at the Hanford Site.

- Section 5.0: Describes the required and expected documentation associated with the use of vadose zone modeling for risk characterization applications.
- Section 6.0: Documents an example of the application of the Federal code selection guidelines for evaluating the adequacy of a code to meet the required attributes and criteria of fate and transport modeling. The code evaluation/selection process is documented for the Subsurface Transport Over Multiple Phases (STOMP) code.
- Section 7.0: Summarizes the manner and extent to which the application of the guidelines concerning the selection and use of an ERM appropriate for Hanford vadose modeling risk characterization applications are consistent with Federal requirements and guidelines.
- Section 8.0: Documents the demonstration of consistency with state regulations concerning the selection and use of ERMs pertaining to vadose zone modeling, including the use of the STOMP code.
- Section 9.0: Provides a summary of the information contained in this document regarding the technical and regulatory requirements and expectations associated with the selection, as well as the use of ERMs and their applications for vadose zone modeling and risk characterization applications at the Hanford Site.
- Appendix A: Provides a synopsis of technical information pertaining to preferential pathways in the context of transport-related mechanisms in the conceptual model for vadose zone system at the Hanford Site.
- Appendix B: Provides an example of the application of published guidelines concerning the manner in which Hanford Site data base information is used in the selection of appropriate, site-specific model parameters, such as instantaneous equilibrium distribution coefficient (Kd) values.

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2.0 REGULATORY REQUIREMENTS, GUIDELINES, AND CRITERIA ASSOCIATED WITH THE USE OF ENVIRONMENTAL REGULATORY MODELS

Federal and state regulations and guidelines identify requirements and recommendations concerning the selection and use of ERMs in risk-based applications (e.g., risk characterization) in environmental remediation efforts. These requirements and recommendations provide guidance on the processes and rationale for the selection of appropriate models and codes, the use of ERMs, and the expected documentation of model results. This section identifies and summarizes the processes and criteria identified in the Federal guidelines concerning the evaluation, selection, and use of an ERM and model code.

2.1 BACKGROUND ON THE USE OF ENVIRONMENTAL REGULATORY MODELS

The selection of ERMs methodology is based on the requirements in the following Federal environmental regulations:

- National Contingency Plan (NCP) (40 CFR 8665–8865 300)
- CERCLA regulations
- RCRA regulations
- *Hanford Federal Facility Agreement and Consent Order* (Tri-Party Agreement) (Ecology et al. 2003).

The Washington State requirements are contained in the following environmental regulations:

- "Hazardous Waste Management Act" (*Revised Code of Washington* [RCW] 70.105)
- "Model Toxics Control Act – Cleanup" (WAC 173-340), in the context of RCRA corrective action, and also where applicable or relevant and appropriate requirements (ARARs) are pursuant to CERCLA. (These regulations are overseen by the Washington State Department of Ecology [Ecology]).

The role of computer models in these Federal and state environmental regulations is to support protection of human health and the environment. Under CERCLA, the EPA is required to assess the risk to human health posed by hazardous and radioactive wastes at sites on the National Priorities List (NPL). Both Federal and state regulations and guidelines recognize the use of ERMs as appropriate methods and tools for assessing and characterizing risk to human health and the environment. The use of ERMs is warranted where contaminant behavior involves media in complex and dynamic systems, such as groundwater and vadose zone pathways.

2.2 RATIONALE FOR THE USE OF ENVIRONMENTAL REGULATORY MODELS

The Federal ERM guidelines indicate that the reason for modeling to support environmental regulatory efforts typically include the following: (1) supporting risk assessment requirements; and (2) identifying, selecting, and designing remedial alternatives (EPA 402-R-93-009). There are many reasons why modeling is needed to fulfill the regulatory requirements associated with the CERCLA remedial action and RCRA corrective action processes are identified in the Federal guidelines (Table 2-1). Among these, the principal reasons (EPA 402-R-94-012) include the following:

1. Assess the actual or potential risk impacts of the site (i.e., assessment of risk)
2. Comply with applicable regulations
3. Define remediation strategies for the site
4. Evaluate alternative remedies.

This information is summarized in Table 2-1, which identifies where and when modeling is likely to be needed and used during different phases of the risk assessment and remedial action evaluation process (EPA 402-R-94-012). The Federal guidelines indicate that, "Notwithstanding the limitations of models, it is difficult to support remedial decisions or the assessment of risk at a site without the use of models" (EPA 402-R-93-009).

The following are examples of the EPA primary guidance documents that provide technical rational and precedents pertaining to the selection and/or use of ERMs, primarily in the context of CERCLA risk assessment requirements:

- The EPA's Agency Task Force on Environmental Regulatory Modeling (ATFERM) guidance states that, "...environmental models...may form part of the scientific basis for regulatory decision making at EPA" (EPA 1999, 2003a).

- ERMs are regarded as appropriate tools throughout EPA guidance on environmental risk assessment (EPA 2001, 2003a; EPA-SAB-EEC-89-012).

- EPA risk assessment supplemental guidance identifies the use of models as being justified where site-specific data or changes in knowledge over time warrant the use of methods different than the basic risk characterization methods and formulas (EPA/540/R-92/003, EPA 1992).

Other Federal and state regulations and guidelines that recognize environmental regulatory modeling as a method for risk assessments and/or the development of media-specific cleanup levels include the following:

- *Report of Agency Task Force on Environmental Regulatory Modeling: Guidance, Support Needs, Draft Criteria and Charter* (EPA 500-R-94-001)

- *A Summary of General Assessment Factors for Evaluating the Quality of Scientific and Technical Information* (EPA 2003b)

- *CERCLA Baseline Risk Assessment Reference Manual for Toxicity & Exposure Assessment and Risk Characterization* (DOE/EH-0484)

- *Proposed Agency Strategy for the Development of Guidance on Recommended Practices in Environmental Modeling* (EPA 2001)

- *Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models* (EPA 2003a)

- *Models Toxics Control Act Cleanup Levels & Risk Calculations (CLARC)*, Version 3.1 (Ecology 94-145)

- "Deriving Soil Concentrations for Ground Water Protection" (WAC 173-340-747).

The main issue concerning ERMs, however, concerns the technical basis and regulatory consistency associated with the selection and use of appropriate models and codes.

Table 2-1. Matrix of Reasons for Modeling in the Remedial Process (from EPA 402-R-94-012, Table 2-1). (2 pages)

	Opportunities for Modeling	Scoping[a]	Site Characterization[a]	Remediation[a]
1.	When it is not feasible to perform field measurements; i.e., • Cannot get access to sampling locations • Budget is limited • Time is limited.	●	○	○
2.	When there is concern that downgradient locations may become contaminated at some time in the future.	●	●	●
3.	When field data alone are not sufficient to characterize fully the nature and extent of the contamination; i.e., • When field sampling is limited in space and time and needs to be supplemented with models • When field sampling results are ambiguous or suspect.	●	●	●
4.	When there is concern that conditions at a site may change, thereby changing the fate and transport of the contaminants; i.e., • Seasonal changes in environmental conditions • Severe weather (floods, tornadoes) • Accidents (fire).	○	●	●
5.	When there is concern that institutional control at the site may be lost at some time in the future resulting in unusual exposure scenarios or a change in the fate and transport of the contaminant; i.e., • Trespassers • Inadvertent intruder • Construction/agriculture • Drilling, mineral exploration, mining • Human interventions (drilling, excavations, mining)	○	●	●
6.	When remedial actions are planned and there is a need to predict the effectiveness of alternative remedies.	○	○	●
7.	When there is a need to predict the time when the concentration of specific contaminants at specific locations will decline to acceptable levels (e.g., natural flushing).	○	●	●
8.	When there is concern that at some time in the past individuals were exposed to elevated levels of contamination and it is desirable to reconstruct the doses.	○	●	○
9.	When there is concern that contaminants may be present but below the lower limits of detection	○	●	○

Table 2-1. Matrix of Reasons for Modeling in the Remedial Process (from EPA 402-R-94-012, Table 2-1). (2 pages)

	Opportunities for Modeling	Scoping[a]	Site Characterization[a]	Remediation[a]
10.	When field measurements reveal the presence of some contaminants and it is desirable to determine if and when other contaminants associated with the source may arrive, and at what levels.	○	●	○
11.	When field measurements reveal the presence of contaminants and it is desirable to identify the source or sources of the contamination.	●	●	○
12.	When there is a need to determine the timing of the remedy; i.e., if the remedy is delayed, is there a potential for environmental or public health impacts in the future?	○	○	●
13.	When there is a need to determine remedial action priorities.	○	○	●
14.	When demonstrating consistency with regulatory requirements.	●	●	●
15.	When estimating the benefit in a cost-benefit analysis of alternative remedies.	○	○	●
16.	When performing a quantitative dose or risk assessment.	○	●	●
17.	When designing the site characterization program and identifying exposure pathways of potential significance.	●	○	●
18.	When there is a need to compute or predict the concentration distribution in space and time of daughter products from the original source of radionuclides.	●	○	○
19.	When there is a need to quantify the degree of uncertainty in the anticipated behavior of the radionuclides in the environment and the associated doses and risks.	●	○	○
20.	When communicating with the public about the potential impacts of the site and the benefits of the selected remedy.	●	○	●

NOTE: Areas shaded denote modeling reasons typically associated with the vadose zone protection of groundwater pathway at the Hanford Site.

[a] Legend:
- ● Denotes an important role.
- ○ Denotes a less important role.

2.3 FEDERAL GUIDELINES FOR THE SELECTION AND USE OF ENVIRONMENTAL REGUALTORY MODELS

Federal guidelines specify that the process for using ERMs begins with the development of the rationale for selecting a modeling method instead of selecting another simpler method for the purpose of the risk assessment. After demonstrating that the use of an ERM is the appropriate method, the documentation defines the model objectives. The EPA guidance then recommends adhering to guidelines pertaining to the selection and use of appropriate model type and codes to accomplish those objectives. The following sections identify and summarize the processes and criteria identified in the Federal guidelines concerning the evaluation and selection of model types and model code(s) used for ERMs.

The selection of an appropriate method/model involves consideration of the strategy for assessing the risk to human health and the environment posed by waste site contaminants. That strategy includes identifying the type and quality of information needed to evaluate the risk associated with the waste site(s). The risk information can include simple screening criteria, quantitative assessments and characterization of the risk, and/or the determination of soil cleanup levels that are protective of human health and the environment. Other criteria include consideration of the characteristics of the pathway and/or system of interest, and the level of model complexity that is consistent with the quality of the information appropriate for meeting the modeling objectives.

2.4 MODEL AND CODE SELECTION GUIDELINES

Federal guidelines identify a technically based processes for model and code selection (EPA 402-R-93-009, EPA 402-R-94-012) and provide guidance on the evaluation and application of ERMs (CREM 2003). The merits of this process include the following:

- It is the product of nearly two decades of consensus building among subject matter experts on the development, evaluation, and application of ERMs within the scientific community.
- It meets the objectives and intent of Federal and state regulations and guidelines in terms of describing and explaining the selection process, as well as the scientific reasoning, rationale, and assumptions associated with the process.

The intent of applying this process is to provide a valid technical basis for the selection of the model. Although there is no formal corresponding state process for ERM method/model selection (e.g., in accordance with WAC 173-340-747, Federal guidelines addresses the intent and expectations of both Federal and state requirements to document the technical basis of the ERM, including the reasons, rationale, and logic for model and code selection). As noted in Federal guidelines, model selection and code selection are different but related activities, as described in the following paragraphs.

The EPA technical guidelines indicate that the model selection process begins with defining the objectives and identifying the type of predictive tasks to be included in the model (EPA 402-R-94-012). This step is followed by the development of a site conceptual model, which is divided into conceptual model components. The conceptual model components help to identify the important factors such as the site features, events, and processes (FEPs) to be included in the model. Model selection involves identifying the type of predictive tasks to be included in the model, consistent with the objectives and purpose of the problem, and determining the attributes necessary for a meaningful simulation. These elements of the model selection process are summarized in the following and are illustrated in Figure 2-1:

1. Define the regulatory purpose of the problem, and describe the rationale/need for modeling.
2. Define the project and site-specific objectives for the use of the ERM.
3. Determine model selection criteria and attributes:
    a. Develop a conceptual model and conceptual model components.
    b. Determine principal FEPs and phenomena to be modeled.
    c. Identify other factors, requirements, or attributes to be included in the selection criteria.

   d. Determine the level of model sophistication or capability required to meet the criteria and attributes.

   e. Select/identify an appropriate model type.

4. Select a code capable of meeting the criteria and attributes:

   a. Identify candidate code(s).

   b. Evaluate the administrative criteria associated with the candidate code(s).

   c. Evaluate/document adequacy of code(s) to meet model criteria/attributes.

   d. Select/identify appropriate modeling code.

5. Document the use of the ERM:

   a. Describe the model and code selection process and rationale.

   b. Identify the sources of information and the rationale used to develop the input parameters.

   c. Present the model results.

   d. Identify the uncertainties in the model and model results, and describe their possible impact on the results.

   e. Identify, provide the rationale, and describe the impact on the model results for the assumptions used in the model.

   f. Identify the limitations of the model and limitations associated with the interpretations of the model results.

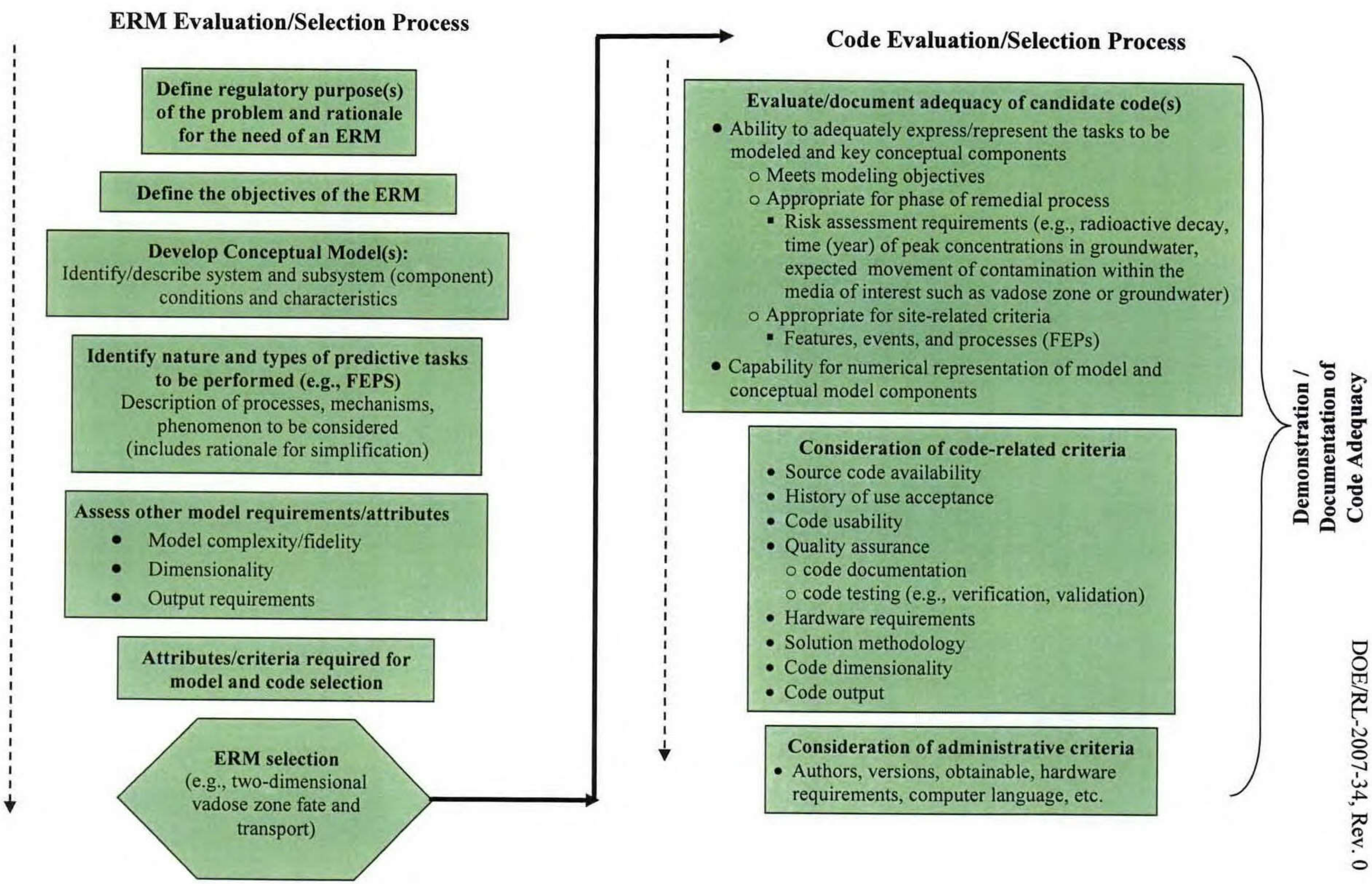
The code selection process focuses on the evaluation and identification of one or more code(s) that meet the required/necessary modeling criteria and attributes, as well as any administrative criteria (e.g., availability, computer language, and hardware requirements) that must be factored into the code selection decision (EPA 402-R-94-012). Code selection involves choosing one or more specific computer codes that are capable of performing the simulation(s) in a manner that satisfies and incorporates the required/necessary modeling criteria and attributes.

2.5 MODEL SELECTION PROCESS

2.5.1 Problem Statement, Objectives, and Modeling Need

The EPA's technical guidelines indicate that the first step in the model selection process is to develop the problem statements. The problem statements define the regulatory purpose of the ERM, determine the objective(s) of the task at hand, and explain the reasons and rationale for using a model to meet the objective(s) (EPA 402-R-94-012, CREM 2003). The documentation of these elements serves as the top-level criteria for model selection. The project-specific objectives (e.g., determining cleanup levels) drive the specific quantitative results required from the model. Combined with the objectives, an initial high-level description of general characteristics of the system(s) and pathway(s) can be identified prior to formal development of the conceptual site model (e.g., involving a groundwater and/or vadose zone system).

Figure 2-1. Summary of the U.S. Environmental Protection Agency Model (ERM) and Code Evaluation/Selection Process.



2.5.2 -Conceptual Site Models

The development of the conceptual site model, integral to the conduct of risk assessments, is the next step in the model selection process (EPA/540/R-92/003, EPA 402-R-94-012, ASTM 1999, CREM 2003). The conceptual model is the set of characteristics and behavior that reflect the actual site system(s) (EPA 402-R-94-012). The conceptual model serves as the basis for determining the processes, mechanisms, and phenomenon to be considered in the selection and use of ERMs (EPA/540/R-92/003). The EPA guidelines state that the required capabilities of the ERM are based on the nature and type of predictive tasks to be performed, and on information in the conceptual model that concern the site's physical and chemical characteristics, conditions, and system processes (EPA/540/R-96/003). The conceptual model also serves as the basis for the selection of appropriate site-specific model input parameters and for evaluating uncertainties, assumptions, and limitations of the model.

The development of the site conceptual model is based on field, laboratory, literature, and other relevant data and descriptive site information (EPA 402-R-94-012, ASTM 1999, CREM 2003). The approach to developing an appropriate conceptual model of the site involves integrating the generalized knowledge of physical and chemical processes with the available site-specific information. Thus, the conceptual model provides a simplifying framework in which information can be organized and linked to processes that can be simulated with predictive models (EPA 402-R-94-012).

Typical examples of conceptual model components for vadose zone and groundwater systems include the geology, hydrology, and the nature and extent of contamination. Each conceptual model component incorporates FEPs[1] for inclusion in the consideration of the necessary modeling capabilities. The principal FEPs associated with the conceptual model components are those that must be simulated to achieve the modeling objectives. These generally include a combination of general physical and/or chemical behavior (e.g., porous media fluid transport and chemical partitioning) and site-specific factors (e.g., geologic stratigraphy and recharge). Conceptual models and conceptual model components may also include simplifying assumptions that are based upon mathematical or scientific rationale, which are necessary and appropriate to simulate the principal FEPs.

Other factors, requirements, or attributes to be included in the model selection criteria are then identified. These can include model complexity, dimensionality, model output requirements, and code-related attributes. Model complexity includes consideration of spatial and temporal discretization, solution methods, model dimensionality, quality and quantity of data, and output requirements.

2.5.3 Determination of Environmental Regulatory Model Selection Criteria and Attributes

The next phase in the model selection process involves identifying and determining the model attributes necessary to meet the objectives of the modeling. These attributes also serve as criteria for model selection. The ERM attributes and selection criteria are related to and derived from the site conceptual model in the manner described in Figure 2-2.

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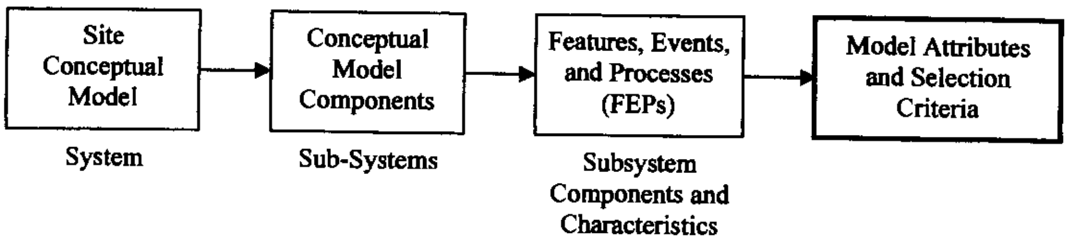
[1] FEPs refers to physical and chemical features, events, and processes of the system that ERMs are required to simulate. The use of "FEPs" stems from the approach used by the Nuclear Energy Agency (NEA) to assess the conceptual model components in the context of the combinations of relevant features, events, and processes, and U.S. Nuclear Regulatory Commission (NRC) reference to "processes, mechanisms, and phenomena" as FEPs, to define the nature and type of predictive tasks necessary to be performed by a computer model (NEA 2000, Bailey and Billingham 1998, PNNL-14702a).

Figure 2-2. The Relationship of ERM Model Attributes and Selection Criteria to the FEPs and the Site Conceptual Model.



2.5.4 Principal Features, Events, and Processes

The determination of the principal FEPs involves consideration of the actual physical and chemical systems and processes in the conceptual model component system (e.g., the hydrologic system in groundwater). ***Features*** are generally physical characteristics and systems that define or describe the area being modeled (e.g., geologic system). ***Events*** are significant occurrences that introduce some stress or change, either natural or artificial, to the area being modeled (e.g., climate-related events such as groundwater recharge or waste site operation events). ***Processes*** are the mechanisms, phenomena, and/or driving forces associated with the system being modeled (e.g., fluid transport processes, geochemical processes). For example in vadose zone modeling, the conceptual model integrates the site-specific knowledge of such items as the site geology (*feature*), hydrologic regime (*feature*), soil properties (*feature*), waste site discharges (*events*), waste site remediation (*event*), recharge (*process*), and distribution of contaminants (*process*).

2.5.5 Other Model Attributes and Criteria to Be Considered

Identifying other model attributes and criteria involves combining the FEPs with other relevant criteria that collectively describe the attributes of the model necessary to achieve the modeling objectives. Other model attributes considered in addition to the primary criteria associated with the FEPs include the following:

- Model complexity and solution methodology
- Model dimensionality
- Output requirements
- Other application-specific requirements.

The following is a summary of model attributes and criteria commonly considered in the selection of ERMs.

2.5.5.1 Model Complexity and Solution Methodology

The necessary degree of sophistication or complexity of the modeling is a key attribute. The necessary degree of sophistication of the modeling must be evaluated in terms of both the site-related issues (FEPs) and modeling objectives (EPA 402-R-94-012). Federal guidelines indicate that the factors with the greatest influence on determining the type and complexity of modeling needed are (1) the objectives of the modeling; (2) the environmental conditions and characteristics of the site; and (3) the nature, extent, and behavior of the contaminants. The combination of these factors determine the modeling needs and type (EPA 402-R-93-009).

Federal guidelines indicate that ERMs should begin with the simplest models and codes that satisfy the objectives, and then progress toward more sophisticated models/codes until the modeling objectives are achieved (EPA 402-R-94-012). However, an overly conservative approach may be contradictory to the objectives of the optimization between remedial activities and the accompanying reduction in risk (EPA 402-

R-93-009). Complex or semi-complex models, for example, are warranted when FEPs criteria cannot be adequately simulated with simpler analytical methods.

2.5.5.2 Model Dimensionality

The determination of the number of dimensions that a code should be capable of simulating is based primarily upon the data available, the modeling objectives, and the dimensionality of the FEPs. Certain FEPs (e.g., geologic layer thickness or recharge rates) may vary spatially and require multiple dimensions in the model to describe them adequately. Lower dimensionality models tend to be more conservative in their predictions, and their use frequently limited to screening analyses (EPA 402-R-94-012). Available data can also affect model dimensionality, because the utility of two- or three-dimensional analysis depends on whether the quantity and dimensionality of the data are consistent with, and/or support, the number of dimensions in the model.

2.5.5.3 Modeling of Radionuclides

In accordance with Federal requirements for the use of ERMs in risk assessment applications involving radionuclides (OSWER Directive 9200.4-18), the models must take into account the factors listed below and the adequacy of numerical models to accommodate these factors:

- Radioactive decay
- Time (year) peak concentrations in groundwater
- (Spatial) movement of contaminants within and between media.

2.5.5.4 Summary of Guidelines for Identifying Key FEPs and Modeling Attributes

Once the key FEPs have been identified, the model attributes delineate the required capability of the model to incorporate the FEPs adequately while meeting the objectives of the model. Together, the FEPs and attributes are criteria used to select the appropriate model type. Model selection involves matching the FEPs and the model attributes to determine the level of model complexity required to meet the objectives of the model. These criteria are used in the identification of needed model input parameters and assumptions.

2.6 CODE SELECTION PROCESS

The code selection process involves identifying and evaluating one or more codes that meet the modeling needs after the model attributes have been determined (EPA 402-R-94-012). The evaluation process identified in Federal guidelines (EPA 402-R-94-012) involves evaluation of the capability of the code to meet the following:

- Modeling objectives
- Required model attributes
- Code-related criteria
- Administrative criteria.

The following subsections describe the requirements and expectations associated with the evaluation and use of the model type attributes and criteria, code-related criteria, and administrative criteria in the code selection process.

2.6.1 Code-Related Selection Criteria

The regulatory code-related criteria considered in the code acceptance process (EPA 402-R-94-012) include the code's fidelity, usage, and acceptance in the scientific community; the code's quality assurance (QA) and quality control (QC) requirements; and the code's output capability. The technical code-related criteria considered include the code's ability to simulate the site-specific primary FEPs to the level of detail according to the required model attributes. Administrative criteria such as the authors, availability, obtainable version updates, hardware requirements, and computer language are also considered in the code evaluation and selection process. The code-related criteria recommended in the Federal guidelines for consideration in the code acceptance process (EPA 402-R-94-012) include the following:

- Source code availability
- History of use and acceptance in the scientific community
- Code usability
- QA
  - Code documentation
  - Code testing (e.g., verification and validation)
- Hardware requirements
- Solution methodology (consistency with model attribute requirements)
- Code dimensionality (consistency with model attribute requirements)
- Code output (consistency with model attribute requirements).

Application of the code selection and evaluation process ensures that the selected code is capable of mathematically representing the site, the pathway-related FEPs, and the discrete components of the conceptual model. The application of this approach can be reduced to three considerations: (1) each key component (attribute) of the conceptual model is adequately described by the mathematical model, (2) each of the separate mathematical models has been successfully integrated to where the sum of the parts is equal to the whole, and (3) the code is accessible and executable (EPA 402-R-94-012). Documentation of the evaluation and selection process, which includes a description of the adequacy of a specific code to meet these criteria, serves as the technical basis and rationale for code selection.

2.7 GUIDELINES FOR ENVIRONMENTAL REGULATORY MODEL USE AND DOCUMENTATION

Documentation of the technical basis and rationale associated with the selection and use of ERMs is necessary for the demonstration of meeting Federal and/or state requirements (EPA 2003a) and guidelines. The general model documentation elements recommended by EPA's Committee on Regulatory Environmental Modeling (CREM) (CREM 2003) are summarized in Table 2-2.

Table 2-2. Recommended Model Documentation Elements (amended from CREM 2003), Associated with the Common Model Use Aspects of the Hanford Vadose Zone System.

Recommended ERM Documentation Elements	Relationship to This Document	Location in Document
Model/Code Selection		
Management objectives	• Method/model selection • Aspects common to Hanford vadose zone modeling	Sections 1.0, 2.0, and 3.0
Conceptual model	• Model type selection • Aspects common to Hanford vadose zone modeling	Sections 3.0 and 4.0
Choice of technical approach	• Model type/code selection • Aspects common to Hanford vadose zone modeling • State requirements	Sections 3.0, 4.0, and 8.0
	• Code selection • State requirements	Sections 6.0 and 8.0
Model Use		
Parameter estimation	• Aspects common to Hanford vadose zone modeling • State requirements	Sections 4.0, 5.0, and 8.0 and Appendix B
Uncertainty/error evaluation	• Aspects common to Hanford vadose zone modeling • State requirements	Sections 5.0 and 8.0
Assumption evaluation	• Aspects common to Hanford vadose zone modeling • State requirements	Sections 3.0, 4.0, 5.0, and 8.0
Evaluation of model results	• Not applicable; • Application-specific	Not applicable
Limitations in the applicability of model results	• Aspects common to Hanford vadose zone modeling	Section 5.0
Conclusions of analysis in relationship to management objectives	• Aspects common to Hanford vadose zone modeling	Section 7.0
Recommendations for additional analysis, if necessary	• Not applicable • Application-specific	Not applicable to this document; see site-specific/waste site-specific document

These elements are intended to encompass the documentation necessary for the demonstration of meeting Federal and/or state requirements and guidance regarding the use of ERMs. The general documentation expectations required for meeting Federal guidelines for the selection and use of ERMs are summarized in Figure 2-3 and also in the context of sequential elements in Table 2-3.

2.7.1 Parameter Estimation Guidelines

The consideration of model parameters in the use of ERMs involves two aspects: (1) evaluation and selection of model parameters, and (2) evaluation of parameter uncertainty. The following is a summary of Federal guidelines associated with the evaluation and selection of model parameters in the use of ERMs.

Figure 2-3. Summary of the Sequential Steps in the Federal Guidelines for ERM Selection and Use Processes and Documentation Expectations.

These processes involve two main subdivisions: (1) elements associated with model and code selection, and (2) elements associated with model use. Note that the ERM selection process illustrated here refers to both model type and code. The documentation requirements and expectations associated with these processes are highlighted in pink.

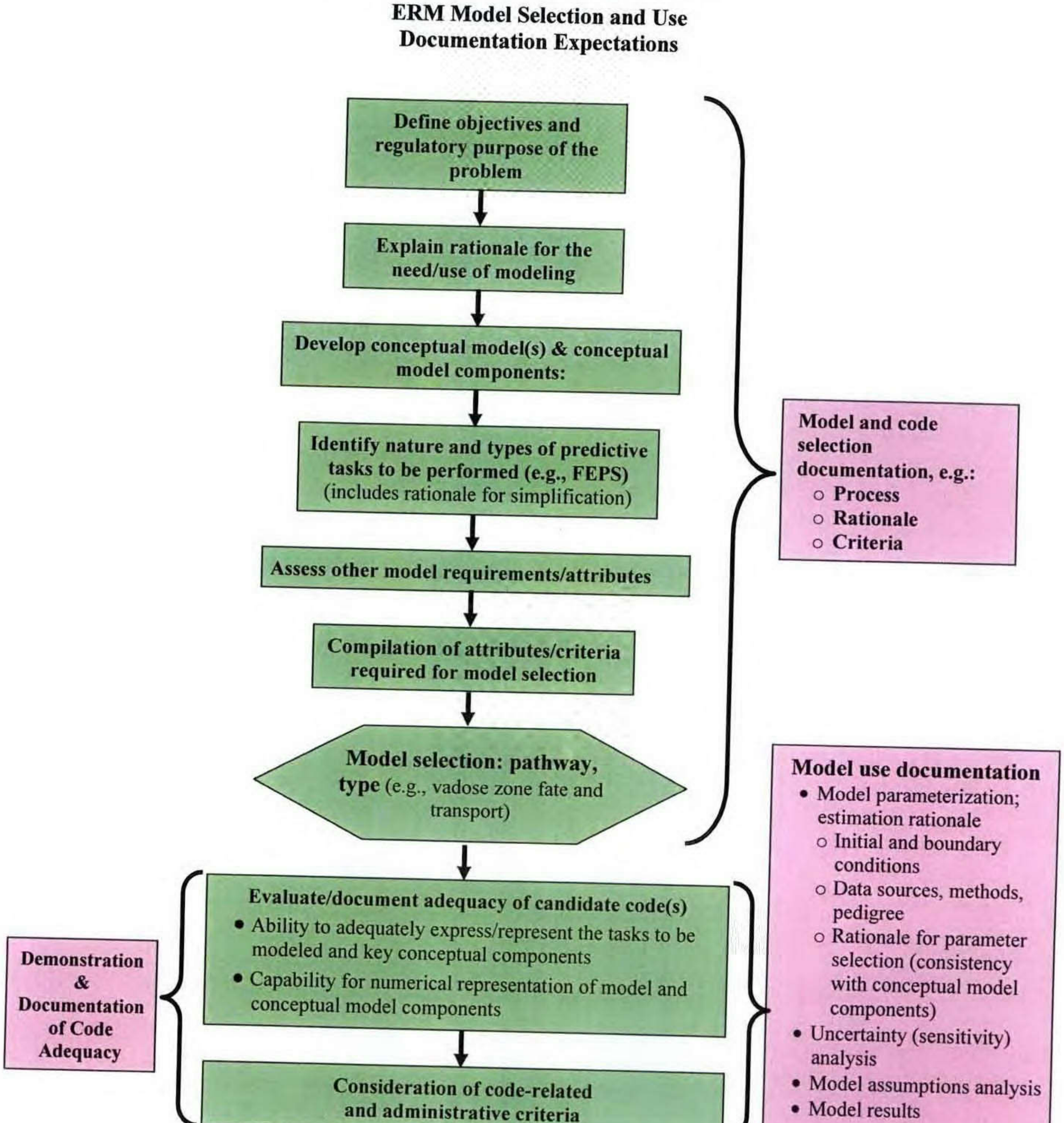


Table 2-3. Comparison of Federal and State Requirements and Elements Pertaining to the Selection and Use of Alternative Fate and Transport Modeling for the Derivation of Soil Levels Protective of Groundwater.

<table>
<tr><th colspan="4">Federal Compliance Elements and Requirements for the Selection and Use of Environmental Regulatory Models for Risk Based Applications</th></tr>
<tr><td rowspan="6">Model/Method Selection</td><td colspan="3">Purpose/Objectives</td></tr>
<tr><td colspan="3">Rationale of need/use for modeling</td></tr>
<tr><td colspan="3">Conceptual model(s); description of processes, mechanisms, phenomenon, site and system (i.e., vadose zone) characteristics to be considered</td></tr>
<tr><td colspan="3">Determine nature and types of primary system (i.e., vadose zone) FEPs and predictive tasks to be modeled</td></tr>
<tr><td colspan="3">Assess/determine other required model requirements/attributes</td></tr>
<tr><td colspan="3">Method selection/documentation</td></tr>
<tr><td rowspan="2">Code Selection</td><td colspan="3">Evaluation/assessment of adequacy/capabilities of candidate codes (vs. required model attributes)</td></tr>
<tr><td colspan="3">Consideration of code-related criteria (characteristics, QA, etc.) and administrative criteria</td></tr>
<tr><td rowspan="8">Model Use Documentation</td><td rowspan="3">Model Parameterization</td><td colspan="2">Boundary conditions</td></tr>
<tr><td colspan="2">Data sources, methods, pedigree</td></tr>
<tr><td colspan="2">Rationale for parameter estimation & selection</td></tr>
<tr><td rowspan="5">Evaluation of results</td><td rowspan="3">Uncertainty / Sensitivity Analysis</td><td>Dominant factors, parameters</td></tr>
<tr><td>Parameter/variable ranges</td></tr>
<tr><td>Magnitude & direction of parameter variability on model results</td></tr>
<tr><td>Model Assumptions Analysis</td><td>Magnitude & direction of effect on model results</td></tr>
<tr><td colspan="2">Limitations of Modeling & Results</td></tr>
<tr><td colspan="4">Conclusions, Recommendations</td></tr>
</table>

<table>
<tr><th colspan="3">State Compliance Elements for the Derivation of Soil Concentrations for Groundwater Protection, and the Selection and Use of Alternative Fate and Transport Models</th><th>State Requirement, Driver</th></tr>
<tr><td rowspan="4">Method Selection</td><td colspan="2">Purpose/Objectives</td><td>WAC 173-340-740/745; WAC 173-340-747</td></tr>
<tr><td colspan="2">Model (Type) selection; model attributes</td><td>none</td></tr>
<tr><td colspan="2">Method selection/documentation</td><td>WAC 173-340-747</td></tr>
<tr><td colspan="2">Code Selection: Demonstration of adequacy, QA/QC</td><td>WAC 173-340-702 (14, 15, 16)</td></tr>
<tr><td rowspan="2">Model Parameterization</td><td colspan="2">Specified parameters</td><td>WAC 173-340-747(8)(b)</td></tr>
<tr><td colspan="2">Other parameters</td><td>WAC 173-340-702 (14, 15, 16)</td></tr>
<tr><td rowspan="7">Documentation of model application and results</td><td colspan="2">Burden of proof (Asssumptions, RME, point of compliance/calculation)</td><td rowspan="7">WAC 173-340-702 (14, 15, 16)</td></tr>
<tr><td colspan="2">(New) Scientific Information</td></tr>
<tr><td rowspan="5">Adequacy and Quality of Information</td><td>Data/information acceptability, sources, references</td></tr>
<tr><td>Accepted methods</td></tr>
<tr><td>Assumptions, uncertaintes, conservatism/protectiveness</td></tr>
<tr><td>QA/QC, model limitations</td></tr>
</table>

The EPA guidance concerning the evaluation and selection of model parameters for use in ERMs stipulates consideration of the following criteria in the selection of model parameters:

1. Values that yield a "reasonable maximum exposure" (EPA/540/1-89/002)
2. "Best-estimate" values for the actual site conditions and/or properties (EPA 540-R-02-002).

Values that have the lowest uncertainty and/or greatest accuracy, therefore, contribute the least amount of uncertainty to the model results (EPA 540-R-02-002).

The selection of parameters in the context of these considerations also depends on the extent to which parameter values are known, or can be estimated. Parameter variability and data gaps are the two main sources of parameter uncertainty in the use of ERMs (EPA 2001). Where reasonable site data are available, the parameter estimation can be based on a measured distribution of parameter values. The parameter variability (due to inherent heterogeneity or diversity of the parameter) is typically manifested in the range of values. Where parameter data are sparse or data gaps exist, additional conservatism in parameter estimation may be warranted to account for the associated uncertainty.

Best-estimate values are generally values determined from the reasonable range of measured parameter variability and best represent the actual site conditions or properties. They are the most probable and least uncertain values, but they can also represent conservatively biased values where the range of parameter variability is not well defined. In the context of uncertainties due to parameter variability, the average values within the parameter ranges have the greatest accuracy and lowest uncertainty (PNNL-13091) and are, therefore, often considered the best-estimate values (NUREG/CR-6565).

Parameter estimation associated with data gaps or sparse data, however, may require assumptions regarding the selection and use of estimated or surrogate parameter values (EPA 1999). CERCLA guidance recommends the use of "best professional judgment" when data gaps are encountered in risk analysis (EPA/600/Z-92/001). Although best professional judgment is itself a source of uncertainty, EPA's position is that, "Expert opinion based on years of observation of similar circumstances usually carries more weight than anecdotal information" (EPA/600/Z-92/001).

2.7.2 Guidelines and Expectations for Addressing and Documenting Model Uncertainty, Assumptions, and Limitations

As noted in Figures 2-3 and Table 2-3, another primary expectation regarding the use of ERMs concerns the evaluation of model results, particularly in the context of uncertainty evaluations (EPA/540/1-89/002). The primary expectations of uncertainty evaluations prescribed in the Federal guidelines include the identification and analysis of uncertainties, summary/analysis of assumptions, and description of the modeling limitations, and these are summarized in Table 2-4.

Federal guidelines indicate that a common problem with modeling efforts is the lack of discussion and documentation dealing with uncertainties, including uncertainties in data, sensitivities, and assumptions (EPA 540-F-96/002). Environmental risk assessments, particularly in Superfund applications, focus on providing information necessary to justify action at a site and to select the best remedy for that site (EPA/540/1-89/002). The Federal guidelines indicate that the evaluation of model uncertainties is intended to gauge the extent to which the model results are useful or sufficient for assessing the risk at the site in order to make remedial action decisions. It is not intended to be a quantification of the accuracy of the model for the sake of accuracy alone. These guidelines state that it is more important to identify the key site-related variables and assumptions that contribute most to the uncertainty than it is to precisely quantify the degree of uncertainty in the risk assessment (EPA/540/1-89/002).

Table 2-4. Primary Expectations For Uncertainty Evaluations Associated with the Use of ERMs.

• Identification of uncertainty factors and parameters in the model to include the following: – The primary factors and parameters that dominate the risk and/or model results – The variables and values used in the risk characterization – Description of the selection rationale – The range of expected values (as appropriate) – Which variable have the greatest range and impact on the results – Justification for the use of values that may be less certain.
• Analysis of uncertainties (e.g., quantitative, semi-quantitative, or qualitative).
• Summary of the major assumptions in the modeling, the magnitude and direction of the effect on estimated risk and/or model results.
• Description of the limitations of the modeling.

2.7.2.1 Sources of Uncertainty

Consistency with requirements and expectations for the evaluation and documentation of model uncertainties requires understanding of the main sources of potential uncertainty in the model. Potential sources of uncertainty in ERMs can be divided into three categories (EPA 540/R-02-002):

- Model uncertainty: Uncertainty associated with the model structure/design and simplifying assumptions.
- Scenario and conceptual model uncertainty: Uncertainty associated with missing or incomplete information on the FEPs important for the model simulation of the intended system(s).
- Parameter uncertainty: Uncertainty in the estimates of input variable in a model.

Some of these sources of uncertainty can be quantified, while others (e.g., scenario uncertainty) are best addressed qualitatively (EPA/540/1-89/002).

Model uncertainties are associated with the model structure/design and simplifying assumptions. These uncertainties also include code-specific factors pertaining to the adequacy, benchmarking/calibrations, and QA/QC of the selected code.

Scenario and conceptual model uncertainties concern the uncertainties associated with the translation of qualitative conceptual model components into a quantitative mathematical model, which involves simplification of the system being modeled. A conceptualization of geologic stratigraphy, for example, may be represented in a mathematical model as a simplified, layered geology with discrete homogeneous layers. The validity of the conceptual model can be evaluated by comparing measurements made at the site to predictions from a mathematical model of the site. The conceptual model and/or the mathematical model may be modified as a result of new data or observations (PNNL-13091).

Parameter uncertainty refers to uncertainty or variability in parameter values and is generally the focus of most uncertainty analyses. Federal risk assessment guidance recommends general quantitative (statistical), semi-quantitative (sensitivity), or qualitative approaches for parameter uncertainty analyses (EPA/540/1-89/002). Sensitivity analyses are normally used to identify influential model input variables (EPA 1985, EPA 540-R-02-002). Sensitivity analyses can be used to develop bounds on the exposure or risk. Alternatively, the guidelines indicate that the most practical approach to characterizing parameter uncertainty is often the development of a quantitative or qualitative description of the uncertainty for each parameter and simply indicating the possible influence of these uncertainties on the final risk estimates (EPA/540/1-89/002).

2.7.2.2 Sensitivity Analyses

Federal guidelines recommend performing sensitivity analyses to indicate the magnitude of uncertainty associated with a model, especially when there is an absence of field data for model validation (EPA/540/1-89/002, EPA-SAB-06-009). Sensitivity analyses demonstrate the extent to which model results and risk assessment are affected by the variability within a plausible range of model parameter values. The design and results of sensitivity analyses are documented on a site-specific, model-specific basis.

The results of sensitivity analyses can be used to indicate the relative importance of parameter uncertainties to the model results, specifically in terms of the magnitude and direction of the change in the model results caused by the variability in the input parameter. The importance of parameter uncertainty is greatest when the value of the parameter is relatively uncertain and the model results are sensitive to the parameter's value, and the importance is lowest when either the model results are insensitive to the parameter value or the value of the parameter is well known (PNNL-13091). These relationships can be defined as the product of: the sensitivity of the model result to the parameter value and the uncertainty in the parameter (as measured by its coefficient of variation):

Importance of parameter to uncertainty in model result	$\propto$	Sensitivity of model results to parameter value	$\times$	Uncertainty in parameter value

These relationships can be useful in assessing the importance of modeling parameters when there is information available on the statistical uncertainty, the model sensitivity to parameter values and/or ranges, or both.

Table 2-5 is a generic example from an uncertainty analysis for a vadose zone hydrogeologic modeling case, showing the relative importance of parameter uncertainties to the model results. Evaluation of uncertainty magnitude serves to prioritize the relative importance of vadose zone modeling parameters and their uncertainties to the model results. Similar evaluations and summaries can be customized for site-specific analyses, accompanied by the technical basis and rationale to justify or prioritize the relative importance of the parameters.

2.7.2.3 Assumptions Analysis

Federal guidelines underscore the importance of identifying key model assumptions (e.g., linearity, heterogeneity/homogeneity, steady-state conditions, and equilibrium) and their potential impact. However, there is as yet no specific guidance on the conduct of assumptions analyses. The only expectations presented in EPA/600/Z-92/001 refer to identifying the key model assumptions and discussing their potential impacts on the model results. Most assumptions result from the simplification of the representation of the FEPs in the model and/or assumptions associated with parameter selection. The evaluation provides a qualitative estimate of the relative conservatism of the assumptions in terms of the direction and magnitude of change in the model results caused by the inclusion of the assumption.

Table 2-5. Generalized Example of Portraying the Relative Importance of Vadose Zone Hydrogeologic Modeling Parameters in Uncertainty Analyses (from PNNL-13091).

		Uncertainty Due to Variability and/or Lack of Knowledge		
		Low	**Medium**	**High**
Model Sensitivity	**High**	UZ thickness		Distribution coefficients Net infiltration rate
	Medium	Effective porosity Bulk density	Darcy velocity Unsaturated water content	SZ exposure parameters SZ hydraulic conductivity
	Low	Porosity	Soil-type exponent Field capacity	UZ saturated hydraulic conductivity Dispersivity

UZ = unsaturated zone
SZ = saturated zone

2.7.2.4 Evaluation of Model Limitations

The evaluation of model limitations must consider two types of limitations: (1) limitations associated with the model, and (2) limitations associated with the applicability of the model results. Model limitations primarily depend on the model capabilities, model design assumption, model input parameters, and model/code ability to represent simulations of complex combinations of dynamic FEPs. Limitations associated with the applicability of the model results concern the extent to which the results are relevant and applicable for different purposes and objectives, or different conditions, parameters, or assumptions.

Federal guidelines (EPA 540/F-96/002) state that proper documentation of model results should also address and answer the following questions that are related to model limitations:

1. Do the objectives of the simulation correspond to the decision-making needs?
2. Is the modeler's conceptual approach consistent with the site's physical and chemical processes?
3. Can the model satisfy all the components in the conceptual model, and will it provide the results necessary to satisfy the study's objectives?
4. Are there sufficient data to characterize the site?
5. Are the model's data, initial conditions, and boundary conditions identified and consistent with geology and hydrology?
6. Are the conclusions consistent with the degree of uncertainty or sensitivity ascribed to the model study, and do these conclusions satisfy the modeler's original objectives?

These six questions align with the model documentation elements recommended in the EPA's CREM documentation guidelines summarized in Table 2-2 (CREM 2003).

2.8 STATE REQUIREMENTS

State regulations also identify pathway-specific models for use in establishing "protectiveness" for RCRA sites and/or as ARARs for CERCLA sites. The Washington State regulation most pertinent to risk-based applications involving the assessment of soil (vadose zone) contaminant levels protective of groundwater is WAC 173-340-747, "Deriving Soil Concentrations for Ground Water Protection." The state regulations concerning soil cleanup standards for unrestricted land use (WAC 173-340-740), and for industrial properties (WAC 173-340-745), both direct users to the WAC 173-340-747 for the determination of soil levels:

> *"...that will not cause contamination of ground water at levels which exceed ground water cleanup levels established under WAC 173-340-720 as determined using the methods described in WAC 173-340-747."*

Factors specifically identified in CERCLA guidance (40 CFR 300.400) for the consideration to whether a requirement is appropriate include the following:

- Goals and objectives of the remedial actions at the site
- Purpose of the requirement
- Whether the use of the requirement at the site is consistent with the purpose
- Physical characteristics of the site.

The primary requirements associated with the WAC 173-340-747 are (1) selection and use of one of seven specified "methods, for "deriving soil concentrations for groundwater protection"; and (2) additional conditional requirements associated with the selection of one of the specified methods. A summary of the state requirements associated with the WAC 173-340-747 is illustrated schematically in Figure 2-4. The following is a brief description of these requirements and the conditions and expectations associated with them.

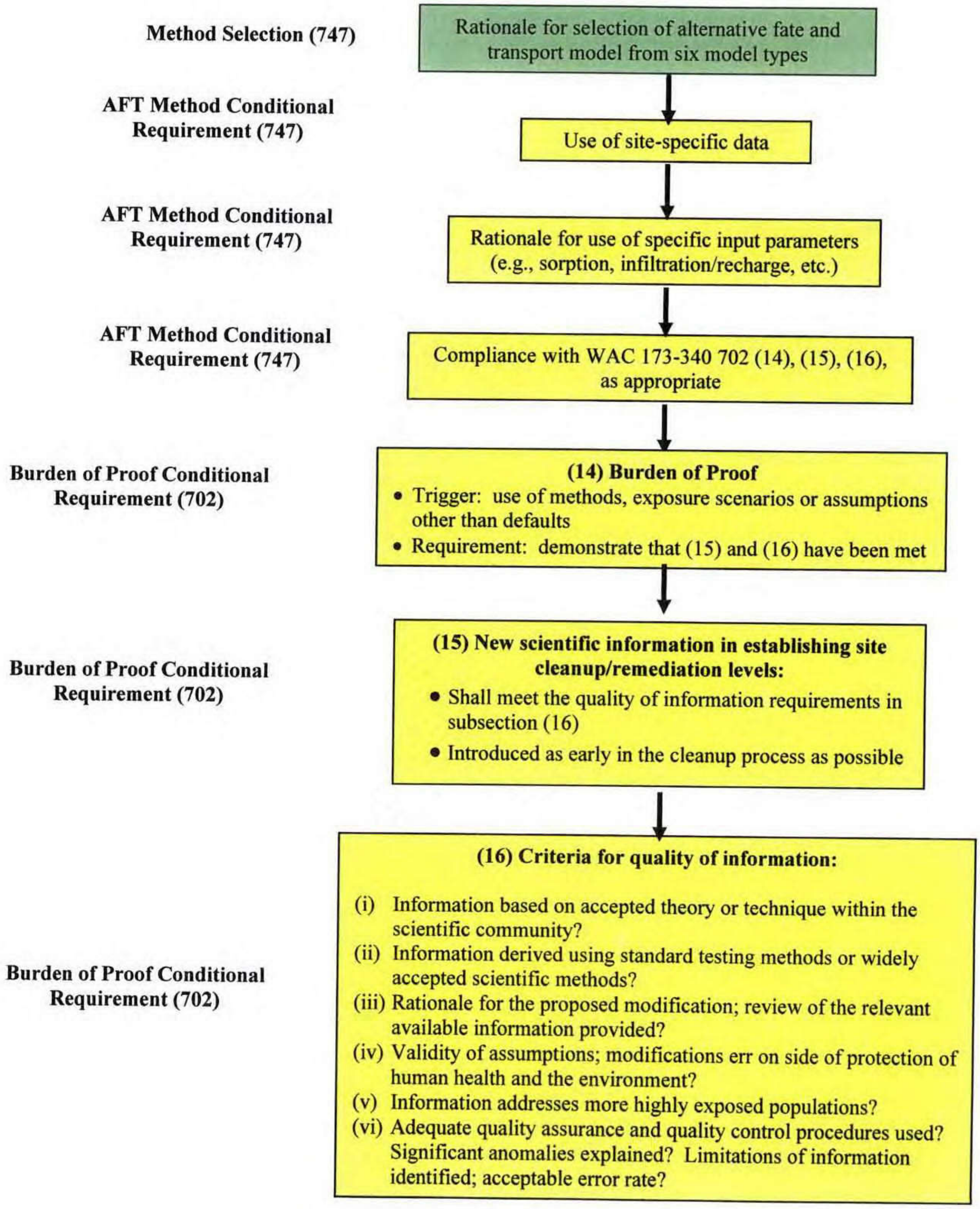
2.8.1 Method Selection

The WAC regulations address the need for a scientifically valid method for determining cleanup levels protective of groundwater. WAC 173-340-747(3), "Overview of Methods," provides an overview of the identified methods that may be used for deriving soil concentrations, and that meet the criteria specified in WAC 173-340-747(2), "General Requirements". WAC 173-340-747(3) states that:

> *"Certain methods are tailored for particular types of hazardous substances or sites. Certain methods are more complex than others and certain methods require the use of site-specific data. The specific requirements for deriving a soil concentration under a particular method may also depend on the hazardous substance."*

Figure 2-4. WAC 173-340-747 Requirements for Deriving Soil Concentrations for Groundwater Protection Associated with the Selection of Alternative Fate and Transport Modeling.

The notations (747) and (702) refer to requirements specific to WAC 173-340-74 and WAC 173-340-702.



WAC 173-340-747(2), "General Requirements," stipulates that one of seven methods specified in WAC 173-340-747(4) through (10) shall be used to determine the soil concentration that will not cause an exceedance of the groundwater cleanup level established under WAC 173-340-720, "Ground Water Cleanup Standards." The following are the methods identified in WAC 173-340-747(4) through (10):

1. Fixed parameter three-phase partitioning model (WAC 173-340-747[3][a] and [4])
2. Variable parameter three-phase partitioning model (WAC 173-340-747[3][b] and [5])
3. Four-phase partitioning model (WAC 173-340-747[3][c] and [6])
4. Leaching tests (WAC 173-340-747[3][d] and [7])
5. Alternative fate and transport model (WAC 173-340-747[3][e] and [8])
6. Empirical demonstration (WAC 173-340-747[3][f] and [9])
7. Residual saturation (WAC 173-340-747[3][g] and [10]).

The WAC 173-340-747 (3) requirements contain no specific provisions or criteria concerning method or code selection. However, the conditional requirements invoked by the selection of specific methods include requirements concerning the adequacy and quality of information.

2.8.2 Conditional Requirements

Additional conditional requirements are associated with the selection of each of the methods identified in WAC 173-340-747(4) through (10). The conditional requirements associated with the selection of the "alternative fate and transport models" method appear to involve the full range of conditional requirements identified in WAC 173-340-747 for all of the methods listed. The remainder of this section, therefore, addresses and describes the conditional requirements associated with the selection of the "alternative fate and transport models" method.

The conditional requirements associated with the selection of the "alternative fate and transport models" method include the following:

- Use of site-specific data

- Documentation concerning the technical basis and rationale for the selection of values for several specific model parameters

- Additional evaluation criteria requirements involving documentation of the technical basis and rationale concerning the proposed fate and transport models, input parameters, and model assumptions (WAC 173-340-702[14], [15], and [16]).

The conditional requirements associated with the selection of the "alternative fate and transport models" method are described in WAC 173-340-747(8) for "...the use of fate and transport models other than those specified in WAC 173-340-747(4) through (6)..." that are used for establishing soil concentrations. As specified in WAC 173-340-747(8):

> *"These alternative models may be used to establish a soil concentration for any hazardous substance... Site-specific data are required for use of these models... "Proposed fate and transport model, input parameters, and assumptions shall comply with WAC 173-340-702 (14), (15), and (16)."*

The selection of the "alternative fate and transport models" method in accordance with WAC 173-340-747(8) also specifies that, "When using alternative models, chemical portioning and advective flow may be coupled with other processes to predict contaminant fate and transport...", with the provision that conditions are met concerning the selection and use of a number of specific parameters. The following are the specific parameters associated with this requirement:

- Sorption (deriving Kd from site data)
- Vapor-phase partitioning
- Natural biodegradation
- Dispersion
- Decaying source
- Dilution
- Infiltration (site-specific).

The conditions for consistency with this requirement are inferred to involve documentation of the regulatory conditions for consistency, identification of the parameter values selected for use in the model, and the technical basis and/or rationale for the derivation and/or selection of the parameter value(s).

The conditional "evaluation criteria" states that consistency with the "burden of proof" requirements (found in WAC 173-340-702[14], [15], and [16] concerning the method/model, model parameter values, and/or assumptions) is also required for the selection and use of the "alternative fate and transport models" method. These "burden of proof" conditional requirements are invoked as follows:

> *"For any person responsible for undertaking a cleanup action ...who proposes to:*
>
> - *Use a reasonable maximum exposure scenario other than the default provided for each medium*
> - *Use assumptions other than the default values provided for in this chapter*
> - *Establish a cleanup level under Method C, or*
> - *Use a conditional point of compliance."*

WAC 173-340-702(14) "Burden of Proof" requirements involve *"...demonstrating to the department that requirements in this chapter [WAC 173-340-702(14), (15), and (16)] have been met to ensure protection of human health and the environment."*

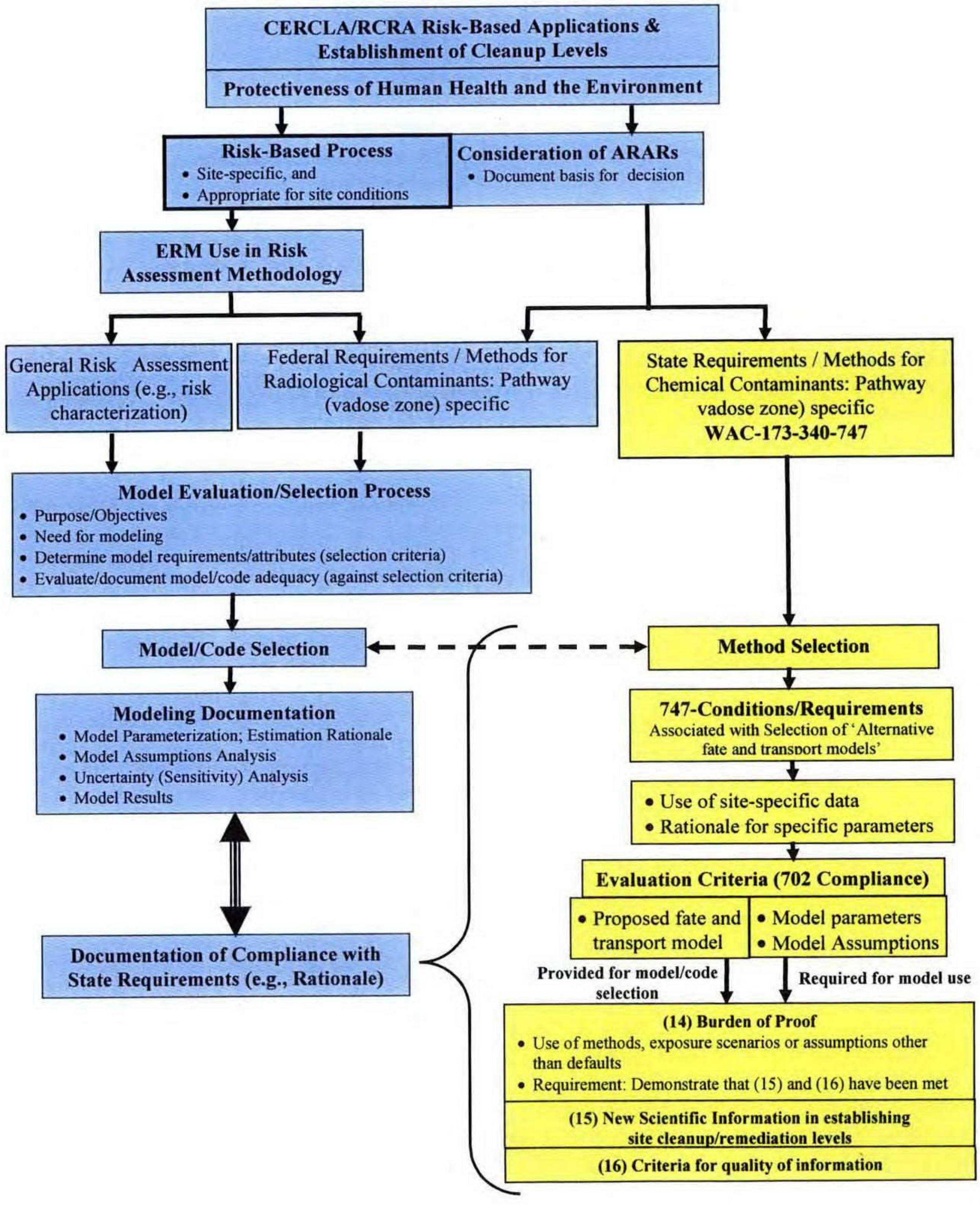
These requirements primarily concern the appropriateness of the data and information used in the model and the "burden of proof" to demonstrate the adequacy of the science and quality of information concerning model input parameters and assumptions. The elements of these "burden of proof" requirements (WAC 173-340-702[14, [15], and [16]) are summarized in Figure 2-4. The WAC 173-340-747 and WAC 173-340-702 requirements are also summarized in Table 2-3.

2.9 COMBINING THE STATE REGULATIONS AND FEDERAL GUIDANCE FOR THE SELECTION AND USE OF ENVIRONMENTAL REGULATORY MODELS

The state and Federal regulations and guidelines pertaining to the selection and use of ERMs each have specific requirements but, overall, most of the requirements and expectations are largely comparable or can be shown to be essentially equivalent. The alignment of the Federal guidelines and state requirements concerning the selection and use of ERMs shown in Figure 2-5 illustrates the general correspondence and comparability of the requirements and consistency criteria. The portions of Figure 2-5 highlighted in ***blue*** refer to the aspects of the framework pertaining to the model and code selection process recommended by Federal guidelines. The portions of Figure 2-5 highlighted in ***yellow*** refer to the parts of the framework that pertain to the state method selection requirements and attendant conditional requirements. The vertical organization of the figure is intended to indicate the logical sequence of these requirements, both in the Federal and state segments.

Figure 2-5. Framework for Identifying the Processes and Requirements for Demonstrating Consistency with Federal and Corresponding State Requirements for the Use of Fate and Transport Modeling for the Derivation of Soil Remedial Action Goal Values.

Blue highlighted sections denote Federal requirements; Yellow highlighted sections denote State requirements. Horizontal alignment of Federal and state requirements illustrate corresponding elements and/or processes.



In this context, the state requirements associated with method/model selection, the modeling objectives, and application must be consistent with the risk assessment process and methodology. This, in turn, implies consistency with Federal guidelines for selection and use of environmental models that are relevant and appropriate to support environmental risk assessment applications. Thus, the technical basis for the demonstration of consistency with the fundamental requirement of both the Federal and state regulations (i.e., protectiveness) requires the use of appropriate risk-based methods and processes.

The logic flow in Figure 2-5 illustrates the role of ERMs for risk-based applications (e.g., risk characterization) where such methods are valuable or necessary. From this point forward (downward in the figure), the main elements of the Federal processes concerning method/model and code selection, model use, and model documentation can be reasonably well aligned with the WAC 173-340-747 and WAC 173-340-702 state requirements. The framework shown in Figure 2-5 indicates that the pertinent state and Federal requirements and expectations, although structured differently, are largely comparable or equivalent and can be aligned reasonably well. The following discussion demonstrates the comparability of the individual state requirements for consistency with corresponding Federal counterparts.

The state's conditional requirements concerning the use of site-specific data, model parameterization, and the "burden of proof" requirements concerning method/models, input parameters, and assumptions are effectively consistent with elements of the Federal guidelines for the selection and use of ERMs. The state requirements concerning the use of site-specific data correspond to the Federal requirements to use site-specific information in the conduct of risk-based assessments. Finally, the state conditional requirements regarding model parameter selection are consistent with Federal guidelines concerning the identification and documentation of the basis for the parameter estimates used to represent the system FEPs from the conceptual site model.

Other comparable aspects of the "burden of proof" requirements in WAC 173-340-702(14), (15), and (16) also have corresponding counterparts in the Federal guidelines. The primary emphasis of WAC 173-340-702(14) is to demonstrate that protection of human health and the environment has been ensured, which is comparable to the Federal guidance to provide documentation of the basis and rationale for the model to ensure protection of human health and the environment. The WAC 173-340-702(15) requirement concerns the use and availability of new scientific information and is consistent with the Federal guideline requirements to document the basis and rationale for parameter estimates, model complexity, and code selection. WAC 173-340-702(16) contains criteria for the quality of information, which is relevant to model, method, and code selection; assumptions; and the technical basis for the selection of model parameter values. The requirements concerning model uncertainties, assumptions, and limitations in WAC 173-340-702(16) correspond to requirements in the Federal guidelines for the analysis of model uncertainties, assumptions, and limitations of the model and model results.

A more detailed side-by-side comparison of the Federal and state requirements and elements associated with the selection and use of ERMs for vadose zone modeling is shown in Table 2-3. The alignment and comparability of the main elements of method/model/code selection and model use documentation in the Federal and state requirements and guidelines are clearly indicated in Table 2-3. This comparison serves to illustrate that the Federal regulations and guidelines for the selection and use of ERMs are comparable and consistent with those in the state regulations for the derivation of soil concentrations for groundwater protection.

2.10 SUMMARY OF REGULATORY REQUIREMENTS AND GUIDELINES

The use of an ERM for characterization of impacts/risk to groundwater at the Hanford Site involves observance of, and consistency with, pertinent Federal and state requirements and guidelines. Federal regulations and guidelines concerning the selection and use stem from the recognized use of ERMs in determining protection of human health and the environment. The Federal regulations and guidelines identify processes for the method/model/code selection and documentation requirements associated with the use of ERMs. The identification of these requirements and guidelines provide a basis for understanding the expectations and criteria necessary for technically validity and consistency with the Federal requirements and expectations. Documentation of the technical basis and rationale associated with the various elements of the method/model and code selection processes and model use are necessary to meet and comply with these expectations and requirements. The documentation elements associated with model and code selection processes include descriptions of the modeling objective, the site/system conceptual model, the FEPs to be simulated, and the attributes and criteria used in the selection processes. The documentation elements associated with model use include the technical basis and rationale for model parameterization, model results, and analyses of model uncertainties, assumptions, and limitations.

The state requirement most relevant to the use of vadose zone modeling for risk-based applications is WAC 173-340-747 and the conditional requirements associated with certain subsections of WAC 173-340-702.

There is a comparability of the elements of Federal and state requirements and guidelines pertaining to the use of ERMs for the assessment of impacts/risk to groundwater from vadose zone contaminants at Hanford. Based on the overall comparability of these elements that serve as criteria, it is indicated that demonstration of consistency with the Federal guideline requirements addresses all of the requirements and expectations associated with the state regulations and can be regarded as appropriate and acceptable for the demonstration of consistency with the requirements in the state regulations.

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3.0 RATIONALE FOR THE SELECTION AND USE OF ENVIRONMENTAL REGULATORY MODELS FOR VADOSE ZONE MODELING AT THE HANFORD SITE

Consistency with the Federal and state regulations and guidelines for the selection and use of ERMs typically requires information related to site-specific modeling applications. The ERM use for risk characterization applications associated with the vadose zone system at the Hanford Site involves a purpose and objectives common to essentially all potential applications: evaluation of the impact to groundwater from vadose zone contamination. The primary characteristics and conditions of the vadose zone system are also largely common for much of Hanford. Most vadose modeling applications at Hanford have (1) common purpose and objectives, (2) largely common conceptual model and conceptual model components, and (3) a largely common group of principal FEPs.

3.1 DESCRIPTION OF RISK CHARACTERIZATION METHODS AND MODELS

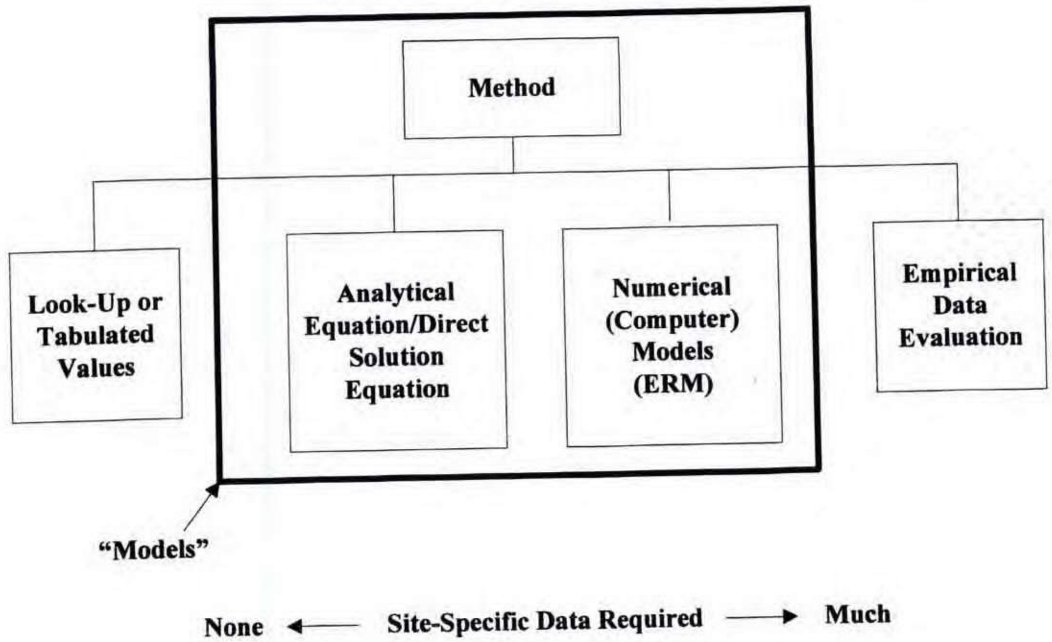
Risk characterization computation and solution methods range from simple analytical/algebraic equations with direct and exact solutions, to complex systems of (differential) equations that require the use of computer-based programs (i.e., codes) to solve. In general, the amount of site-specific data required for the selected computation and solution method depends on the complexity of the method. Figure 3-1 depicts the range of methods most commonly considered for the risk characterization step of the risk assessment process.

The simplest method to estimate soil contaminant levels that are protective of groundwater is the use of look-up or tabulated values typically determined from generalized assumptions, background levels, or minimum laboratory detection limits. This method requires essentially no site-specific data or information and no site-specific calculations of risk. The levels are protective and are also typically very conservative because they generally do not account for site-specific conditions or processes. Empirical data evaluation represents the other end of the spectrum of risk characterization methods. Use of this method requires sufficient waste site data that support certain/specific "protectiveness" conclusions on the basis of certain/specific conditions/trends exhibited by the data. The method does not involve site-specific calculations of risk levels because the conclusions are based solely on interpretation of the data.

The remaining two methods involve computation and solution methods that require varying amounts and quality of site-specific data. These methods use predictive modeling to calculate site-specific risk levels on the basis of the available data.

The risk characterization methods most appropriate for the protection of groundwater from contamination in the vadose zone at Hanford involve modeling. Modeling is the only "method" that involves predictive calculations for the levels of exposure point contamination and associated risk. In this context, the terms "method" and (mathematical) "model" are often used synonymously. The terms refer to any computational approach designed and appropriate for the purpose of risk characterization of the system or systems of interest (e.g., natural systems). Both simple and complex computation methods can be considered to be "models" because both use mathematical equations to represent or approximate natural systems. Further explanation regarding the uses and meanings of the terms "method" and "model" is presented in Section 3.5.

Figure 3-1. Illustration of the Relationship Between Method and Model Types in the Context of Environmental Regulatory Model Use. The boxed areas denote the methods that require the use of model for risk characterization applications.

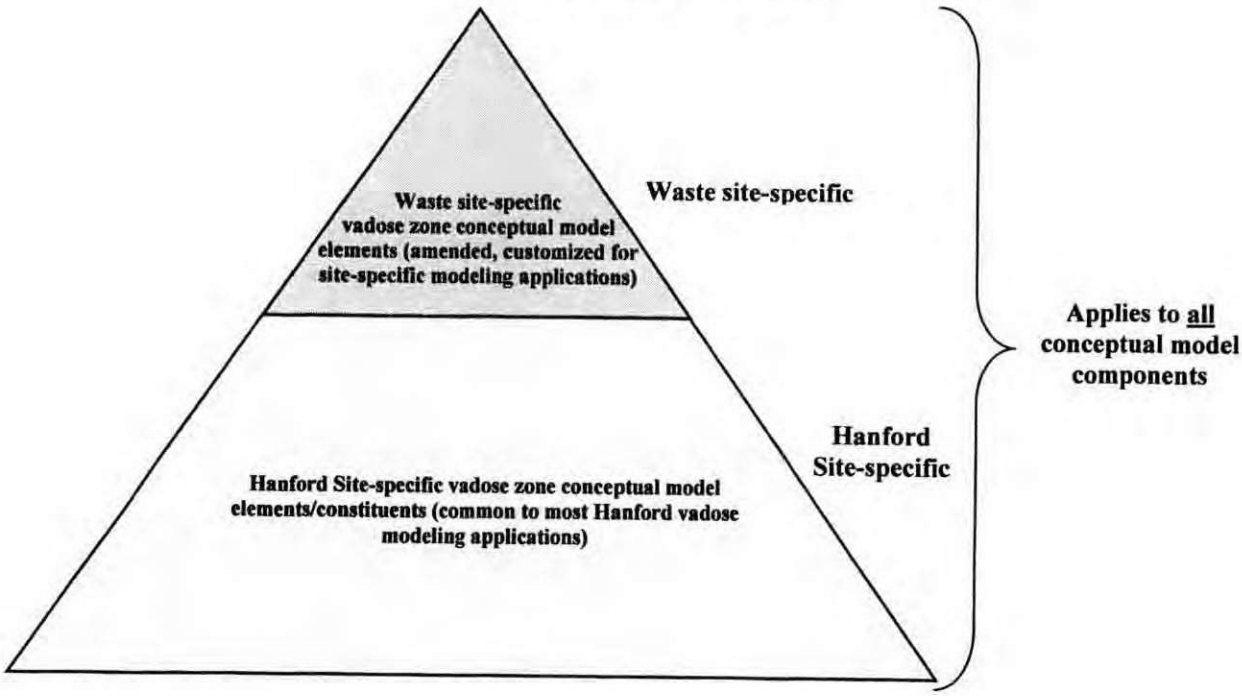


3.2 IMPLICATIONS OF VADOSE ZONE SYSTEM COMMONALITIES FOR MODEL TYPE SELECTION

The extent to which the elements of the ERM model and code selection processes can be applied and documented here is based on the commonalities in the characteristics, conditions, and processes of the vadose zone system on the regional scale of the Hanford Site. Consistency with the Federal model type and code selection processes requires a thorough documentation of the technical basis and rationale. An integral element of this documentation is a description of the aspects of the conceptual model and conceptual model components that are common to the vadose zone system. This Hanford Site-specific "basic" conceptual model provides the information necessary to identify selection of a model type and code capable of meeting the objectives of vadose zone modeling. The "basic" vadose zone conceptual model provides a basis for the development of waste site-specific conceptual models, which incorporates waste site-specific information in the manner illustrated in Figure 3-2.

The application of the Federal guidelines for the selection of an ERM type appropriate for evaluations concerning impacts/risk to groundwater from contaminants in Hanford vadose zone soils is documented in Section 4.0.

Figure 3-2. Relationship of the Hanford Site-Specific "Basic" Vadose Zone Conceptual Model to Waste Site-Specific Conceptual Models.



3.3 IMPLICATIONS OF VADOSE ZONE SYSTEM COMMONALITIES FOR CODE SELECTION

The commonalities in the vadose zone system also impact the evaluation and selection of codes that are capable of implementing the model type appropriate for most Hanford vadose zone modeling. The common model attributes and criteria must result in the identification of codes that are also applicable and acceptable for most Hanford vadose zone modeling applications. Thus, documentation of the code evaluation process, conducted in accordance with the Federal guidelines, also requires only a single, thorough description of the technical basis and rationale for the evaluation of candidate codes. Demonstration of the use of the Federal guidelines regarding the code selection for the model type appropriate for most vadose zone modeling at the Hanford Site is presented in Section 6.0. This documentation describes the evaluation process, presents an evaluation of the STOMP code in accordance with the process, and validates the use as an appropriate model code for vadose zone modeling at Hanford.

3.4 IMPLICATIONS OF VADOSE ZONE SYSTEM COMMONALITIES FOR MODEL USE AND ASSOCIATED DOCUMENTATION

Site- and application-specific information is also required for complete evaluations and documentation of the model use elements. However, there are also many aspects of model use that are common to most vadose zone modeling at Hanford. As described in Section 2.7 and in Table 2-2, these model use elements primarily include model parameters, model uncertainties, model assumptions, and model limitations.

The description of the common aspects of model use for most Hanford vadose zone modeling applications and the extent to which they are generally relevant and applicable to these applications are presented in Section 5.0. Documentation concerning the relationship of these commonalities to the overall model use documentation requirements is relevant to the evaluation of the impact of uncertainties, model assumptions, and model limitations. This documentation provides a basis and framework for consistency with the Federal and state requirements concerning model parameterization, as well as the evaluation of model uncertainties, assumptions, and limitations.

3.5 RISK CHARACTERIZATION METHODS AND MODELS TERMINOLOGY

It is important to recognize that the terms "method" and "model" referred to here and in subsequent sections are often used interchangeably in the context of ERMs, but the terms can have somewhat different meanings in the state and Federal regulations and guidelines. This section provides a clarification of these and related terms and describes the context of their use. The general relationship between "methods" and "models" is illustrated in Figure 3-1. The "method" generally refers to the approach used to quantitatively identify or assess risk levels and/or levels of protectiveness.

Much of the EPA guidance concerning method selection and model selection refer to "models" only in the context of computer-based methods. They consider simple analytical/algebraic-type equations as a distinct method rather than a model type. However, the terms "method" and "model" are used interchangeably in WAC 173-340-747. Therefore, the terms "method" and "model" are largely used interchangeably in this document to refer to any appropriate risk characterization computational method (simple or complex "model"). In this document, the terms "method selection" and "model selection" both refer to the decision about whether to use simple analytical/algebraic equations or complex systems of equations that require computer programs (i.e., codes) to solve. In this context, method/model selection focuses primarily on the necessary level of complexity required for adequate representation of the natural system for the purpose of risk characterization. The term "environmental regulatory model (ERM)" in this document refers to a specific computational method (computer-based model) that is selected and developed for the purpose of risk characterization in accordance with state and Federal requirements and guidelines. "Vadose zone modeling" in this document refers collectively to ERMs developed for the purposes of risk characterization for the protection of groundwater pathway (vadose zone) at Hanford.

4.0 APPLICATION OF THE MODEL SELECTION PROCESS FOR THE HANFORD VADOSE ZONE SYSTEM: CONCEPTUAL MODEL; FEATURES, EVENTS, AND PROCESSES; AND IDENTIFICATION OF MODEL ATTRIBUTES

The selection of an appropriate model type (as described in Section 2.5) for assessing the impact/risk to groundwater from contaminants in Hanford vadose zone involves the following steps:

1. Identify the problem and define the objectives and regulatory purpose of the modeling.
2. Develop a conceptual model and conceptual model components.
3. Determine principal FEPs to be modeled.
4. Identify other factors and requirements to be considered as required model attributes and selection criteria.
5. Select an appropriate model type:
    a. Evaluate candidate methods/models possessing the required attributes for their ability to meet the model criteria.
    b. Select the appropriate ERM model type that possesses the required model attributes and is capable of meeting the modeling objectives.

The following sections use these steps in describing the manner in which the model selection processes have been implemented.

4.1 PROBLEM IDENTIFICATION: PURPOSE AND OBJECTIVES OF VADOSE ZONE MODELING AT THE HANFORD SITE

As described in Section 1.0, the primary purpose of this document is to address the need to select a technically appropriate ERM that meets regulatory requirements to determine the potential risk (impact) to groundwater from vadose zone contaminants at the Hanford Site. This purpose also involves the need to understand the technical and regulatory requirements for the technical adequacy of the risk assessment, and to attain consistency with the requirements and intent of the Federal and state regulations and guidelines for ERM selection and use.

The need for vadose zone modeling at Hanford is based on the requirement for evaluation of risk associated with the protection of groundwater pathway from vadose zone contamination. In accordance with EPA guidance on risk assessment (EPA/540/1-89/002), risk assessments performed for CERCLA are required to evaluate risks associated with all relevant pathways. This pathway often yields the lowest soil cleanup levels among the relevant pathways for protection of human health and the environment. It is, therefore, important that the selection and use of the appropriate ERM model type is technically justified and consistent with the requirements and intent of the pertinent Federal and state regulations and guidelines.

After defining the purpose and objectives of the ERM, the model selection process requires the development of a site conceptual model, identification of the conceptual model components, and determination of the FEPs. The conceptual model, conceptual model components, and FEPs are also used as a basis for the identification of model attributes, criteria, which are then used in the selection of an

ERM model type and computer code that are appropriate for most vadose zone modeling needs at Hanford.

4.2 CONCEPTUAL MODEL FOR HANFORD SITE VADOSE ZONE SYSTEM

The general conceptual model for the Hanford vadose zone system focuses on the characteristics, conditions, and associated FEPs that are largely common to Hanford vadose zone conceptual models. The Hanford Site-specific conceptual model provides the fundamental information necessary to identify the criteria for selecting the most appropriate model type and code.

The conceptual model for the vadose zone to groundwater (protection of groundwater) pathway at Hanford is based on the basic nature, characteristics, and behavior of the vadose zone system on a regional scale. Many aspects of the conceptual model of the vadose zone to groundwater pathway are largely common for most vadose zone risk characterization model applications, especially for the Central Plateau where the vadose zone is the thickest. These aspects include the general site conditions, the dominant transport mechanisms, and the driving forces and related factors. Many of the FEPs in the conceptual model components pertain to regional characteristics and conditions that are common to the vadose zone system in general. Therefore, this conceptual model can serve as template for both regional and OU/waste site scale models.

The conceptual model framework for the Hanford vadose zone system can be divided into key conceptual model components, which include descriptions of the subsystems and associated FEPs that are important for description of the vadose system as a whole. The key conceptual model components that are common Hanford vadose zone conceptual models include the following:

- Model domain and boundary conditions
- Geologic setting
- Source term
- Groundwater domain
- Hydrogeology and fluid transport
- Recharge
- Geochemistry.

These conceptual model components are consistent with those identified in EPA guidelines for the evaluation of the protection of groundwater pathway (EPA 402-R-94-012, OSWER Directive 9200.4-18, HNF-5294). The principal FEPs associated with these conceptual model components include the following:

- A relatively thick vadose zone composed of predominantly similar sediments (geologic setting conceptual model component)

- A semi-arid region (recharge conceptual model component) and an underlying unconfined aquifer (groundwater domain conceptual model component)

- A relatively limited number of contaminants of concern (COCs) in the vadose zone soils (source term) that have potential impacts to groundwater.

The key conceptual model components listed above, as well as the FEPs associated with them, are discussed in the following subsections. The discussion includes the rationale and basis for each of the conceptual model components. This Hanford Site-specific conceptual model for the vadose zone system incorporates key conceptual model components and FEPs and can also include information such as typical parameter types, parameter ranges, and sources of data (e.g., Hanford Site databases). This conceptual model can be amended with waste site-specific conceptual model component information (e.g., source term, geologic units, hydrogeologic properties, site-specific recharge, and local groundwater conditions). As such, this conceptual model also provides a common technical basis and rationale for identification of the attributes and criteria used for selection of an ERM model type and code. It also provides for consistency in the use of the vadose zone models for the various site-specific applications (see Figure 3-2).

4.2.1 Model Domain and Boundary Conceptual Model Component

4.2.1.1 Rationale and Basis

Model domain and boundary conditions define the physical extent and constraints on the flow and transport simulated at the boundaries of the model domain, respectively. Boundary conditions are assigned to approximate the chemical and hydraulic characteristics of the model at the extent of the model domain because they are necessary to solve flow and transport model equations. For risk assessment purposes at Hanford, the model domain for simulations of flow and transport in the vadose zone is commonly represented numerically as a two-dimensional, vertical cross-section aligned with the direction of groundwater flow. Aligning the vertical cross-section with the direction of groundwater flow allows contaminant concentrations to be calculated downgradient of the waste site(s). The following is a summary of the model domain and boundary condition requirements for vadose zone modeling at Hanford:

- Model domain (length, width, height, node spacing, and depth to groundwater)
- Waste site dimensions
- Grid size (horizontal and vertical node spacing, and total number of nodes)
- Boundary conditions (flow and transport assigned to the top or ground surface, sides, and bottom of the model domain).

4.2.1.2 Assumptions

Boundary conditions are prescribed input values and form one basis of the solution of the numerical model equations. Because boundary conditions must be assumed, boundary conditions are typically established where the domain boundary is reasonably well defined or far enough away to minimize interference with the solution of the numerical model equations in the area of interest. In vadose zone models, boundary conditions must be defined for flow and transport at the top, sides, and bottom of the model domain. Boundary conditions applied at the top boundary, representing ground surface, vary spatially and temporally depending on (1) site conditions, (2) location and physical dimensions of the waste site, (3) time of waste operations, and (4) surface remedy. Boundary conditions at the sides of the model domain, located far enough away to avoid interfering with the solution in the area of interest (assuming that they do not intersect a prominent geologic feature beforehand), are usually assumed to be "no flow" in the vadose zone and "constant head" or prescribed flux in the saturated zone. In the event that the boundary conditions do intersect a prominent geologic feature, the boundary conditions are established in accordance with the feature. The bottom boundary of the model in groundwater is usually defined as a vertical no-flow condition.

4.2.1.3 Features, Events, and Processes

Because the model domain and boundary conditions establish the framework for the numerical model, their development typically affects the integrity of the solution of the numerical model. For this reason, they are located or prescribed to minimize interference with the solution of the numerical model equations in the area of interest. The model domain and boundary conditions incorporate those FEPs that can limit the model domain or impact the approximations of the chemical and hydraulic characteristics of the model at the boundaries.

4.2.1.4 Impact on Results

Models are constructed with the intent that the model domain and boundary conditions exert as little influence on the solution of the model equations as possible, except where the boundary conditions are defined on the basis of available data and information.

4.2.2 Geologic Setting Conceptual Model Component

4.2.2.1 Rationale and Basis

The geologic setting conceptual model component contains information on Hanford Site geologic units, their spatial relationship to one another and groundwater, physical characteristics, and structures.

The geologic setting is fundamental to the conceptual model and integral in the assessment of risk associated with the vadose zone and groundwater processes at the Hanford Site because of the unique geologic province, the Channeled Scablands (Bretz, 1928, 1969; RHO-ST-23; RHO-BWI-ST-14; Baker et al. 1991; DOE/RL-92-24). Characteristic features of the Channeled Scablands geographic province include the extreme erosional scouring (channels) associated with the Ice Age cataclysmic (Missoula) floods (DOE/RL-92-23) and the attendant deposition of this erosional material elsewhere within the province. These flood deposits that comprise the Hanford vadose zone extend to over 91.4 m (300 ft) thick and are composed predominately of a series of clastic sediments. Many of the hydrogeologic properties and parameters associated with fate and transport modeling reflect their geologic environment and are strongly influenced by other related processes, including the geochemical, recharge, and hydrologic transport conceptual model components.

The Hanford Site geology, particularly the subsurface geology, has been extensively studied, characterized, and documented (e.g., Newcomb et al. 1972, RHO-ST-23, Fecht et al. 1987, WHC-SD-EN-TI-008, DOE/RL-2002-39, RPP-23748, and DOE 2005). Most of the information in these documents focuses on site-specific subsurface geology obtained from an extensive collection of well and borehole drilling data, sediment sampling and analysis, and geophysical logging. These data provide considerable information and insight into the lithology, stratigraphy, structure, hydrologic, and geochemical information. For the geologic setting conceptual model component, lithology, stratigraphy, and structure are the key features.

4.2.2.2 Features, Events, and Processes: Lithology, Stratigraphy, and Structure

The vadose zone at the Hanford Site consists of sediments from Holocene glaciofluvial to Miocene/Pliocene fluvial/ lacustrine deposits (e.g., DOE/RL-92-23, DOE/RL-96-61, and DOE/RL-98-48). These sediments range in thickness from less than 1 m (3.3 ft) along the Columbia River in the 100 and 300 Areas to more than 91.4 m (300 ft) on the Central Plateau in the center of the Hanford Site.

The general stratigraphy of the Hanford vadose zone consists of three main geologic formations (PNNL-14702a) including glaciofluvial deposits of the Pleistocene-Age (Hanford formation), fluvial and/or eolian deposits and paleosols of the Pliocene/Pleistocene Age (Cold Creek unit), and fluvial/lacustrine deposits of the Miocene/Pliocene Age (Ringold Formation). About 85% of the vadose zone sediments throughout the Hanford Site are the immature, poorly consolidated glaciofluvial clastic sediments of the Hanford formation deposited during the Ice Age cataclysmic floods (DOE/RL-92-23). The detailed stratigraphy varies significantly across the Central Plateau of the Hanford Site, which is a large-scale sedimentary flood bar. However, the general stratigraphy of the vadose zone and uppermost parts of aquifer on the scale of the Central Plateau is relatively similar overall in the context of a thick vadose zone over 91 m (300 ft) in places, composed predominately of poorly consolidated glaciofluvial clastic sediments of the Hanford formation, underlain by the Cold Creek unit (which is discontinuous and/or absent to the eastern part of the plateau), which is in turn underlain by the upper Ringold Formation. While the thickness of the different geologic layers varies across Hanford, the consistency in the sedimentary composition indicates that the generic features of the vadose zone can be described by a "basic" Hanford vadose zone system conceptual model. For site-specific applications, the geology conceptual model requires site-specific information describing and/or estimating unit thicknesses and composition.

4.2.2.3 Hanford Formation

Hanford formation sediments occur as a succession of alternating and discontinuous layers of high-energy, coarse-grained gravels to low-energy, sand silt deposits resulting in vertical and lateral variability. The variable physical characteristics of these sediments are primarily attributable to differences in the proportions of the constituent size fractions and sedimentary structures, which include size grading (vertically and laterally), cross-bedding, draping, and channeling with lateral variations in layer thicknesses.

Despite the physical heterogeneity of these sediments, there is consistency in the types of materials that dominate the finer-grained size fractions among these sedimentary facies (layers). One to two-thirds of the finer-grained size fractions consist of clastic basaltic material, along with variable proportions of quartz, feldspar, and other subordinate minerals (DOE/RL-92-23). On a regional scale, Hanford formation sediments are closely related in terms of their provenance, as well as basic sedimentary characteristics, and have been shown to comprise a single compositional population of sediments (DOE/RL-92-23).

4.2.2.4 Cold Creek Unit

The Cold Creek unit is one of the most significant lithologies affecting vadose zone transport in the 200 West Area and parts of the 200 East Area because it physically retards water transport and chemically retards moderately mobile contaminants. The Cold Creek sedimentary sequence overlies the older Ringold Formation and underlies cataclysmic flood deposits of the Hanford formation (DOE/RL-2002-39).

Cold Creek sediments consist of overbank eolian, calcic paleosol, mainstream alluvial, colluvial, and side stream alluvial deposits. These deposits occur as fine- to coarse-grained, laminated, massive layers; fine- to coarse-grained calcium-carbonate cemented layers; and coarse-grained, multi-lithic basaltic layers. The layers range in thickness from 1 m (3.3 ft) in the calcic paleosol facies in the southern portion of the 200 West Area to a 15-m (49.2-ft) sequence of layers north of the 200 West Area (DOE/RL-2002-39) and pinching out of the carbonate layers in the 200 East Area. The degree of cementation varies considerably within the Cold Creek unit and contains many weathering products (oxides and carbonates) that chemically react with transported wastes. Where it occurs as continuous layer, the indurated caliche represents a potentially substantial physical "barrier" to inhibit and/or divert the downward transport of liquids and contaminants to deeper levels in the vadose zone. Although discharge water from Hanford operations have been observed to have ponded on it, the degree of cementation varies considerably and can be fractured and/or laterally discontinuous.

Immediately overlying the carbonate-cemented layers of the Cold Creek unit are fine-grained, laminated, massive layers with high moisture-retention capacity and correspondingly low permeability that tend to retard the downward movement of moisture and contaminants. These fine-grained facies may also contain calcareous components. Recent studies confirm that the fine-grained Cold Creek sediments are highly sorptive for contaminants such as uranium and act to chemically retard migration (Qafoku et al. 2005).

4.2.2.5 Upper Ringold Formation

The Upper Ringold Formation is above groundwater in places where it comprises less than 10% of the volume of the vadose zone. These sediments lie below the Cold Creek unit (where present) or below the Hanford formation (where the Cold Creek unit is absent). The Upper Ringold Formation filled the Pasco Basin to an elevation of approximately 275 m (900 ft) with fluvial-lacustrine deposits in the Miocene/ Pliocene period (WHC-SD-EN-EE-004, DOE/RL-2002-39). The fluvial-lacustrine Ringold Formation consists of semi-indurated clay, silt, pedified mud, fine- to coarse-grained sand, and granule to cobble gravels. The Upper Ringold (Unit E) facies in the vadose zone in the 200 West Area include the basaltic gravel and fanglomerate unit overlain by an overbank and lacustrine mud and lesser sand unit where it is not eroded (Newcomb et al. 1972, SD-BWI-DP-039, DOE/RW-0164, Lindsey and Gaylord 1990). The contact between Ringold Unit E and the Hanford formation is important because the saturated hydraulic conductivity for the Upper Ringold Units can differ up to two orders of magnitude between each other and/or the gravel-dominated sequence of the Hanford formation or Cold Creek unit.

4.2.2.6 Facies, Stringers, Clastic Dikes, and Sills

Both the Ringold and the Hanford formations contain relatively thin, fine-grained stringers that contribute to the lateral spreading of moisture and slow the vertical movement of water and contaminants within the vadose zone. Low-permeability layers within the Ringold Formation often occur as single, relatively thick (meters or more) continuous layers. Low-permeability layers within the Hanford formation are relatively thin (0.5 m [1.6 ft] or less) and laterally discontinuous. Low-permeability layers within the sand-dominated facies of the Hanford formation are generally thicker and more continuous than those in the gravel-dominated facies. Paleosols and some facies changes (i.e., the contact between fine-grained and coarser grained facies) have been observed to be fairly continuous and promote lateral spreading of crib effluent over the range of at least 100 m (328 ft) (PNNL-14907, PNNL-14702b).

Clastic dikes and sills are of particular interest because of their potential for allowing water and contaminants to bypass vadose zone continuum fate and transport processes. Clastic dikes and sills are thin (generally less than 1 m [3.3 ft] thick), discordant, and concordant features (respectively) that occur in the vadose zone. They are typically fine-grained, silty units that extend up to tens of meters in length. Features such as clastic dikes, sills, and tectonic structures typically considered responsible for creating preferential flow paths, are described further in Section 3.4.5, Appendix A, and in more comprehensive summaries of Hanford Site geology (BHI-01103, RPP-23748, PNNL-15955).

4.2.2.7 Assumptions

The primary assumption is that the geologic stratigraphy can be adequately represented by the geometric approximation of the geologic layers in the numerical grid and as a porous media continuum.

4.2.2.8 Impact on Results

The geology at the Hanford Site has a large impact on the fate and transport of contaminants. The geology at Hanford, particularly the thickness and sediment types of the vadose zone in the 200 Areas, is one of the major reasons that the decision to dispose of liquid waste in buried cribs appeared to be a satisfactory answer to the problem of liquid waste disposal (HW-9671). In fate and transport models, the distance between the source and the aquifer impacts the peak groundwater concentration, especially if the travel time of contaminants to groundwater encompasses changes in the surface that impact the recharge rate (DOE/ORP-2005-01). Estimates in DOE/ORP-2005-01 indicate that without ongoing discharge, but with relatively high recharge resulting from infiltration through the tank farm surface gravel (100 mm/yr), mobile contaminants starting 45.7 m (150 ft) below ground surface (bgs) at Waste Management Area S/SX and 39.6 m (130 ft) bgs require approximately 40 to 60 years to produce peak concentrations in groundwater.

4.2.3 Source-Term Conceptual Model Component

4.2.3.1 Rationale and Basis

The source-term conceptual model component defines the nature and extent of the contamination, including the contaminant inventory, characteristics of the release (type of release [e.g., crib, trench, pond, waste tank, pipeline, surface spill, etc.], as well as the release or discharge volume and the chemistry of the solution), and the resulting distribution of the contaminants. The type of waste site where the release occurred, either planned or unplanned, provides an indication of where contamination is expected to be found. Discharge to high-volume structures (e.g., ponds, cribs, and certain trenches) resulted in deeper contamination than discharge to low-volume structures (e.g., french drains or specific retention trenches) or surface spills. Descriptions and approximations of these features and events are based on vadose zone characterization data (contaminant concentrations and depths), operational information relevant to estimates of contaminant inventories, timing and magnitude of discharges, contaminant release mechanisms and rates, effluent chemistry, estimates of the extent of contamination, estimates of contaminant distributions, and concentration profiles based on characterization and/or contaminant inventory data.

4.2.3.2 Features, Events, and Processes

During Hanford's operational history, both planned and unplanned releases of hazardous chemical and radioactive materials were made to the soil on an immense scale. Waste production overwhelmed the available waste storage capacity, and much of the waste was disposed directly to the ground or subsurface. According to current estimates, over 1.7 trillion L (450 billion gal) of contaminated liquid were discharged to the ground beginning in 1944, primarily through engineered drainage structures (e.g., cribs and trenches), but also through ponds and retention basins. The Waste Information Data System (WIDS) database (DOE/RL-88-30) contains a list of 2,963 waste sites at Hanford. Each listing contains information describing the extent of each waste unit and the waste it contains. Most of Hanford's inventory of hazardous chemical and radioactive wastes is located in the 200 Areas in the Central Plateau region. About 1.3 trillion L (346 billion gal) of waste were discharged to the soil in this area. The key assumption of these waste disposal operations was that radioactive contaminants with long half-lives would migrate very slowly, if at all, through the soil column (HW-9671). Contamination of the groundwater outside of the 200 Areas from crib discharge is known to have occurred beginning in January 1956 (HW-43149).

The main types of structures used to dispose liquid waste were ponds, cribs, trenches, french drains, and reverse wells. Ponds were located in natural depressions and received large volumes of relatively uncontaminated process water. Crib construction consisted of an excavation, usually containing one or more timber box frames filled with soil and/or crushed gravel. Cribs often received large quantities of waste and stopped operating when contamination was detected in the groundwater beneath the crib. Trench construction consisted of an unlined excavation. Some trenches received large volumes of relatively uncontaminated wastewater. Specific retention trenches were designed to receive a specific volume of low-level or intermediate-level radioactive waste. The french drain construction consisted of a shallow, buried, open-ended or perforated pipe filled with rock. Reverse well construction consisted of a deep vertical pipe with the lower end open or perforated.

The 200 Areas also contain the Hanford Site's 177 large-capacity, high-level waste tanks that hold a combined total of approximately 200 million L (54 million gal) and 200 million curies of high-level radioactive waste. It is currently estimated that as much as 3.8 million L (1 million gal) (1 million curies) have leaked from the waste tanks to the underlying soils. Additionally, over 379,000 m^3 (496,000 yd^3) of solid waste, an estimated 4.8 million curies of radioactive materials, are buried in disposal trenches in the 200 Areas. Waste also entered the environment as a result of unplanned releases, such as those from the waste storage tanks, diversion boxes, or releases from pipelines used to transport waste.

4.2.3.3 Assumptions

Inventory estimates associated with many waste sites depend on often incomplete disposal and discharge records and estimates, along with process knowledge about the waste streams, to quantify contaminant inventories (RPP-26744, RPP-23405). The distribution of contaminants in the subsurface is approximated from very limited field data, especially at depths requiring boreholes to access. Substantial quantities of certain contaminants have reached groundwater; hence, estimating the contaminant mass remaining in the vadose zone requires another estimated quantity. Consequently, vadose zone models either simulate the discharge release of the inventory at the time of occurrence on the basis of the disposal and discharge records and estimates, or the vadose zone models approximate inventory and distribution on the basis of characterization data.

One example of a model simulating an inventory discharge release can be found in PNNL-16198. Additional examples of models using assumed or approximated contaminant distributions include those described in RPP-7884, RPP-10098, DOE/RL-2003-23, and RPP-23752, which include simulations using various hypothesized contaminant distributions.

Many assumptions are necessary for estimating contaminant inventory or approximating the current contaminant distribution. The choice of assumptions used will depend on the objectives of the model, which is consistent with EPA guidance on the conduct of environmental regulatory modeling. The emphasis, according to the guidance in CREM (2001), is placed on documenting the assumptions, their rationale, and evaluating their range of impact on the results. Federal guidelines favor the development of a general constitution of principles for developing, applying, or otherwise evaluating a model rather than compiling a lengthy compendium of methodologies. When developing a modeling strategy EPA's Model Evaluation Action Team recommends that it not be "too specific, long, or burdensome," because it may be too unwieldy to meet the needs of the decision makers (EPA 402-R-94-012, CREM 2001).

4.2.3.4 Impact on Results

The source-term conceptual model component has a large impact on the results. The groundwater concentration and risk results are often proportional to the contaminant inventory. The depth of the contaminants may also strongly impact the results, depending on the contaminants' mobility. The vertical distribution of contaminants, within ranges of comparable depths, does not appear to have as great an effect on the results. A comparison of the results in RPP-7884, RPP-10098, and RPP-23752 indicates that different hypothesized contaminant distributions produced minimal differences in the results. The contaminants in those distributions were mostly located within 45.7 m (150 ft) of the ground surface, with most of the contamination located within close proximity to the center of mass.

4.2.4 Groundwater Domain Conceptual Model Component

4.2.4.1 Rationale and Basis

Risk assessment or establishing soil cleanup goals for the protection of groundwater pathway includes the mixing of the vadose zone leachate (recharge transporting contaminants) with groundwater in the underlying aquifer. The resulting contaminant concentration in groundwater provides the basis for the evaluation of risk assessment and soil cleanup goals. In addition to local groundwater contamination concerns, the aquifer system provides a possible pathway for transport of contaminants to offsite receptors. The groundwater conceptual model includes the uppermost unconfined aquifer system that exists within Ringold and Hanford formation sediments. Similar to the Hanford Site's geology, the groundwater and aquifer system have been studied extensively throughout Hanford's operational history (USGS-WP-7) and with renewed interest after contamination associated with crib discharges was discovered in groundwater outside of the 200 Areas (HW-43149, HW-60601).

Most recently, PNNL-14753, PNNL-10886, and PNL-10195 have provided summaries of Hanford geologic and hydrologic data for the unconfined aquifer. Other documents that provide the basis for the hydrogeologic interpretations of the 100, 200, and 300 Areas of the Hanford Site include the following: WHC-SD-EN-TI-008, WHC-SD-EN-TI-011, WHC-SD-EN-TI-012, WHC-SD-EN-TI-132, WHC-SD-EN-TI-133, WHC-SD-EN-TI-155, WHC-SD-EN-EV-027, WHC-SE-EN-TI-052, WHC-SD-EN-TI-014, and WHC-SD-EN-TI-019.

4.2.4.2 Features, Events, and Processes

Groundwater in the unconfined aquifer at Hanford generally flows from the west and discharges into the Columbia River. Some northerly flow occurs through the gap between and to the north of Gable Mountain and Gable Butte. Artificial discharge resulting from Hanford operations greatly altered the flow regime. Because of the cessation of large operational liquid discharges to the ground, the water table in the Central Plateau is expected to continue declining for more than 100 years, according to the most recent estimates (PNNL-14753). The saturated thickness of the unconfined aquifer on the Hanford Site ranges from zero (where basalt ridges associated with Gable Mountain and Gable Butte extend above the water table) to greater than 61 m (200 ft) around the 200 West Area. Depth to the water table ranges from less than 0.3 m (approximately 1 ft) near the Columbia River to more than 100 m (330 ft) near the 200 Areas (PNNL-10886). Perched water-table conditions, caused by the liquid discharges to the surface, have been encountered in sediments above the unconfined aquifer in the 200 West Area (WHC-MR-0206, PNL-8597).

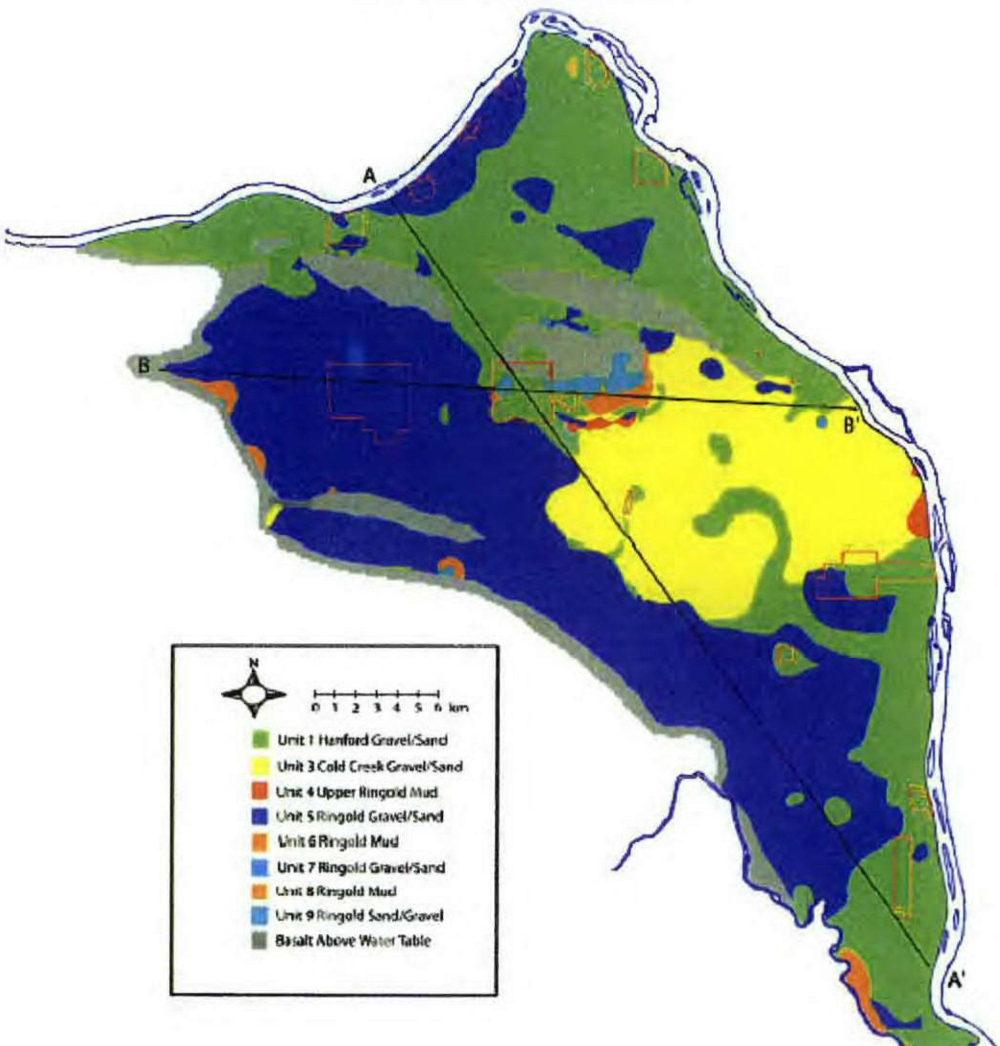
PNNL-14753 identifies eight distinct hydrogeologic units comprising the Hanford Site unconfined aquifer system and provides a brief description of the units provided in BHI-00184:

- Hanford formation gravel, sand, and silt (dominated by gravel and sand within the aquifer)
- Coarse-grained multilithic facies of the Cold Creek unit
- Silt and clay facies of the Upper Ringold Unit
- Ringold gravel Units E and C, also including sand facies of the Upper Ringold Unit where it directly overlies the other gravel units
- Ringold fine-grained overbank and paleosol deposits that separate Ringold gravel Units B and D in the eastern part of the Hanford Site

- Ringold gravel Units B and D
- Lower Ringold Mud Unit
- Ringold Unit A, gravel and sand facies dominated by sand in the western part of the Pasco Basin.

Figure 4-1 (adapted from PNNL-14753) presents the distribution of the different units as they occur at the estimated water table of 1944, which is assumed to represent steady-state conditions. For long-term risk assessment and establishing soil cleanup goals, the distribution from this figure is used to identify the aquifer unit for the specific area addressed by an individual waste site-specific model, and the estimated water table of 1944 provides the basis for estimating the hydraulic gradient. The groundwater conceptual model includes information (presented in PNNL-14753) that describes the physical characteristics and transport parameters of the hydrologic system: hydraulic conductivity, total porosity, effective porosity, dispersivity, and horizontal to vertical and anisotropy.

Figure 4-1. Distribution of Hydrogeologic Units Present at the Water Table for 1944 (Pre-Hanford) Conditions.



NOTE: Figure adapted from Figure 5-5 in PNNL-14753, Rev. 1.

4.2.4.3 Assumptions

Leachate from the vadose zone is assumed to enter the aquifer and mix with the groundwater by advective and dispersive processes. Concentrations calculated in the model for a specified depth, elevation, or interval in the aquifer are assumed to be comparable to concentrations that would be measured by sampling a well with a well screen at the same location. Because the model domain can extend beyond the edge of the waste site, the estimated concentration in groundwater downgradient of the waste site can be calculated. However, for two-dimensional vadose zone models, all flow and transport in the vadose zone and aquifer remains confined within the two-dimensional cross-section of the model.

4.2.4.4 Impact on Results

The groundwater domain conceptual model component has a large impact on the results. The groundwater concentration and risk results are often proportional to the flow of water in the aquifer, as determined by the hydraulic conductivity and hydraulic gradient.

4.2.5 Hydrogeology and Fluid Transport Conceptual Model Components

4.2.5.1 Rationale and Basis

The hydrogeology conceptual model components represent the structure within which fluid transport through the vadose zone occurs. The porous media continuum assumption (an extended form of Darcy's Law for vadose zone applications) and the soil relative permeability/saturation/capillary pressure relations provide the basis for vadose zone flow and transport modeling (PNNL-11217). In the model domain, the hydraulic properties describing fluid transport characteristics associated with each geologic layer are approximated by average values, with each unit having different flow and transport parameter values (hydraulic conductivity, bulk density, and dispersivity). The model describes bulk (or mean) flow and contaminant transport behavior in the vadose zone, limiting the evaluation to estimating the overall and eventual contaminant impacts to groundwater.

Features such as clastic dikes, sills, and tectonic structures can allow water and contaminants to bypass vadose zone continuum fate and transport processes. However, there is little evidence of enhanced transport in these preferential pathways in arid and semi-arid climates with low-water flux in the vadose zone, particularly where soils are coarse-grained such as in Hanford formation sediments. While these features may form preferentially faster flow pathways under saturated conditions, under unsaturated flow conditions, these features tend to act as barriers to transport. Precipitation at arid sites is usually too low (in relation to saturated hydraulic conductivity) to invoke preferential flow. Much of the water in the dry soils is simply retained on grain surfaces by capillary forces and does not move along preferential pathways (see Appendix A for additional information).

4.2.5.2 Features, Events, and Processes

The fluid transport and soil moisture-retention conceptual model component describes the hydrogeologic flow and contaminant transport characteristics of the subsurface environment flow and transport phenomena in terms of the soil hydraulic properties. Soil hydraulic properties control the movement of water and contaminants through the vadose zone. They describe the amount of water that the soil is capable of containing, the capillary pressure at which the soil retains a certain quantity of water, and the rate at which water is capable of moving through the soil. Capillary pressure refers to the suction exerted by the soil to hold water in place. Measurable soil properties of interest are bulk density, porosity, saturated moisture content, and soil moisture-retention (moisture content measured at different capillary suction pressures).

Using an analytical equation and a curve-fitting process, soil moisture-retention characteristic curves (moisture content as a function of capillary pressure) and relative permeability curves (permeability as a function of capillary pressure) may be fit to the soil moisture-retention data determined by physical properties testing. The characteristic curves allow the relationship to be expressed for the entire continuum of values, which is a necessity of modeling. Moisture content is often expressed in terms of saturation (the amount of water contained by the soil relative to the maximum amount the soil could contain). Residual moisture content (or saturation) refers to the minimum amount of water retained by the soil regardless of the amount of pressure applied. Residual saturation represents water so tightly bound to the soil that is does not move regardless of the capillary pressure gradient. It is not measurable but is determined through the curve-fitting process.

Much of the information needed to determine effective values of parameters from small-scale samples in conjunction with information on the fine-scale structure of these sediments exists, and is integrated into the model along with upscaling and volume-averaging methods. One approach has been to assign flow and transport parameters based on the similarity between grain-size statistics of the different soil textures at the site and at previously characterized sites (PNNL-14907). Hydraulic properties are estimated based on similarities in grain-size statistics (mean grain size and sorting index) between sediments at the waste site and other characterized sites on the Hanford Site (PNNL-13672) using pedotransfer functions. Grain-size distributions are obtained from a database (i.e., ROCSAN). Effective, large-scale diffusion coefficients for the different textures are assumed to be a function of volumetric moisture content. Measured hydraulic properties are obtained from databases for the immobilized low-activity waste and Sisson and Lu sites (RHO-ST-46-P). Fluid flow parameters for the vadose zone include soil moisture-retention characteristics and saturated hydraulic conductivity. Variable or saturation-dependent anisotropy was used as a framework for simulating the effects of saturation on lateral spreading using laboratory measurements on undisturbed directional cores.

Another approach is to estimate the effective unsaturated hydraulic conductivity tensor of an equivalent homogeneous medium using the Richards' equation and the evolution of spatial movements in a moisture plume (Yeh et al. 2005). A hierarchical geostatistical analysis is performed to examine the large-scale geologic structure for the entire field site; subsequently, small-scale features within different layers are investigated.

Based on the analysis of the injection experiment data at the Sisson and Lu site, the effective hydraulic conductivities compare well with the laboratory-measured conductivities for core samples. Spatial movements of the simulated plume based on the effective hydraulic conductivities agree with those for the observed plume. This approach provides a way to estimate effective Kd and allows the previously developed moisture-dependent anisotropy concept to be quantitatively evaluated. It also appears to be a useful practical tool for estimating effective unsaturated hydraulic conductivities based on snapshots of moisture movement in a large-scale vadose zone and is applicable to column- or field-scale problems (Yeh et al. 2005).

4.2.5.3 Assumptions

The average parameter values for different soil types are assumed to adequately represent the bulk contaminant flow and transport processes occurring in the vadose zone. Small-scale heterogeneity is important with respect to contaminant deposition and impacts flow and transport in the vadose zone (PNNL-15443). PNNL-15443 indicates that model results from upscaled homogeneous parameters with constant anisotropy match the centroid of an injected water plume reasonably well, even without accounting entirely for the effects of small-scale heterogeneity. To approximate the bulk flow, upscaling the parameters incorporates the effects of small-scale textural contrasts that introduce heterogeneity into the flow parameters.

4.2.5.4 Impact on Results

The hydraulic parameter values for the vadose zone units do not appear to have a large impact on the results. DOE/RL-2005-01 indicates that increasing or decreasing the hydraulic conductivity of the vadose zone units by a factor of 10 increased or decreased the peak concentration in groundwater of the mobile contaminants by less than a factor of 2. The change in the results for moderately mobile contaminants (Kd = 0.2 mL/g) was even less. DOE/ORP-2000-24 included sensitivity cases that treated the entire vadose zone as having the properties of sand or gravel. The results indicated that little difference from the base case results occurred for the mobile contaminants.

4.2.6 Recharge Conceptual Model Component

4.2.6.1 Rationale and Basis

Recharge is the amount of water that enters the groundwater from the vadose zone. It can be defined as the net difference between the water entering soil by infiltration at the surface or by subsurface discharge and the water stored indefinitely by the soil or returned to the atmosphere by evapotranspiration processes. It is the driving force for the movement of contaminants in the vadose zone to groundwater; therefore, recharge is a primary parameter in vadose zone fate and transport processes. When recharge is combined with residual soil moisture content, it determines the flux of water available for transport through the vadose zone. The recharge conceptual model component documents the technical basis, data, and rationale used in the selection of recharge rate parameters in Hanford vadose zone models. Recharge rates for the Hanford have been estimated from UNSAT-H models, whose use at Hanford was agreed upon via the *Hanford Federal Facility Agreement and Consent Order* (Tri-Party Agreement) (Ecology et. al. 2003) process (DOE/RL-91-44).

4.2.6.2 Features, Events, and Processes

Regional recharge rates depend on climate in terms of (average) precipitation and evaporation rates, on vegetation (which determines transpiration rates), and on soil type (which determines the rate and extent of water infiltration into the soil). Recharge rates can also vary locally where there are local differences in soil and vegetation conditions. Any factors that impact these processes, conditions, or events can potentially affect the episodic recharge rate, including the frequency and magnitude of rangeland fires and other factors affecting the nature and rate of revegetation. Site-specific measurements or estimates of recharge rate are, therefore, dependent on the scale of the site.

Significant effort has gone into site-specific determinations of recharge rates across the Hanford Site based on data from lysimeter measurements over extended periods (20+ years) and chlorine isotopic measurements (Gee et al. 1992, 2005a, 2005b; PNNL-13033; PNNL-14744; Murphy et al. 1996). These data and other relevant information have gone into the development of a Hanford recharge database that serves as the primary technical basis for estimates of the recharge rate in this region as a function of soil type and vegetative conditions.

These data have been compiled and summarized in a Hanford Site database by geographic area in terms of major baseline soil types and plant community (vegetation) for the following four conditions (PNNL-14702a, PNNL-14725a, PNNL-14725b):

- No vegetation
- Cheatgrass
- Young shrub-steppe assemblage
- Mature shrub-steppe assemblage.

The compilation of recharge rate databases at the Hanford Site enable tabulated recharge rate values to be estimated for most site-specific or waste site-specific conditions on the Site. PNNL-13033, PNNL-14702a, and PNNL-14702b provide "best-estimate case" (mean values) and "reasonable bounding case" (upper and lower bounds) recharge rates for the main baseline soil types. The upper-bound values refer to the highest value for each soil and vegetation type, and lower-bound values to the lower 1 percentile of lognormal distributions. The "best-estimate" recharge rates are a function of soil type, the four vegetation conditions provided in the data summarized above (PNNL-14702a), and various time intervals (e.g., site use conditions). Recharge rate data for site-use conditions have been assembled into a suite of recharge classes that describe probability distribution functions for recharge rates appropriate for pre-Hanford, operations, post-remediation, and post-Hanford conditions. The basis for assignment of recharge values for the four vegetation conditions listed above is to base the "no vegetation" and "mature shrub-steppe" recharge rates on site-based field measurements, to assign the recharge rate for "cheatgrass" as 50% of the "no vegetation" values, and "young shrub-steppe" estimates as two times the "mature shrub-steppe" values. Data and interpretations summarized in PNNL-14702a and PNNL-14725 estimate site-specific recharge rates for Hanford that meet or exceed the criteria for applications to environmental regulatory and risk assessment modeling, and also meet or exceed the requirements of WAC 173-340-747(8)(b)(vii) for estimating recharge in RCRA applications or for applications as ARARs in CERCLA activities. More recently, best-estimate recharge rates values for post-remediation recharge classes were updated to include values for the short-term, post-remediation transitional recovery period (e.g., 30 years); barriers; and long-term recharge values (final long-term recharge class) (PNNL-14725b).

These guidelines, the recharge data package (PNNL-14744), and the Geographic and Operational Site Parameters List (GOSPL) (PNNL-14725a, PNNL-14725b) facilitate the identification and selection of the most appropriate site-specific recharge rates and surface soil conditions for use in vadose zone modeling at each waste site. Soil conditions and recharge estimates were derived from a suite of available field data and computer simulation results (PNNL-14725a, PNNL-14725b).

4.2.6.3 Assumptions

Annual recharge estimates incorporate the effects of episodic infiltration events and spatial heterogeneity within individual soil types and surface conditions into a single steady-state value. Infiltration is an inherently episodic process. Data measuring the net infiltration of winter rains through bare sand surfaces at Hanford show that the pulses do not appear to penetrate beyond 3 m (9.8 ft) below the surface, and a near steady-state drainage condition prevails below this depth (PNNL-14115). This allows for the use of time-averaged recharge rates for risk assessment applications of vadose zone modeling. The PNNL-14702a identifies appropriate parameter values and/or ranges for use in vadose zone fate and transport modeling.

4.2.6.4 Impact on Results

The recharge conceptual model component typically has a large impact on the results, especially with respect to long-term recharge rates such as those associated with post-remediation conditions. However, because recharge may undergo transient changes, the effects vary depending on the quantity of recharge, duration, and location and mobility of the contaminants in the vadose zone. The groundwater concentration depends upon the flux rate of the contaminant into the groundwater, which depends on the recharge entering the aquifer. Changes in the recharge rate, applied at ground surface in the model, require some duration of time for the perturbation to impact the flux rate of water from the vadose zone to the aquifer. DOE/ORP-2005-01 evaluated several recharge sensitivity cases and noted that increased or decreased recharge increased or decreased the peak concentration, but only if the recharge rate was sufficient to transport the contaminants to groundwater at the time when the increased or decreased recharge occurred.

4.2.7 Geochemical Conceptual Model Component

4.2.7.1 Rationale and Basis

Geochemical conceptual models primarily provide a technical basis for contaminant release and retardation mechanisms. The parameters describe contaminant mobility (Kd values) and provide rationale for simplifying assumptions in vadose zone modeling. The dynamic interaction of contaminants with the geologic media (physical and chemical environments) in the vadose zone impacts the geochemical conceptual model and is variably dependent on contaminant and waste site composition. Contaminant behavior in Hanford vadose zone is complex and dependent on many transient factors. Dominant geochemical processes are contaminant-specific, but contaminant mobility can be described in terms of highly mobile, moderately mobile, relatively immobile, and variable groupings in terms of behavior. The importance of geochemical processes on the transport of contaminants through the vadose zone is described in the U.S. Department of Energy's (DOE's) state-of-knowledge and preliminary concept documents (DOE/RL-98-48), the international list of FEPs, and the list of relevant Hanford Site FEPs (BHI-01573). The geochemical conceptual model provides the technical basis for the understanding of contaminant behavior and the rationale for making simplifying assumptions in vadose zone modeling.

Guidelines are available to assist users in selecting appropriate Kd values from the Hanford Kd database (PNNL-13895). The Kd values for a given COC can be selected on the basis of geographic location, site-specific area designation, specific waste sites, the stratigraphic units within the area of interest, waste site type (operations), waste chemistry group, and source categories (PNNL-14702a, PNNL-14725a, PNNL-14725b). Best-estimate, minimum, and maximum Kd values have been projected based on data distributions from the Hanford Kd database. In cases of sparse data, distributions were developed from the best existing data using professional judgment for the distribution construct. This approach is consistent with EPA risk assessment guidelines for the use and application of professional judgment and the consideration of data uncertainties (EPA/540/1-89/002, EPA/600Z-92/001). A process for using these documents to select Hanford Site-specific Kd values for vadose zone applications is summarized in Appendix B.

4.2.7.2 Features, Events, and Processes

The range of geochemical processes associated with fate and transport of contaminants in the vadose zone at Hanford include oxidation/reduction, aqueous speciation, adsorption/desorption, precipitation/dissolution, diffusion, colloid-facilitated transport, and anion exclusion (PNNL-13037, Rev. 1). Summaries of these processes and their implications for geochemistry conceptual models have been documented (e.g., EPA 1999 and EPA 402-R-04-002C). Site-specific behavior and the associated geochemistry of contaminants at Hanford have been documented in many project reports and investigations (e.g., PNL-8889, PNL-10722, PNL-10379, PNNL-11485, PNNL-11966, PNNL-13895, PNNL-15502, PNNL-15121, and Qafoku et al. 2005).

Geochemical behavior of contaminants in the Hanford vadose zone can be described in terms of the primary geochemical processes affecting contaminant transport, including adsorption/desorption (ion exchange) and precipitation dissolution (PNNL-13037, Rev. 1). Adsorption/desorption typically controls contaminant retardation in areas where low concentrations of dissolved radionuclides exist, such as those associated with the far-field environments of disposal facilities or spill sites. Precipitation/dissolution is typically an important process where elevated concentrations of dissolved radionuclides occur, such as in the near-field environment of waste site facilities (PNNL-13037, Rev. 1).

Some Kd measurements are only applicable for a specific set of conditions because Kd value variability cannot be confidently estimated beyond the range of chemical conditions under which it was measured.

This limitation is not a significant problem as long as site-specific conditions being modeled do not deviate significantly from those for which Kd measurements are available (PNNL-13037, Rev. 1). The Kd values from the Hanford contaminant distribution coefficient database that have been measured multiple times, preferably in separate studies with suspect outliers excluded from consideration, are the most reliable (PNNL-13895). The Kd values selected for modeling purposes are typically the lowest, or close to the lowest, value for the sake of conservatism (PNNL-13037, Rev. 1). This conservative approach tends to over-estimate the transport of the contaminants, leading to the selection of overly conservative remedial actions and wasted efforts. The linear adsorption (Kd model) approach has been shown to adequately describe contaminant behavior in modeling vadose zone fate and transport for Hanford Site sediments under most circumstances involving far-field and/or low-impact sites where geochemical conditions remain fairly constant and contaminant loading of adsorption sites is low (PNNL-13895).

PNNL-13895 contains 90% of the existing site-specific data on contaminant distribution coefficients applicable to sediment and related materials in the vadose zone and groundwater at Hanford. This database includes documentation of contaminant concentrations in the solution phase and solid phase, sediment mineralogy, physical properties, experimental procedures used, the availability of the original reference, availability of sediment characterization data, a comprehensive bibliography of published documents containing useful distribution coefficient data applicable to Hanford, and ratings and evaluations of the data in terms of quality of documentation for each value. For situations associated with large changes in chemical condition, especially in near-field environments and/or certain disposal chemistry conditions (e.g., large variations in pH, alkaline concentrations, or complexing agents), the linear adsorption model may not be appropriate due to the departure from dilute solution behavior implicit in the use of the Kd model and/or other dominance of other geochemical processes (e.g., aqueous complexation or solubility-controlled behavior) (RPP-10098, Qafoku et al. 2005).

Other factors that have potential impacts on the geochemistry conceptual model include the aging of sediments after adsorption of a contaminant and kinetically controlled contaminant release. The effects of sediment aging after the adsorption of a contaminant can alter the physical and/or chemical processes that dominate the subsequent desorption and transport of the contaminant. Contaminant deposition and adsorption can occur in a geochemical environment that has been altered because of the characteristics of the waste discharges. In time, the buffering capacity and other natural processes in the vadose soils mitigate the impacts of the waste discharges. As the geochemical environment changes, the release and desorption characteristics of the contaminant can also change. Water and contaminants entering dead-end pores can result in the subsequent contaminant release becoming kinetically controlled, especially if the contaminant solubility changes as a result of sediment aging. As sediments drain and desaturate, a fraction of the porewater and total sorbed inventory can become isolated from the advective transport pathway (Qafoku et al. 2005). Diffusion through micropores within sediments can physically isolate contaminants from advective transport and increase the importance of diffusion controls in the release process for some contaminants. This can result in an increase in effective Kd values over time and/or higher desorption Kd values. Porewater isolation also has implications with respect to multiple porosity.

A synopsis of nitrate, technetium-99, and uranium (COCs) geochemistry in vadose zone soils is provided below. These contaminants represent some of the more common COCs evaluated for the protection of groundwater. The synopsis includes the technical basis and rationale regarding the contaminant behavior conceptual models and the selection of Kd values for these contaminants in the protection of groundwater pathway.

Nitrate

Nitrate is one of the most widespread contaminants associated with past Hanford operations. It is highly mobile and does not precipitate or readily adsorb on minerals under the near-neutral or slightly alkaline pH conditions common in sediment systems. As anions, their adsorption is expected to be high under acidic conditions, decrease with increasing pH values, and be essentially zero in basic pH conditions. Based on measurements of nitrate Kd values, PNNL-13895 concluded that nitrate adsorption under most Hanford Site-relevant conditions is essentially zero (Kd = 0) within experimental error. However, under some conditions (e.g., acidic), nitrate adsorption may be higher.

Technetium-99

Of the several technetium isotopes produced as fission products in nuclear reactors, only technetium-99 is a potential hazard at DOE defense waste sites because of the specific activity and long half-life (2.11 x 105 years) of this isotope (EPA 402-R-04-002C). The most stable and characteristic oxidation state of technetium in slightly acid, neutral, or basic aqueous solutions in equilibrium with the atmosphere is pertechnetate ion (TcO_4 -) in which technetium is in the +7 oxidation state (Hanke et al. 1986). The adsorption of technetium(VII) oxyanion TcO_4 - is expected to be very low to zero, with Kd values of approximately 0 mL/g at near-neutral and basic pH conditions and increasing when pH values decrease to less than 5.

PNNL-13895 compiled the Kd values measured from Hanford sediments for radionuclides and contaminants of environmental concern to the vadose zone and groundwater. The data indicate that technetium(VII) adsorption is low under nearly all conditions relevant to the Hanford vadose zone and upper unconfined aquifer, with Kd values ranging from zero (0) to a high of approximately 1 mL/g. PNNL-13895 concludes that, under normal Hanford Site conditions, zero is the most appropriate Kd value for technetium(VII), and 0.0 to 0.1 mL/g is the best estimate for the range for technetium(VI) Kd values.

Uranium

The geochemical behavior of uranium is complex, and has been extensively studied (Langmuir 1978, 1997; Burns and Finch 1999). In studies conducted at Hanford, uranium is found primarily in the +6 valence state (PNNL-14022, RPP-10098). It is often the only COC that is associated with geochemical release and retardation processes. The release model(s) for uranium for remedial action goal modeling is (are) based on consideration of sorption, and precipitation and solubility controlled release.

The dissolved concentrations of uranium(VI) beyond the very near field are controlled by adsorption processes in the Hanford vadose zone (sediments) and unconfined aquifer system (PNNL-13037, Rev. 1), making the selection of appropriate Kd values highly dependent on disposal chemistry, soil type, pH, chemistry of the leachate/porewater, and the concentration of dissolved carbonate/bicarbonate in solution. uranium(VI) has been found to range from highly mobile to highly immobile in Hanford vadose zone systems depending on the combination of conditions. In the presence of alkaline, bicarbonate-rich waste streams, uranium(VI) exists as strong aqueous anionic uranium(VI) complexes, which do not readily adsorb to the naturally negatively charged Hanford Site sediments at neutral-to-alkaline pH conditions. Under mildly alkaline conditions, aqueous uranyl carbonate species may adsorb onto reactive surfaces present in soil minerals (Bargar et al. 1999), soils (Duff and Amrhein 1996), and sediments (Qafoku et al. 2005).

Precipitation and co-precipitation processes are important for uranium(VI) under some environmental conditions. Dissolved calcium uranyl carbonate complex has an important effect on the geochemical behavior of uranium(VI) in calcium-rich aqueous systems at near-neutral to basic pH conditions. Characterization studies at the Hanford, Fernald, Oak Ridge, and Savannah River sites indicate that uranium-containing minerals or co-precipitates may be present in sediments and soils contaminated from disposal or spills of uranium-containing liquid wastes (Delegard et al. 1986, PNNL-14022, RPP-10098, Catalano et al. 2004, Buck et al. 1994, Morris et al. 1996, Roh et al. 2000, Bertsch et al. 1994, Hunter and

Bertsch 1998). These studies show that uranium (VI) dissolution from the contaminated sediments containing uranyl-silicate mineralization is a pseudo-first-order rate kinetic process(ck) characterized by an initial fast rate, and reaching constant concentration solubility-controlled release after period of 30 to 200 days. The rate and extent of uranium dissolution is dependent on the pH, electrolyte (i.e., porewater) composition, and bicarbonate/carbonate concentration. Initial kinetic reaction rates were observed to be slower, and uranium concentrations lower for release from calcareous sediments. These results were caused by rapid dissolution of the uranyl silicates from grain surfaces and cavities, with dissolution kinetics of the precipitated uranyl minerals regulating the slow release (Liu et al. 2004). The solubility of uranium(VI) decreases significantly as pore/leachate water compositions become increasingly equilibrated by interaction with the vadose zone sediments (solubilities are greater than five times higher in calcite-saturated deionized water than in calcite-saturated, sodium- and silicon-rich electrolytes) (Qafoku et al. 2005). Surface secondary uranium mineralization in the deep vadose zone sediments extended to groundwater.

4.2.7.3 Assumptions

The empirical distribution coefficient, Kd construct, through the application of the empirical linear adsorption model, will be used at Hanford waste sites for key contaminants and system performance activities. The rationale for the utility of the empirical linear adsorption model or Kd approach is that it is a simple, useful, and practical approach for modeling contaminant adsorption and transport in geologic systems. Additionally, a considerable database is available for Hanford Site-specific Kd values measured under a variety of conditions (PNNL-13895). Experiments have been conducted with site-specific sediments, water resembling natural recharge and/or vadose zone porewater, and actual or simulated contaminant materials for most of the sorption data (PNL-8889, PNNL-14022, PNNL-14594, PNL-10722, PNL-SA-10390, PNNL-11485, PNNL-11966, PNNL-15502, PNNL-15121). PNNL-13037 (Rev. 1) summarizes the key attributes and shortcomings of the empirical construct and mechanistic models for application to vadose zone and groundwater modeling at Hanford. Empirical modeling involves the collection of representative data for model building and validation. PNNL-13895 directs that geochemical environments will be mechanistically studied. Mechanistic models are based on fundamental knowledge of the mechanisms governing the process and provide the necessary paradigms on which technically defensible empirical Kd values must be based. These models involve experiments to define model structure and data found in the model validation process. An alternative is to use a combination of fundamentals and process knowledge for the model structure and empirical procedures thereafter.

4.2.7.4 Impact on Results

The geochemical conceptual model component typically has a large impact on the results. Contaminant mobility is a major factor in the model results.

4.3 DETERMINATION OF MODEL SELECTION ATTRIBUTES AND CRITERIA

The FEPs within the conceptual model components identified as important for vadose zone modeling at the Hanford Site are summarized in Table 4-1. The following is an evaluation of these FEPs in the consideration of the model complexity and type needed for the objectives of this modeling, as well as the identification of the attributes and criteria for model selection.

Table 4-1. Examples of Principal Features, Events, and Processes Identified as Important for Vadose Zone Modeling at the Hanford Site.

Conceptual Model Component	Features, Events, and Processes
Location and geologic setting	• Waste site type • Geologic stratigraphy
Characteristics of the discharge or unplanned release event	• Discharge or release event • Contaminant inventory • Discharge chemistry • Discharge volume • Plume size and location
Infiltration and recharge characteristics of the surface soils	• Infiltration • Recharge • Drainage[a]
Vadose zone fluid and contaminant transport	• Vadose zone hydrogeology • Vadose zone geochemistry • Contaminant geochemical characteristics
Contaminant mixing and transport in the capillary fringe	• Capillary fringe unit's hydrogeology and geochemistry • Contaminant geochemical characteristics • Capillary fringe flow
Contaminant mixing and transport in the groundwater	• Groundwater unit's hydrogeology and geochemistry • Contaminant geochemical characteristics • Groundwater flow

[a] Drainage, in the context of the features, events, and processes identified in this table, refers to the downward movement of water artificially introduced into the subsurface environment.

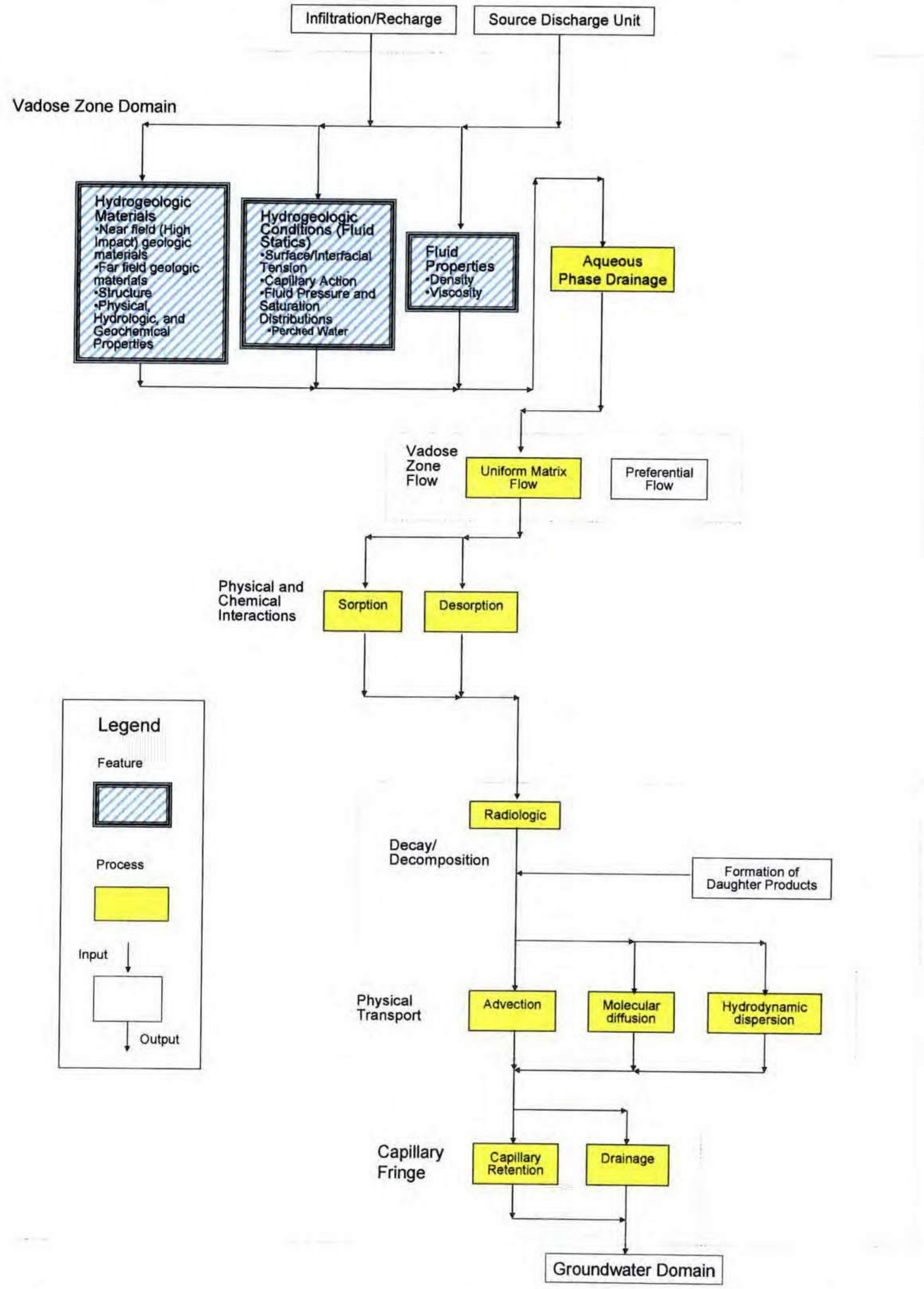
The combination of FEPs relevant to model selection for Hanford vadose zone system is depicted in Figure 4-2 in the manner recommended by the Nuclear Energy Agency (NEA) for this type of evaluation (NEA 2000). This approach is comparable to the process relationship tool developed by PNNL (PNNL-SA-34515). This depiction of the features and processes illustrates the relationships between them in the conceptual model components and their ability to facilitate identification and selection of adequate model capabilities (i.e., required model attributes and criteria).

Two of the most important FEPs required for meaningful simulation of vadose zone processes at the Hanford Site are (1) the uncommonly thick sequence of vadose zone sediments with associated hydrologic properties, and (2) the infiltration rates imposed by the semi-arid climatic conditions in this region. The following is an example of the association provided in the Federal guidelines:

> *"If the risk assessment is based on arrival times and peak concentrations of contaminants (and radionuclides) arriving in groundwater, then consideration of transport through even a thin unsaturated zone is significant"* (EPA 402-R-93-009).

The Federal guidelines further specify that flow, fate, and transport models are needed for vadose zone models in remedial processes and/or remedy selection and design applications. The model criteria identified in Tables 4-1 and Figure 4-2 also indicate that that fluid flow and contaminant fate (i.e., retardation) are integral for adequately describing fluid and contaminant transport in Hanford vadose zone models.

Figure 4-2. Features and Processes Potentially Relevant for Vadose Zone Model Types



NOTE: The primary features and processes most relevant to the vadose zone models at the Hanford Site are highlighted (adapted from PNNL-14702a).

Federal guidelines associate the level of complexity needed to accommodate the principal FEPs for most vadose zone models with the attributes and criteria necessary for fate, flow, and transport models (EPA-402R-93-009) (also referred to as "fate and transport models"). As noted in Section 2.5.5, Federal guidelines indicate that risk assessments should begin with the simplest models that satisfy the objectives, progressing toward more sophisticated models/codes as necessary to accommodate the principal FEPs and achieve the modeling objectives (EPA 402-R-94-012). The guidelines also state that a conservative, simplistic method or approach should not be taken to avoid modeling, because an overly conservative approach may be contradictory to the objectives of the optimization between remedial activities and the accompanying reduction in risk (EPA 402-R-93-009). An evaluation of the appropriate level of complexity for the Hanford vadose zone models is summarized in Table 4-2, which compares principle FEPs with model complexity. Based on the characteristics of the Hanford Site's unsaturated zone and the types and nature of associated features and processes identified in Table 4-1 and Figure 4-2, it is indicated in Table 4-2 that "complex" models are required versus the use of "simple" or "semi-complex" models.

This conclusion is consistent with Federal guidelines which indicate that complex fate and transport models are needed for systems involving the following types of FEPs, which are all principal FEPs for the Hanford vadose zone:

- Thick vadose zone
- Layering or heterogeneous lithology
- Sub-regional recharge
- Step-wise release and attenuation of contaminants versus a simple, single partitioning event
- Unsaturated flow.

In accordance with Federal requirements for the use of ERMs in risk assessment applications involving radionuclides (OSWER Directive 9200.4-18), the level of model sophistication must also take into account and accommodate the factors listed below:

- Radioactive decay
- Time (year) peak concentrations in groundwater
- (Spatial) movement of contaminants within and between media.

Generic or simple models incapable of adequately addressing these FEPs are not considered suitable for long-term contamination assessments at the Hanford Site. Complex or semi-complex models in the context of these factors are required when FEPs criteria cannot be adequately simulated with analytical methods. This is because analytical models do not generally account for many of the flow and transport processes that require more complex models (EPA 402-R-93-009).

Model complexity also refers to the required numbers of dimensions in the model domain. While simulations in three spatial dimensions may provide the most accurate representation of the Hanford vadose zone system, such numerical models require computational capability that exceeds most accessible contemporary computers. Thus, the dimensionality of the FEPs must be balanced against the available computation capability and data. Two-dimensional models appear to be adequate to incorporate the spatial variability in the key FEPs (e.g., sloping geologic layers and variability in recharge) without introducing excessive demands for computational resources.

Table 4-2. Model Complexity, Dimensionality and Other Factors in Consideration of Model Attributes and Criteria/Model Selection.

Model Complexity	**Vadose Zone Dimensions (Geology) and Hydrogeology**	**Chemical Fate and Transport Processes**	**Scale and Temporal Factors**	**Degradation and Decay Processes**
Simple	• One-dimensional • 4 to 6 horizontal layers • Homogeneous, isotropic	• Aqueous phase transport • ***Linear sorption isotherm (Kd)***	• ***Step-wise steady state*** • One site per area per waste type	• ***Radioactive decay*** • Biological pseudo-decay • Homogeneous, isotropic
Moderately complex	• *Two-dimensional* • ***Up to 10 sloping layers*** • Homogeneous, isotropic	• Density and temperature effects • ***Linear sorption isotherm (Kd)*** • ***Peak arrivals***	• Long-term climate changes • Sites on finer grid	• ***Radioactive decay*** • Biological decay
Complex	• Two- and three-dimensional • >10 complex layers • ***Heterogeneous and anisotropic*** • Preferential flow paths • Chemically enhanced permeability	• Multi-phase transport • Colloidal transport • Barometric effects • ***Reactive transport*** • Wind and water erosion	• Episodic, seasonal variations • Long-term climate changes • ***Scale on site-specific basis*** • Near- and long-term	• ***Radioactive decay*** • Biological decay • Inorganic decay (oxidative/reductive)

NOTE: Principal features, events, and processes for the Hanford Site vadose zone are shown in bold/italics.
Kd = instantaneous equilibrium distribution coefficient

These evaluations based on the principal FEPs identified in the conceptual model components and the Federal model selection process serve to collectively identify the model capabilities required of an ERM model type for vadose zone modeling at Hanford. It is clearly indicated from this evaluation that the most appropriate model type capable of incorporating the characteristics and conditions of the Hanford vadose zone, and meeting the modeling objectives for most risk characterization applications concerning the vadose zone pathway, is "fate (flow) and transport" modeling. Based on this evaluation, a two-dimensional fate and transport model type is necessary to account for the distinct geologic, hydrologic, and meteorological conditions of the Hanford vadose zone system and to adequately accommodate the other principal FEPs, attributes, and criteria identified in conjunction with the implementation of the Federal model selection process. The results and conclusions of this model selection process are also regarded as appropriate and adequate for most vadose zone modeling at the Hanford Site. These model attributes and criteria serve as conditions and criteria for the identification and selection of one or more codes for implementation of the fate and transport model type.

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5.0 APPLICATION OF GUIDELINES FOR THE USE AND DOCUMENTATION OF ENVIRONMENTAL REGULATORY MODELS FOR THE HANFORD SITE VADOSE ZONE SYSTEM

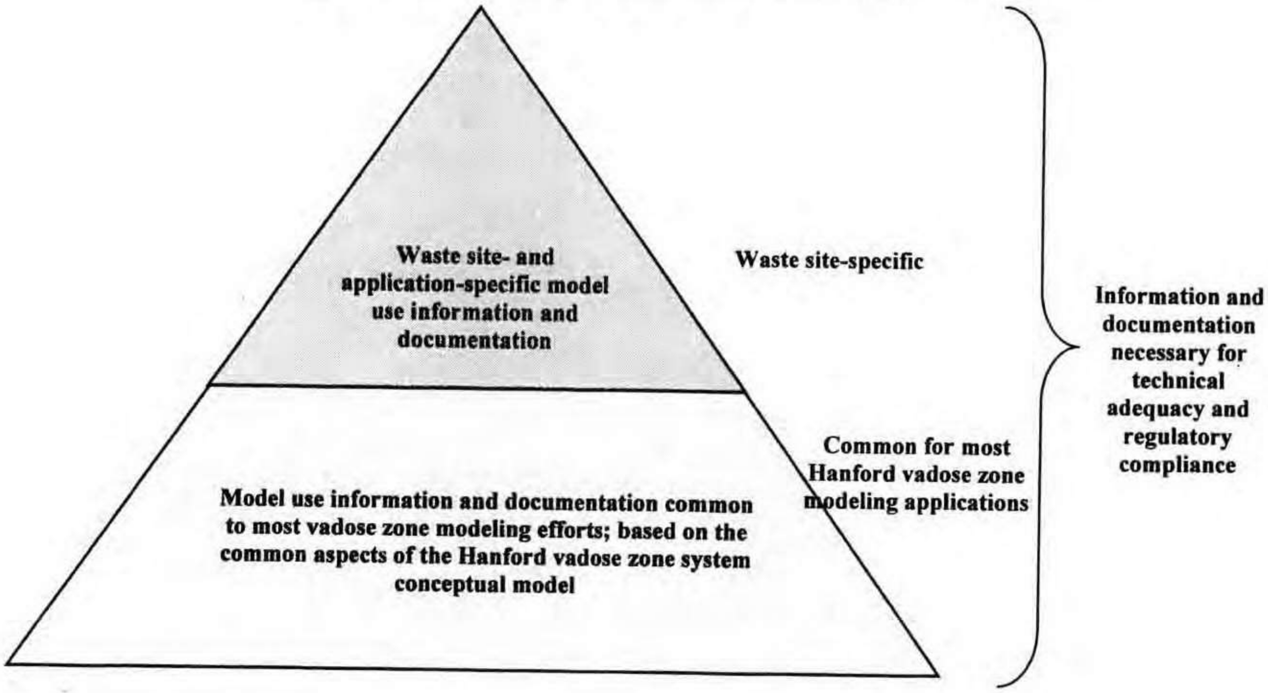
There are many common aspects of the requirements and expectations concerning ERM selection, use, and documentation for most vadose zone modeling applications at the Hanford Site. The following are the general model documentation elements recommended by EPA (2003a) and identified in Section 2.4 concerning the selection and use of ERMs:

- Describe the model and code selection process and rationale.
- Identify the sources of information and the rationale used to develop the input parameters.
- Present the model results.
- Identify the uncertainties in the model and model results, and describe their possible impact on the results.
- Identify, provide the rationale, and describe the impact on the model results for the assumptions used in the model.
- Identify the limitations of the model and the limitations associated with the interpretations of the model results.

These documentation elements are also identified and segregated in Table 2-2 under the categories of model selection and model use. Section 4.0 presents documentation associated with the selection of an appropriate model type for the Hanford vadose zone system. This section documents the application of the requirements and guidelines concerning the use and documentation of the vadose zone fate and transport model type at Hanford for risk characterization applications. As indicated in Table 2-2, model use elements that require substantiating documentation (in addition to the model results) primarily include model parameterization, as well as the evaluation of model uncertainties, assumptions, and limitations.

Although complete evaluations and documentation of these elements of model use require site-specific and application-specific information, there are underlying assumptions, considerations, and factors common to most vadose zone modeling at the Hanford Site. The common aspects of the model use elements described here provide a fundamental basis for waste site-specific modeling documentation. This information is intended to serve as a foundation and framework for the information and documentation necessary for most vadose zone modeling efforts at Hanford in the manner illustrated in Figure 5-1. The information and documentation for complete technical adequacy and regulatory consistency requires the inclusion of those elements that are common for the vadose zone system, amended with site- and application-specific information and documentation. The relationship of the documentation on the common aspects of model use to the overall documentation necessary to demonstrate ERM technical adequacy and regulatory consistency is shown in Figure 5-1. This relationship resembles the relationship shown in Figure 3-2 of the Hanford vadose zone system conceptual model to the site-specific conceptual model required for waste site-specific applications.

Figure 5-1. Illustration of the Relationship Between the Model Use Documentation Associated with the Common Aspects of the Hanford *Site* Vadose Zone System and *That* Associated with Waste Site-Specific Information.



The model use elements documented in the following sections include the basis and rationale for the determination and/or estimation of model input parameters, and for the general aspects common to the evaluation of model uncertainties, model assumptions, and model limitations, all in the context of their impact on and applicability to the model results. The documentation of these elements also contributes to the technical basis for the modeling, and to the demonstration of consistency with Federal and state requirements.

5.1 MODEL PARAMETERIZATION

Vadose zone model parameter estimates are based almost entirely on data from site-specific studies and characterization efforts. This information and data have been compiled, summarized, and evaluated in databases; published in data packages; and/or published in other environmental investigation reports (e.g., limited field investigation reports, field investigation reports, and remedial field investigation reports). These data summaries and evaluations provide a basis for understanding the common aspects of (and fundamental relationships between) the parameter values, data sets, and populations. From the evaluation of the data sets comes the information and insight necessary to determine parameter best-estimate values, parameter ranges, and parameter variability, all of which are considered in the model parameterization and uncertainty analyses. New site-specific data are typically used both to augment these Hanford data sets and for site-specific model applications. A comprehensive list of all of the sources of information relevant to ERM parameterization is beyond the scope of this report, but examples of some of the major source documents that contain data compilations and estimates for the vadose zone conceptual model components parameters include the following: RPP-23748, WHC-SD-EN-TI-008, WHC-SD-EN-TI-012, RPP-26744, PNNL-14753, PNNL-14702b, PNNL-14744, and PNNL-13895.

These and other relevant documents serve as sources of information in the development of the Hanford vadose zone system and site-specific conceptual models, from which model parameter estimates are derived for use in site-specific ERMs. Examples of the types of parameters typically used in vadose zone fate and transport models are summarized in Table 5-1.

5.2 VADOSE ZONE MODEL UNCERTAINTY FACTORS AND CONSIDERATIONS

5.2.1 Model Uncertainties

Factors in the model selection process that can contribute to uncertainties for vadose zone modeling at the Hanford Site are addressed qualitatively in Section 4.0 (e.g., simplifying assumptions). Code-specific factors pertaining to the adequacy, benchmarking/calibrations, and QA/QC of candidate codes in general are addressed in the following subsections and to a specific candidate code in Section 6.0 and Section 8.2.

Table 5-1. Examples of Parameters Typically Used in Vadose Zone Fate and Transport Modeling.

Model Domain and Boundary Conditions
• Model domain dimensions (longitudinal and vertical dimensions, unit width (e.g., 1-m); saturated zone vertical dimension
• Waste site dimensions
• Grid size
• Boundary conditions (flow conditions at surface, sides, and bottom of domain boundaries)
Geologic Setting
• Geologic unit thicknesses; associated geologic properties (see hydrogeologic properties)
Source term
• Source-term (contaminated soil) dimensions (lateral and vertical)
• Source-term depths and depth intervals
• Source-term concentration(s)
Recharge rate(s) & moisture conditions
• Pre-operational, operational, post-remediation recharge rates
Vadose zone fluid transport and hydrogeologic properties
• Particle density
• Dry bulk density
• Saturated moisture content
• Residual moisture content
• Van Genuchten parameters
• Residual saturation
• Vertical saturated hydraulic conductivity
• Total porosity
• Longitudinal dispersivity
• Dispersion anisotropy
Geochemistry
• COC-specific Kd (± geologic unit-specific Kd values)
Groundwater domain and characteristics
• Average water table elevation
• Groundwater thickness
• Hydraulic gradient
• Average hydraulic conductivity

COC = contaminant of concern
Kd = instantaneous equilibrium distribution coefficient

5.2.2 Scenario and Conceptual Model Uncertainties

The conversion of qualitative conceptual model components or FEPs into a quantitative mathematical model typically involves simplifying the system being modeled and introducing uncertainty associated with the simplification. For example, a geologic conceptualization may be represented in a mathematical model as a simplified, layered geology with homogeneous layers. The linear isotherm Kd construct includes the assumption that porewater and soil concentrations equilibrate immediately and proportionally. The conceptual model and/or the mathematical model may be modified to reduce this uncertainty on the basis of new data or observations (PNNL-13091). These new data or observations may also foster improvements to the mathematical model that allow more rigorous representation of the conceptual model components or FEPs. Ultimately, the overall validity or accuracy of the conceptual model in representing the Hanford vadose zone system may or can be evaluated by comparing actual or analogous measurements to predictions or results from the corresponding mathematical model.

5.2.3 Parameter Uncertainties

Vadose zone model parameter uncertainty can result from the lack of adequate data and/or from variability in the data used to quantify a parameter. Parameter estimates based on site-specific data tend to have relatively low uncertainties. In vadose zone modeling at Hanford, parameters associated with the contaminant source term (i.e., quantity, extent, and depth) are the most significant sources of parameter uncertainty affecting model results because they are highly variable and are usually based on limited data. Recharge rate also has a large effect on vadose zone model results, but with less uncertainty because of the available site-specific data that form the basis for the estimates. Apart from waste configuration (contaminant source term), the sensitivity to model parameters also depends on the contaminant type. For mobile contaminants, the most significant parameter is recharge rate. For semi-mobile contaminants, significant parameters are the sorption coefficient (Kd value) and recharge rates. Parameter estimates representing the greatest sources of uncertainty, their nature and magnitude of effect on model results, and the relative confidence of the estimated values are listed in Table 5-2. An understanding of the magnitude and direction of the sensitivity model results to variability in key parameters of the Hanford vadose zone system can be ascertained from the results of the sensitivity analysis that have been performed to date (e.g., DOE/ORP-2005-01 and DOE/RL-2007-35).

Reviewing and comparing vadose zone parameter sensitivity analyses from Hanford and non-Hanford sources is instructive and demonstrates a number of important commonalities among the results. The most notable finding among non-Hanford vadose zone sensitivity analyses of hydrogeologic parameters is that the results consistently have the greatest sensitivity to infiltration/recharge rate, unsaturated zone thickness, and contaminant distribution coefficient parameters (e.g., NUREG/CR-5621, Beyeler et al. 1998, and PNL-7296). The uncertainties and sensitivities associated with most hydrogeologic parameters stemming from natural system heterogeneities have been found to be low (Table 5-2). Uncertainties associated with such parameters are a secondary source of overall uncertainty. The results of these sensitivity analyses appear to be consistent with the results of most vadose zone modeling sensitivity analyses conducted at Hanford, in terms of identifying which parameters have the greatest impact on the results. Those parameters representing the greatest sources of uncertainty, nature, and magnitude of effect on model results, as well as the relative confidence of representative best-estimate values, are listed in Table 5-2.

Table 5-2. Evaluation of Primary Parameter Uncertainty Factors in Hanford Site Vadose Zone Modeling.

Primary Parameter Uncertainty Factors	**Effect on Model Results**	**Confidence Level in Best-Estimate Parameters**
	Magnitude	**Qualitative Assessment**
Geologic setting Vadose zone thickness/depth to water table Stratigraphy/geologic units and characteristics (unit thickness, grain size, etc.)	Moderate to high	High
Contaminant source term Mass Depth Concentration Volume and geometry	High	Low to medium
Groundwater domain Hydraulic conductivity Hydraulic gradient	Moderate to high	Medium to high
Hydrogeology and fluid transport Hydraulic conductivity Porosity, permeability Dispersivity Anisotropy	Low	High
Recharge rates Undisturbed (vegetated) soil Operational period (bare, disturbed soil) Post-remediation period (disturbed, vegetated, time-averaged) Artificial recharge (discharge water; volume, timing)	Moderate to high	Medium to high
Geochemistry/contaminant behavior Contaminant release mechanism, parameter values (e.g., Kd, Ksp) Retardation/attenuation mechanism(s); parameter values (e.g., Kd)	Low to high	Medium to high

Kd = instantaneous equilibrium distribution coefficient
Ksp = solubility product constant

5.2.4 Determination of the Relative Importance of Parameters in an Uncertainty Analysis

The relative magnitude of uncertainty for certain vadose zone modeling parameters can be identified and compared using the coefficient of variation (i.e., the standard deviation divided by the mean value). This measure of uncertainty is based on a review of the literature and available databases. The sensitivity of the model results to their parameter values is a function of the model results and the coefficient of variation, which depend on site-specific conditions and exposure scenarios.

The main factors and parameters affecting Hanford vadose zone model results can also be qualitatively and/or semi-quantitatively evaluated using the results of sensitivity analyses from Hanford Site and other case studies. The relationships were described previously for evaluating the importance of model parameters to uncertainty in the model result and the relative importance of parameters in uncertainty analyses. These relationships are significant for Hanford vadose zone modeling because most parameters have low importance to the overall uncertainty in the model result, excluding contaminant source-term parameters (i.e., extent, depth, and mobility). Because the vadose zone model parameters are essentially all derived from site-specific data, most other parameters tend to have relatively low uncertainties.

5.2.5 Uncertainties/Errors Associated with Coupled Processes and Other Effects

The most likely sources of coupled uncertainties are hydrogeologic properties and their relationship to soil moisture-retention characteristics. Changes in soil retention characteristics may change the soil hydraulic conductivity, anisotropy, or recharge through the soil. Soil moisture content has been observed to affect anisotropy, while soil retention characteristics and recharge effect the soil moisture content. These parameters, individually or collectively, may affect the distribution coefficient of contaminants (Kd values). Effects of coupled hydrogeologic parameter variation on vadose zone modeling results are compiled in correlation coefficient matrices for 12 hydrogeologic parameters over a range of clastic sediment types (clay to sand) reported in PNNL-13091. In this summary, some significant positive and negative correlations were noted between several of the hydrogeologic parameters. However, no significant correlations between logically unrelated parameters were observed in the uncertainty evaluation of recent vadose zone modeling results (DOE/RL-2007-35).

Some characteristics that factor into the net average processes controlling fate and transport of contaminants through the vadose zone may or may not be accounted for directly in simplifying assumptions or in sensitivity analyses. Scaling effects for representing hydrogeologic properties (upscaling from laboratory to field-scale), spatial and temporal resolution of data, colloid transport, density effects, and thermal effects (PNNL-14702a) all can introduce uncertainty into vadose zone modeling, but for most risk assessment applications do not introduce uncertainty that is at least accounted for indirectly by the other sources of acknowledged uncertainty. Scaling effects resulting from the assignment of physical properties determined from laboratory studies (e.g., effective permeability, porosity, moisture-retention characteristics, anisotropy, and dispersivity) to larger modeled units can be addressed through physical property sensitivity analysis. Similarly, uncertainty introduced by the spatial and temporal resolution of data can be addressed through sensitivity and assumptions analysis. While certain models may have to include or consider colloidal transport as a key FEP, colloid formation or colloid-facilitated transport is not consequential at most waste sites at Hanford because of the low water contents and relatively simple geochemistry (PNNL-14702a). Likewise, thermal and density effects are not considered consequential in most, but not all, vadose zone model applications because below 10 m (32.8 ft) bgs, the temperature varies by less than 1°C (33.8°F) during the seasons. While the waste releases introduced immediate density and thermal gradients into the vadose zone, the gradients have been buffered by the capacity of the vadose zone and the time since the releases occurred, and they appear to have limited impact on contaminant transport in the future (RPP-7884).

5.3 EVALUATION OF VADOSE ZONE MODELING ASSUMPTIONS

An evaluation of the primary and largely common assumptions associated with the traditional vadose zone modeling approach at the Hanford Site is summarized in Table 5-3. The type (category) of assumptions, the magnitude and direction in which they impact model results, and the rationale for the assignment of model impacts are summarized in Table 5-3. In the context used here, "conservative" refers to conditions or parameter values that include a bias to yield model results with higher concentrations in groundwater and earlier arrival times than might reasonably be expected. Usually the bias compensates for some feature or process that is not well defined or insufficient data exist to characterize it adequately.

Table 5-3. Summary of the Type (Category) of Assumptions, Magnitude, and Direction in Which They Impact Model Results, and Rationale for the Assignment of Model Impacts. (3 pages)

Category	Assumption	Model Parameter Affected	Direction and Risk Impact of Model Result	Magnitude of Effect on Risk Estimate	Rationale/Evaluation of Assumptions
Geology	Numerical grid approximates geologic layers and sequences	Stratigraphy	Neutral	Low	Resolution and/or size of grid can be adjusted to include representation of the different geologic layers and sequences.
Hydrogeology and soil properties	Single values for associated physical/ hydrogeologic properties for each of the main stratigraphic units in the vadose zone	Hydrogeologic properties	Neutral	Low	Average up-scaled properties represent the bulk or average moisture flow in vadose zone reasonably well, based on evaluation results in the PNNL-15443 and laboratory tests on site-specific materials and field-scale testing reported in that document.
Transport	Vadose zone flow domain is dominated by aqueous phase drainage	Hydrogeologic parameters	None	None	The vadose zone flow domain is defined by aqueous phase drainage as opposed to transport mechanisms associated with other types of fluids (e.g., NAPLs) or phases (vapor-phase transport)
Source term	Entire source terms available for advective transport	Source term	Conservative	Low to high	This assumption is conservative because laboratory studies (e.g., Freehley et al. 2000) indicate that not all contaminants may available for advective transport in porous media (i.e., clastic sediments) due to multiple porosity effects (i.e., part of the mass transfer may be diffusion rather than advection controlled, or isolated in dead-end pore spaces). The assumption that 100% of contamination is available and transported by advective flow can over-estimate the mass transfer rate of contaminants to groundwater and under-estimate arrival times.
Hydrogeology and soil properties	Uniform matrix flow through porous media versus unstable (fingering) flow, preferential pathways	Hydrogeologic	Slightly non conservative	Neutral to low	The effects of the local connectivity and anisotropy structures are reasonably well represented, even when the detailed effects of fine-scale heterogeneities (e.g., preferential flow paths, fingering flow) are not captured (PNNL-15443).
Hydrogeology and soil properties	Horizontal to vertical anisotropy is adequately approximated by a constant 10:1 ratio	Anisotropy	Neutral	Low	This ratio is a conservative estimate describing lateral water movement in the modeling based on comparisons to moisture dependent anisotropy function values presented in Figures D2 through D6 in the RPP-17209, Rev. 1.
Domain	Two-dimensional vadose zone modeling is representative/	Hydrogeologic parameters	Conservative	High (10 to 40 times)	This assumption is conservative because it yields groundwater concentrations that are greater, and arrival times that are shorter, than

Table 5-3. Summary of the Type (Category) of Assumptions, Magnitude, and Direction in Which They Impact Model Results, and Rationale for the Assignment of Model Impacts. (3 pages)

Category	Assumption	Model Parameter Affected	Direction and Risk Impact of Model Result	Magnitude of Effect on Risk Estimate	Rationale/Evaluation of Assumptions
	adequate for purpose of evaluating groundwater risk/impacts				three-dimensional models; the transport of all water and contamination is restricted to the two-dimensional domain compared to more extensive spreading and sediment interaction (retardation) in a three-dimensional domain.
Recharge	Recharge rates are representative	Recharge rates	Conservative	Moderate	Recharge rates are biased toward higher values; the pre-Hanford and undisturbed ground value is regarded as appropriate for representing the natural (undisturbed) recharge conditions at waste sites prior to Hanford operations and for undisturbed soil elsewhere in the area (PNNL-14702a, PNNL-14702b, PNNL-14725a, PNNL-14725b); Best-estimate recharge rates generally represent values at the upper end of data distributions.
Geochemistry	Use of linear sorption isotherm construct (equilibrium partitioning behavior; Kd model) for description of geochemical behavior	Kd	Conservative	Moderate to high	The linear adsorption (Kd model) approach has been shown to adequately describe contaminant behavior when modeling vadose zone fate and transport for Hanford Site sediments under most circumstances involving far-field and/or low-impact sites where geochemical conditions remain fairly constant and contaminant loading of adsorption sites is low (PNNL-13895). However, in situations associated with large changes in chemical condition, especially in near-field environments, and/or certain disposal chemistry conditions (e.g., large variations in pH, alkaline concentrations, or complexing agents), the linear adsorption model may not be appropriate. Guidelines exist for selecting appropriate Kd values from the Hanford Kd database (PNNL-13895). In PNNL-13037 (Rev. 2), the authors note that Kd values selected for modeling purposes are typically the lowest value, or close to the lowest value of the range of values available in order to give a conservative estimate. This tends to over-estimate the transport of contaminants to groundwater.

Table 5-3. Summary of the Type (Category) of Assumptions, Magnitude, and Direction in Which They Impact Model Results, and Rationale for the Assignment of Model Impacts. (3 pages)

Category	Assumption	Model Parameter Affected	Direction and Risk Impact of Model Result	Magnitude of Effect on Risk Estimate	Rationale/Evaluation of Assumptions
Geochemistry	Instantaneous equilibrium between water and contaminants	Numerical model	Conservative	Variable	The assumption of instantaneous equilibrium between water and contaminants is conservative because laboratory studies of contaminated Hanford vadose zone sediments indicate that this assumption over-estimates observed mass transfer rates (PNNL-14594, PNNL-15121).
Geochemistry	Utilization of adsorption Kd values for both adsorption and desorption Kd values (for contaminant release)	Kd	Conservative	Moderate	This assumption is conservative, because laboratory studies show desorption Kd values to be greater than adsorption Kd values for COCs at Hanford (PNNL-14022, PNNL-14594, PNNL-13895).
Geochemistry	Mass transfer rate to groundwater based on Kd-based retardation	Kd	Conservative	Moderate to high	Model assumptions using Kd-based retardation can significantly over-estimate the mass transfer rate to groundwater compared to kinetic or solubility-limited release for some contaminants (uranium), as demonstrated in PNNL-15121, PNNL-14594, and RPP-7884.
Geochemistry	Discharge chemistry effects lower uranium (VI) Kd values	Kd	Conservative	Low to moderate	Assumptions involving the selection of low Kd values for some contaminants due to the observed effects of elevated pH, alkaline, and/or bicarbonate concentrations in porewater to reduce Kd values are not applicable to all waste sites at the Hanford Site or to behavior throughout the vadose zone. These effects on uranium Kd are limited to areas associated with such discharge compositions (tank farms near-field environments, and conditions of contaminant emplacement, but not necessarily contaminant release from contaminant-aged sediments).

COC = contaminant of concern
Kd = instantaneous equilibrium distribution coefficient
NAPL = nonaqueous phase liquid

The evaluation of these assumptions indicates that (1) most of the assumptions involve hydrogeologic and geochemical factors, (2) most of the assumptions are either conservative or neutral, (3) source-term uncertainty is potentially non-conservative, and (4) the majority of conservative assumptions range from moderate to high magnitudes in terms of their potential effect on risk and vadose zone model results. The evaluation of these assumptions indicates that, with the exception of the source-term uncertainty, the assumptions associated with model parameterization are largely conservative. Based on the assumptions evaluation, results of vadose zone modeling at Hanford should provide conservative estimates of risk in terms of impacts to groundwater from soil contaminants. This presupposes that the source term can be reasonably constrained or bounded and that care has been taken to ensure that the selection of parameters from the Hanford Site databases are both appropriate for the model conditions and within the range of plausible parameter variability.

5.4 LIMITATIONS IN THE APPLICABILITY OF VADOSE ZONE MODEL RESULTS

Vadose zone model limitations associated with the FEPs are considered during the model (Section 3.4) and code selection processes (Section 4.0). The limitations also address uncertainties in the model results. Some examples of common vadose zone model limitations at Hanford include the following:

- Simulating only Kd-controlled contaminant geochemical reaction and transport processes, which neglect surface complexation and precipitation

- Simulating contaminant release and retardation based on the assumption of reversible equilibrium conditions (i.e., the same Kd coefficients used for both adsorption and desorption, which neglect differing contaminant adsorption and desorption characteristics)

- Simulating bulk-flow and transport processes as described by the assumption of a porous media continuum, which homogenizes small-scale heterogeneity and discordant preferential pathways

- Simulating only predicted increase in groundwater contaminant concentrations (and incremental risk impacts to groundwater) from site-specific contaminant source terms, which neglects interaction with waste or discharges from other waste sites, or the accumulation of risk from one waste site to the next, unless included in the model domain or otherwise accounted for in the model design.

In general, the applicability of waste site-specific model results is limited by the site-specific conditions, parameters, and assumptions used in the model. The main exceptions are situations for which other site-specific conditions and intended purposes are sufficiently comparable or bounding, based on comparison of the magnitude of the similarities and/or differences in the context of the sensitivity analyses.

However, these may not necessarily represent limitations of the model or code; rather, they represent limitations associated with the most common use of the model/code and the applicability of the model results. Some examples of limitations in the applicability of vadose zone model results obtained using a specific set of waste site conditions and using waste site-specific parameters at Hanford include the following:

- Domain and scale limitations:
  - Results represent incremental groundwater risk/contamination
  - Limited to source-term components within the model domain
  - Limited to discharge impacts within the model domain
- Geologic setting limitations:
  - Results limited to modeled and comparable stratigraphy
  - Portions of the Hanford Site for which the vadose zone characteristics are comparable or bounding in terms of thickness and geology/stratigraphy

- Source-term limitations:
  - Results limited to modeled and comparable source-term distributions
  - Results limited to modeled and comparable source-term release mechanisms
- Groundwater domain limitations:
  - Limited to dilution effects within model domain based on site hydrologic properties
- Hydrogeologic parameter limitations:
  - Flow and transport is dominated by unsaturated porous media flow, with comparable or acceptably bounding moisture content profiles
  - Limited to values within the plausible range expected for the site
  - Limited to constant (unchanging) values over time
  - Limited to porous media continuum behavior
  - Preferential pathways not considered (e.g., discordant voids such as well seals/casing, clastic dikes, and sills)
- Recharge limitations:
  - Conditions similar to, or bounded by, the values of recharge rates evaluated in the models
- Geochemical limitations:
  - Limited to linear isotherm behavior for contaminant release and attenuation
  - Limited to assumption that adsorption Kd and desorption Kd values are equivalent
  - Contaminant behavior similar to, or within the range of, evaluated Kd values.

For the purposes of risk assessment applications, these limitations appear to be acceptable because the results represent reasonable (upper) bounding or limiting conditions, or the risk implications of the results are not sensitive to the limitations apart from those identified through the sensitivity analysis.

5.5 SUMMARY

The common aspects of the vadose zone system at the Hanford Site have implications for model selection and model use documentation. The expected documentation for the determination and/or estimation of model input parameters, and many aspects of the evaluation of model uncertainties, model assumptions, and model limitations share a common basis and rationale. The common aspects of model parameterization primarily involve the data compilations, summaries, and evaluations that collectively provide a basis for understanding the common aspects of, and fundamental relationships between, the parameter values, data sets, and populations for the Hanford vadose zone system. This information provides insight for the determination of parameter best-estimate values, parameter ranges, and parameter variability. The parameters typically used in vadose zone fate and transport modeling, and the parameters that generally have the greatest sources of uncertainty, are identified in Table 5-1. Expected documentation concerning the common aspects of uncertainty evaluations includes the identification of the nature and (qualitative) magnitude of their effect on model results, and a summary of the relative confidence of representative best-estimate values (Table 5-2).

An evaluation of the common assumptions and uncertainties associated with most vadose zone modeling is summarized in Table 5-3. These assumptions include the type (category), the magnitude and direction in which they impact model results, and the rationale for the assignment of model impacts (Table 5-3). It is indicated from the evaluation of these assumptions that most assumptions involve hydrogeologic and geochemical factors. Most assumptions are either conservative or neutral, with the exception of those concerning source terms, which are non-conservative. Also indicated is that the potential effect of the most conservative assumptions on calculated risk and/or vadose zone model results, range in magnitude from moderate to high. The evaluation of these assumptions indicates that the assumptions associated with model parameters are largely conservative, with the possible exception of the source term.

Documentation is also provided on the evaluation of the common aspects of vadose zone model limitations. This evaluation of common limitation includes those associated with the conceptual model FEPs, code selection processes, and uncertainties in the model results. These model limitations appear to be acceptable for risk characterization applications, because the results represent reasonable (upper) bounding or limiting conditions, or the risk implications of the results are not sensitive to the limitations apart from those identified through the sensitivity analysis.

The documentation on these common aspects of model use is intended to provide a basis and framework that supports the technical adequacy and regulatory consistency of most waste site-specific vadose zone modeling applications at Hanford. This documentation is intended to be amended with waste site- and application-specific information and documentation. The documentation of the common aspects of model use presented here fosters the development of the technical basis and the achievement of regulatory consistency.

6.0 APPLICATION OF THE CODE SELECTION PROCESS FOR VADOSE ZONE FATE AND TRANSPORT MODELING AT THE HANFORD SITE

This section presents an application of the code selection process. As noted in Federal guidelines, model selection and code selection are different, but related, activities. Model selection involves identification of the type and attributes of the computer simulation that are necessary for a meaningful simulation of the vadose zone system and code selection involves the choice of one or more specific computer code(s) capable of adequately implementing the selected model type (Section 2.6). Candidate codes are evaluated based on their ability to meet the model objectives, adequately express/represent the tasks to be modeled, and meet the identified requirements and attributes (EPA 402-R-94-012). The main steps associated with the code selection process and their relationships to the model selection process are summarized in Figure 2-1. The evaluation process involves determination of the capability of the code to meet (1) modeling objectives, (2) required model attributes, and (3) code-related criteria (EPA 402-R-94-012).

The following sections apply the code selection process to the STOMP code.

6.1 EVALUATION OF THE SUBSURFACE TRANSPORT OVER MULTIPLE PHASES (STOMP) CODE

The technical criteria in HNF-5294 are consistent with the model attributes and FEPs described in Section 3.5, and the administrative criteria are consistent with the other factors and criteria described in Section 6.2. Appendix A of RPP-18227 contains an evaluation of the STOMP code against these criteria and requirements. Although this evaluation was based on model criteria and attribute requirements identified in HNF-5294, these are comparable to those summarized in Table 6-1 because they were both developed specifically for vadose zone fate and transport modeling at Hanford's Central Plateau. The results of the evaluation show that the STOMP code is capable of meeting or exceeding the identified attributes and criteria necessary for the simulation of vadose zone flow and contaminant transport and assessment of groundwater impacts at Hanford. A summary of the documentation demonstrating the adequacy of the STOMP code for vadose zone fate and transport modeling at Hanford is presented in the following section.

Table 6-1 provides a summary of the main model attributes and code selection criteria that serve as the basis for demonstration of the adequacy of the STOMP code for use in vadose zone modeling at Hanford. The comparison of the code selection criteria to the STOMP code capabilities indicates that the STOMP code is capable of simulating all of the necessary FEPs and meets all of the other required code selection criteria. Several specific aspects of the adequacy of the STOMP code are provided in Section 6.4.1 that address aspects of the code selection criteria, including QA documentation of verification studies for specific model attributes (e.g., unsaturated flow, solute transport, infiltration, and drainage) and discussion of code-related criteria (i.e., intercede comparison, hardware requirements, solution methodology, dimensionality, and output). Information on verification studies not included in or required by the model attributes (e.g., density-driven flow and transport, nonaqueous phase liquid [NAPL] transport, and heat flow) are also included in these discussions for completeness and demonstration of additional capabilities of the STOMP code.

Table 6-1. Summary of the Model Attributes and Code-Related Criteria Required for Vadose Zone Fate and Transport Modeling at the Hanford Site and Comparison to the Capabilities of the STOMP Computer Code. (2 pages)

Code Selection Criteria Based on Model Attributes, FEPs, and Code-Related Criteria	STOMP Code Capabilities
Features	
Fluid properties	X
Hydrogeologic conditions:	X
– Capillary retention	X
– Fluid pressure and saturation distribution	X
– Geology	X
Hydrogeologic material properties:	X
– Porous media	X
– Physical characteristics	X
– Vadose zone thickness (depth to groundwater)	X
Events	
Recharge	X
Source terms/releases:	X
– Water	X
– Contaminants	X
Processes	
Physical transport mechanisms/rates	X
Advection	X
Vadose zone drainage	X
Estimating time (year) of peak concentrations in groundwater	X
Hydrodynamic dispersion	X
Molecular diffusion	X
Spatial movement of contaminants within and between media	X
Physical and chemical interactions:	X
– Desorption	X
– Solubility-based release/precipitate	X
– Sorption	X
Capillary fringe:	X
– Capillary action	X
– Drainage	X
Radioactive decay	X

Table 6-1. Summary of the Model Attributes and Code-Related Criteria Required for Vadose Zone Fate and Transport Modeling at the Hanford Site and Comparison to the Capabilities of the STOMP Computer Code. (2 pages)

Code Selection Criteria Based on Model Attributes, FEPs, and Code-Related Criteria	STOMP Code Capabilities
Groundwater Transport[a]	
Dilution	X
Other Criteria	
Solution methodology	X
Model dimensionality	X
Time (year) peak concentrations in groundwater	X
(Spatial) movement of contaminants within and between media	X
Core-Related Criteria	
Source code availability	X
History of use and acceptance in the scientific community	X
Code usability	X
Quality assurance:	X
– Code documentation	X
– Code testing (e.g., verification and validation)	X
Hardware requirements	X
Solution methodology (consistency with model attribute requirements)	X
Code dimensionality (consistency with model attribute requirements)	X
Code output (consistency with model attribute requirements)	X

[a] Groundwater transport is not a vadose zone FEP. It is included in this table because it is an important factor in calculating the contaminant concentration results for the indicated methods.

FEPs = features, events, and processes

STOMP = Subsurface Transport Over Multiple Phases

6.2 DOCUMENTATION OF THE ADEQUACY OF THE STOMP CODE FOR VADOSE ZONE FATE AND TRANSPORT MODELING AT THE HANFORD SITE

Based on the model and code selection criteria identified and summarized in Table 6-1, the model complexity required for vadose zone fate and transport modeling for risk-based assessments for groundwater protection is a semi-complex, two-dimensional fate and transport model that includes some features from complex models (two-dimensional and three-dimensional). As noted in Table 6-1, the STOMP code possesses the capabilities associated with the level of model complexity necessary for vadose zone modeling at the Hanford Site. The STOMP code is capable of one-, two-, and three-dimensional, multi-phase simulations with essentially unlimited heterogeneous and anisotropic layers. The gridding scheme allows for almost any scale of problem, including some grid refinement techniques to evaluate some preferential flow pathways. Certain add-on modules extend the capability of the code to include chemically enhanced permeability, colloidal transport, and reactive transport, while others extend the capability to include meteorological and barometric effects. The code can accommodate episodic and seasonal variations in input parameters and variations associated with long-term climate changes, and can provide output for both the near and long term. The code can also account for radiological, biological, and inorganic decay.

6.2.1 STOMP Acceptability Documentation

6.2.1.1 Source Code Availability

The STOMP simulator is a finite-difference code developed by and available from Pacific Northwest National Laboratory (PNNL) for analyzing multi-phase subsurface flow and transport. The STOMP code development is managed under a configuration management plan (PNNL-SA-54023) in conjunction with a software test plan (PNNL-SA-54022) (both only available from PNNL) that detail the procedures used to test, document, and archive modifications to the source code. The STOMP code development is also supported by a software specifications document (PNNL-SA-54079), as well as a software design document (PNNL-SA-54078) (both also only available from PNNL).

6.2.1.2 History of Use and Acceptance in the Scientific Community

The scientific theory upon which the code is based is documented in PNNL-12030. Subsurface flow and contaminant transport are generated from the numerical solution of non-linear partial differential equations that describe subsurface environment flow and transport phenomena. The STOMP code's capabilities include the simulation of saturated and unsaturated flow regimes, transport of radioactive elements and non-decaying contaminants, and transport of aqueous phase and nonaqueous phase organics. The STOMP code has also been used extensively at Hanford to simulate vadose zone flow and contaminant transport for various remedial and corrective actions (PNNL-11310, PNNL-12192, PNWD-3111, PNNL-65410, DOE/RL-2003-23).

6.2.1.3 Code Usability

The STOMP code is not a simple code to apply; however, it meets the selection criteria for vadose zone modeling at Hanford. Use of the STOMP code is supported by application guides, user's guides, and theory guides maintained by PNNL. The use and application of the STOMP code requires knowledge and understanding of, as well as experience with Fortran. To augment dissemination and usage of the code in the scientific community, PNNL provides short courses taught by the code developers to instruct new users how to apply the STOMP code to a variety of examples of varying complexity. Additional lecture topics address documentation, governing equations, constitutive relations, numerical solution schemes, algorithms, applications, parallel computing, and future development plans for the simulator (http://stomp.pnl.gov/stomp_course.stm).

6.2.1.4 Quality Assurance

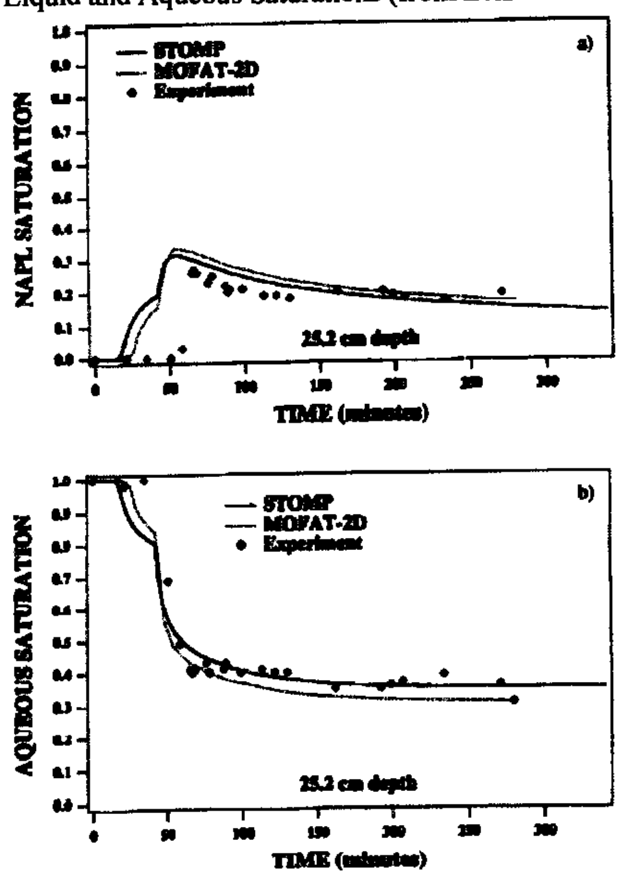
The QC for the STOMP source code is currently maintained under configuration control procedures by PNNL. The STOMP code development is managed under a configuration management plan in conjunction with a software test plan that detail the procedures used to test, document and archive modifications to the source code. Formal procedures for software problem reporting and corrective actions for software errors and updates are maintained and rigorously implemented. Documentation of all verification and validation testing is publicly available.

The QA overview includes the results of verification and validation tests. The process of comparing model output with either analytical or other numerical model results is known as model verification. Model validation, however, compares output from a verified model with independent laboratory or field data. Generally, validation studies are performed at the laboratory scale, where sediments are well characterized and driving forces are controlled. The STOMP code verification and validation studies have been carried out since its inception. As new capabilities are incorporated into the simulator, model results are compared against both analytical and other numerical solutions for both old and new capabilities. Although internal records of tests are maintained at PNNL (and are publicly available upon request), many of the verification and validation studies have been published in PNNL documents and peer-reviewed journals. A brief overview of some of these results is presented in this section.

6.2.2 Initial Verification and Validation Examples

Early in the STOMP simulator's development, three-phase flow verification and validation studies were published in a peer-reviewed journal (White et al. 1995, Lenhard et al. 1995). In this work, the STOMP code was tested against simulation results from a published numerical code, MOFAT-2D (Kaluarachchi and Parker 1989), and against non-hysteretic and hysteretic data from three-phase flow experiments. Figure 6-1 plots NAPL and aqueous saturations against time for a 25.2-cm depth in the experimental column. These results demonstrate good agreement between the STOMP and MOFAT-2D simulations, as well as good agreement between the simulated and measured data.

Figure 6-1. Experimental and Simulation Results at the 25.2-cm Depth for Nonaqueous Phase Liquid and Aqueous Saturations (from Lenhard et al. 1995).



6.2.3 Application Guide Verification and Validation Examples

Additional verification studies for thermal and hydrogeologic flow and transport examples are presented in the STOMP application guide (PNNL-11216). The examples in this guide are selected to demonstrate the STOMP code capabilities, as well as to serve as verification and benchmark cases that could be compared to analytical solutions or to results reported elsewhere in the literature using other computer codes. Results presented in this report verified the STOMP code solution for flow and transport in fully saturated media, flow and transport in variably saturated media, salt-water intrusion and density-driven flow, non-isothermal flow, heat pipe flow and transport, and NAPL flow and transport. The examples presented here were selected based on capabilities needed to represent FEPs and simulate flow and transport at the Hanford Site. For more detailed descriptions of the test examples, see PNNL-11216.

6.2.4 Unsaturated Flow

The STOMP application guide presents verification and validation studies for unsaturated flow and transport. Traditionally, this two-phase flow problem involving air and water is reduced to a single-phase problem by assuming that the air phase is at constant atmospheric pressure. A case is presented that uses this constant atmospheric pressure assumption where results generated by the STOMP simulator are compared to experimental data provided by Ségol (1994). Hills et al. (1989) (as reported by Ségol in a personal communication) used Haverkamp et al. (1977) problem definition and results to test alternative pressure-based and moisture-content-based formulations for infiltration, with the ultimate objective being the development of an algorithm capable of addressing infiltration into very dry soils.

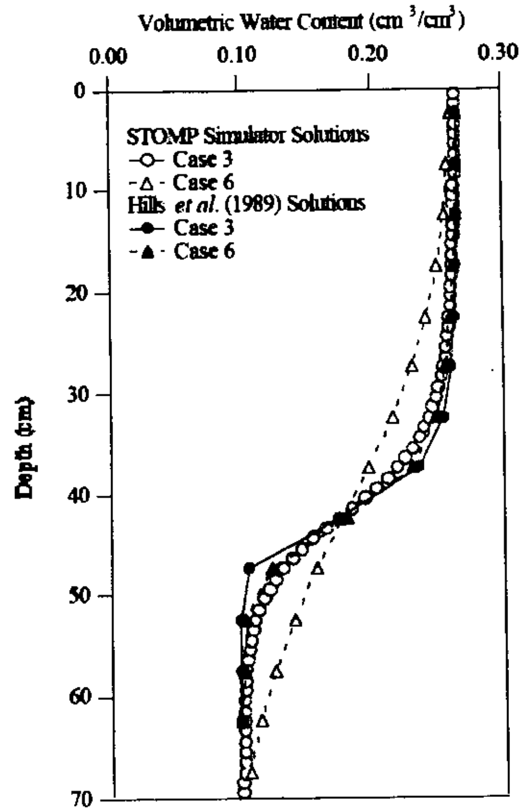
The solutions obtained using the STOMP simulator for two test cases (labeled Case 3 and Case 6) are displayed in Figure 6-2, along with the computational results reported in Ségol (1994). In Case 3, good agreement is obtained between the STOMP code and the Hills et al. (1989) solution; in Case 6, however, the STOMP code wetting front is not as sharp. In the STOMP code, temporal and spatial refinement is required to obtain a sharply defined wetting front that would match the Hills et al. (1989) solution. The Hills et al. (1989) model, however, was optimized for infiltration into very dry soils, and the refined temporal and spatial resolution is not required.

6.2.5 Solute Transport

Also presented in the STOMP application guide are verification examples for solute transport. In a one-dimensional transport example, assuming a fully saturated porous medium, concentration profiles predicted by the STOMP code are compared to results generated by an analytical solution. In Figure 6-3, results are presented for a Peclet number of 0.2 and five different values of the Courant number. (The Peclet number is defined as is a measure of the relative importance of advection to diffusion, whereas the Courant number is the ratio of a time step to a cell residence time). These results demonstrate that for a Peclet number (Pe) of 0.2, both the Patankar and total variation diminishing (TVD) transport schemes yield solutions close to the analytical results. Other results presented in PNNL-11216 demonstrate that when advection dominates (higher values of the Peclet number), the TVD transport scheme is superior to the Patankar scheme in simulating a sharp transport front.

Figure 6-4 provides further verification of the STOMP numerical transport solution, where an analytical solution for a "patch concentration" problem is used (Cleary and Ungs 1978). In this example, a fixed-concentration boundary condition is used as source in a steady, uniform, two-dimensional flow field that represents a fully saturated and confined aquifer. For all three times, STOMP's TVD transport predictions show a good match with the analytical solution.

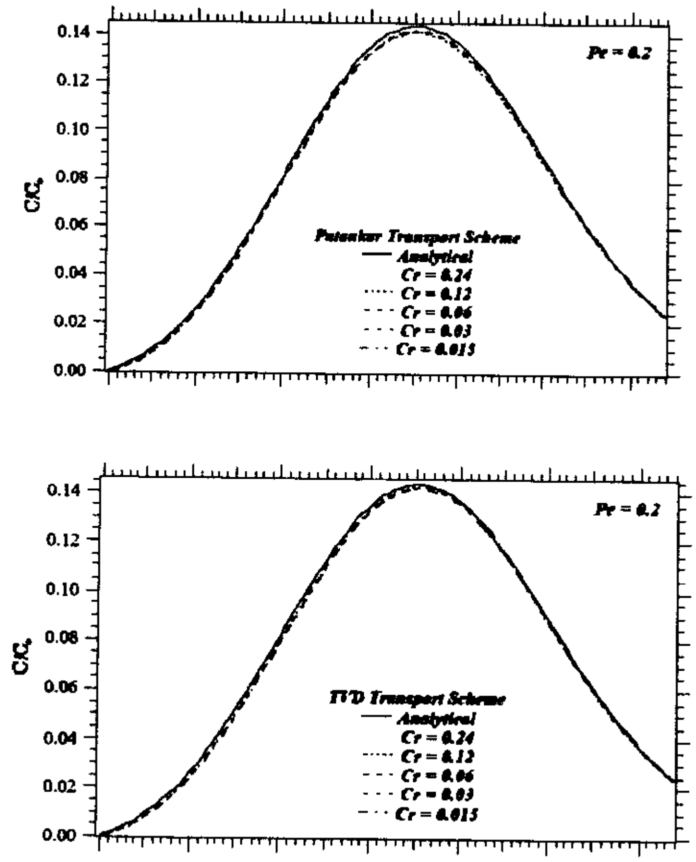
Figure 6-2. Comparison of the STOMP Code and Hills et al. (1989) Solutions to the Haverkamp et al. (1977) Infiltration Example.



6.2.6 Density-Driven Flow and Transport

Henry's Problem is a classic problem that describes the advance of a diffused salt-water wedge in a confined aquifer initially filled with fresh water. This application was presented in the STOMP application guide to demonstrate the coupled flow and transport capabilities of the STOMP simulator. Although these capabilities have been specifically written for salt-water brines, other solutes could be considered by changing the algorithms for computing the brine properties (e.g., density and viscosity). Results of the comparison are shown in Figure 6-5, which demonstrate good agreement between analytical and numerical solutions for the concentration distribution.

Figure 6-3. Comparison of Analytical and Numerical Relative Concentration Data for Two Different Transport Schemes in STOMP.



NOTE: Results are for a one-dimensional transport problem with a uniform, steady flow field (from PNNL-11216).

Figure 6-4. Longitudinal Concentration Profiles at y = 1 Along the x-Direction for the Patch Source Example (from PNNL-11216).

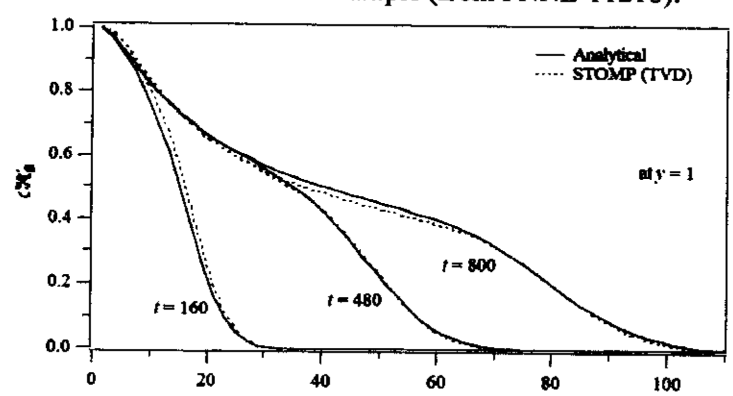
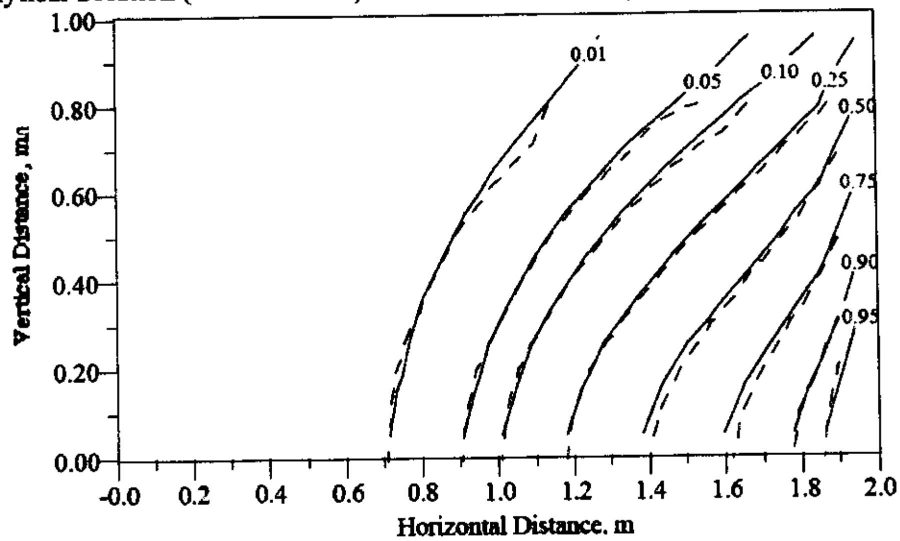


Figure 6-5. Steady-State Concentration Distribution from the STOMP Solution (Solid Lines) with the Ségol Analytical Solution (Dashed Lines) for the Classical Henry's Problem (from PNNL-11216).

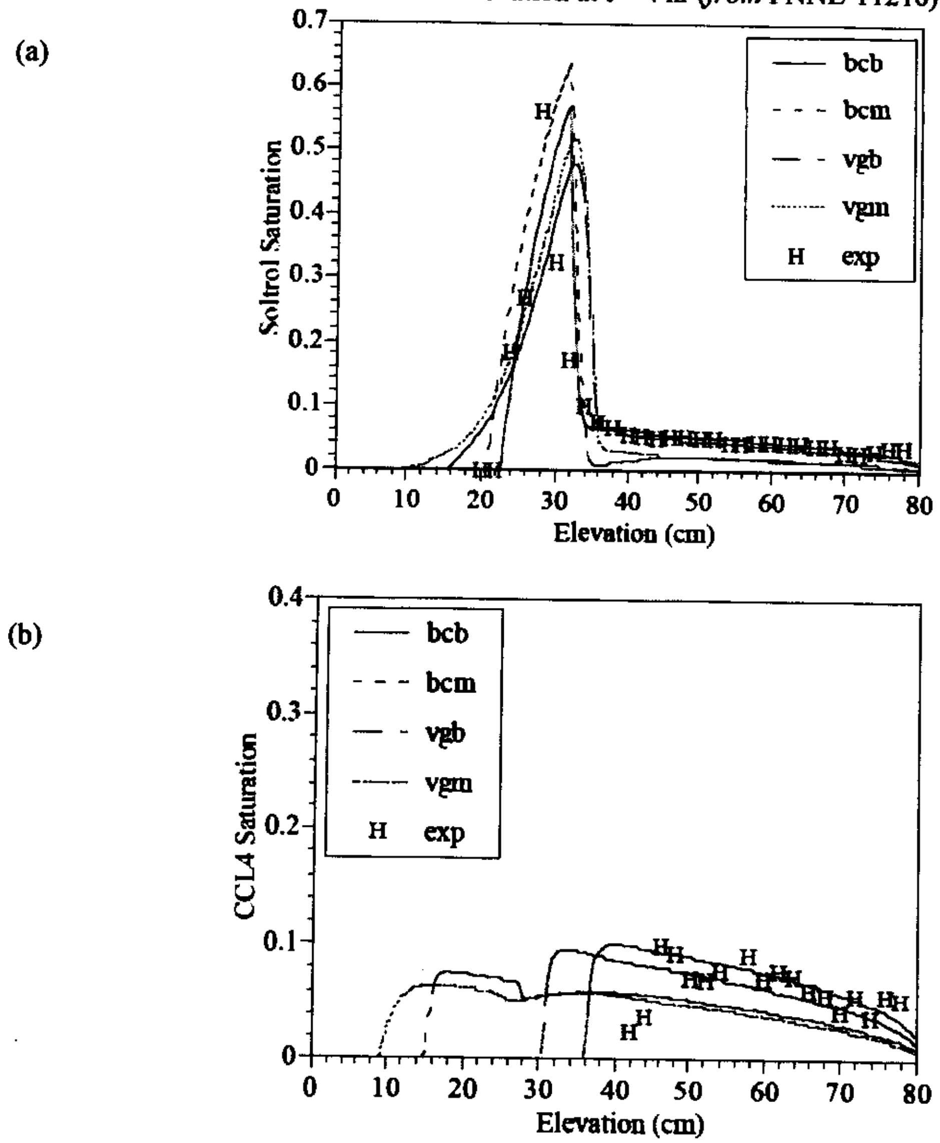


6.2.7 Nonaqueous Phase Liquid Transport

The application guide presents a validation case where STOMP simulation results are compared with experimentally determined fluid saturations during the infiltration and redistribution of a light NAPL (Soltrol®) and a dense NAPL (carbon tetrachloride) in a partly saturated one-dimensional column (Oostrom et al. 1995). The main objective is to evaluate the performance of the Brooks and Corey and the van Genuchten pressure-saturation relations in combination with either the Burdine of Mualem pore-size distribution model. The experimentally determined fluid saturations are compared with simulated results from four relative permeability-saturation-pressure (k-S-p) models. The four models are the Brooks and Corey-Burdine (BCB), Brooks and Corey-Mualem (BCM), van Genuchten-Burdine (VGB), and van Genuchten-Mualem (VGM) models. It was shown (see Figure 6-6) that Brooks-Corey capillary-pressure relations in combination with the Burdine pore-size distribution model yield the best agreement between experimental and simulated NAPL saturations for infiltration and redistribution of Soltrol and carbon tetrachloride in the unsaturated zone of sand.

Soltrol® is a registered trademark of Chevron Phillips Chemical Company, The Woodlands, Texas.

Figure 6-6. (a) Soltrol Saturation versus Elevation at t = 72 hr, and (b) Carbon Tetrachloride Saturation versus Elevation at t = 4 hr (*from* PNNL-11216).



6.3 SUPPLEMENTAL VERIFICATION AND PARTIAL VALIDATION EXAMPLES

Additional verification examples are presented in PNNL-15465 that describe the theory implemented in the STOMP code for the sparse vegetation evapotranspiration model (i.e., engineered barrier). The verification examples include tests for infiltration, drainage, and heat flow in a homogeneous and layered system from the UNSAT-H problem set (PNNL-13249). In addition to these examples, the barrier simulations reported in the intercode comparison found in Scanlon et al. (2002) are included both for verification and to establish a benchmark for STOMP code users. Only brief descriptions of the test examples are presented. For more detailed descriptions, see PNNL-15465.

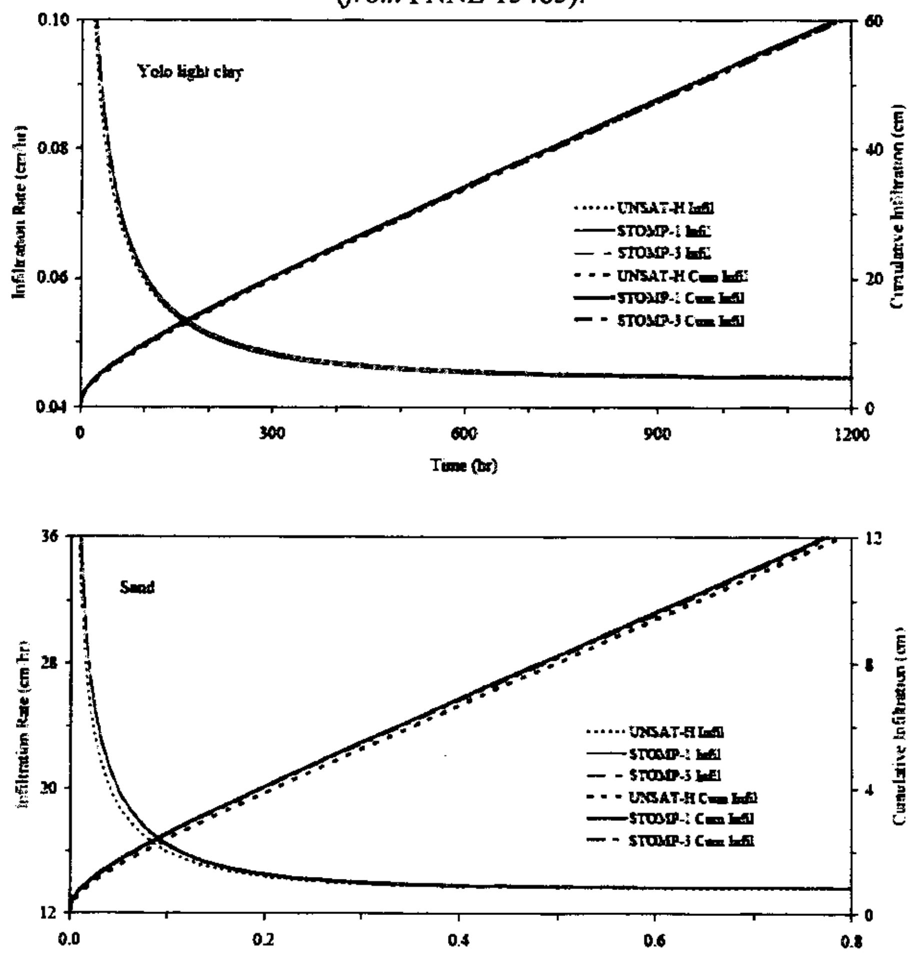
6.3.1 Infiltration

For the infiltration verification and validation, the problem of isothermal infiltration into Yolo light clay and sand, as reported by Haverkamp et al. (1977), was selected. This example is based on the simulation of ponded and non-ponded isothermal infiltration into Yolo light clay and soil, as reported by Haverkamp et al. (1977). The infiltration process was simulated with both STOMP-W (water mode) and STOMP-WAE (water-air-energy). Figure 6-7 compares the results of the STOMP-W and STOMP-WAE simulations with those of UNSAT-H, and demonstrates that the STOMP code converged to the established solutions for the two soils in comparable times. In general, the agreement between the results of UNSAT-H (PNNL-13249) and the STOMP simulator (STOMP-W and STOMP-WAE) is good, thereby verifying the infiltration component of the STOMP code.

Figure 6-7. Infiltration Rate and Cumulative Infiltration Versus Time in Yolo Clay Soil for STOMP-W, STOMP-WAE, and UNSAT-H for (a) Yolo Clay and (b) Sand (*from* PNNL-15465).

(a)

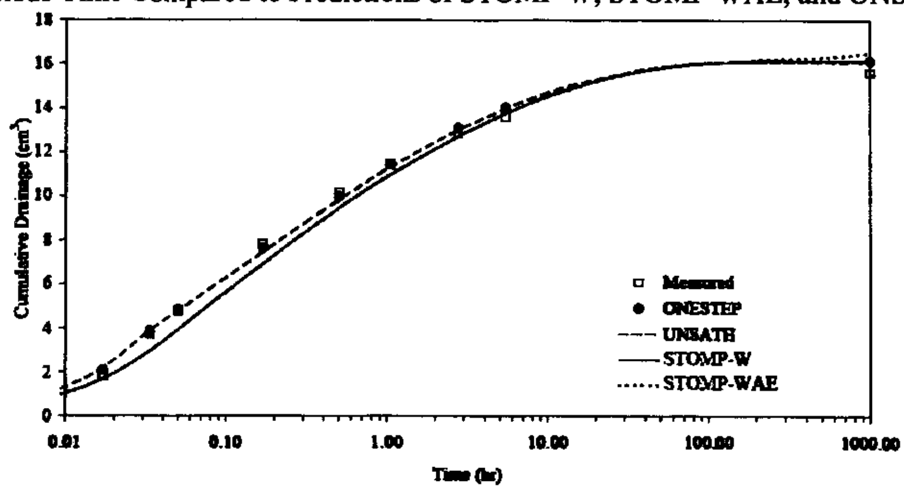
(b)



6.3.2 Drainage

To verify and validate the drainage component of the STOMP code, the experiment of Kool et al. (1985) is simulated with the STOMP code and compared to both the experimental data and the numerical simulation results from UNSAT-H. In the Kool et al. (1985) experiment, drainage was monitored on an undisturbed core of a silt loam from a field in Virginia. Kool et al. (1985) measured the water content and unsaturated hydraulic conductivity in the laboratory, but the unsaturated hydraulic properties used in the van Genuchten equation were obtained by inverse modeling. Figure 6-8 compares the cumulative outflow predicted by UNSAT-H and the STOMP code with the laboratory measurements and predictions from Kool et al. (1985). Overall, the agreement between the STOMP code predictions, the observed data, and UNSAT-H is good. However, neither the STOMP code nor UNSAT-H was able to duplicate the approximation used by Kool et al. (1985) to describe flow in portions of the core that remained saturated during the very early times of drainage. However, this difference between the models should not significantly affect the comparison because saturated conditions in the simulated core disappeared after less than 0.01 hr.

Figure 6-8. Cumulative Drainage Versus Time as Measured by Kool et al. (1985) and Versus Time Compared to Predictions of STOMP-W, STOMP-WAE, and UNSAT-H.



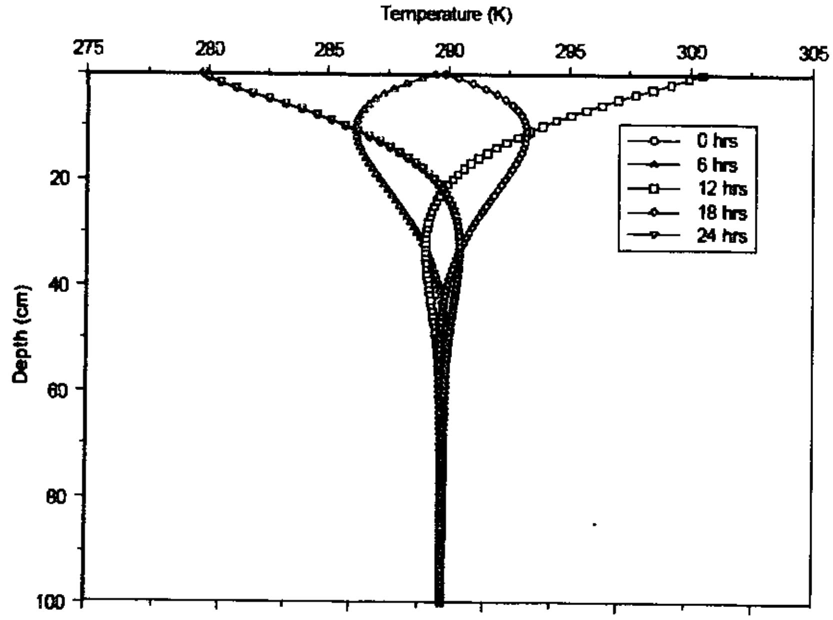
NOTE: STOMP-W and STOMP-WAE are mostly indistinguishable (PNNL-15465).

6.3.3 Heat Flow

In unsaturated soils, water vapor flow is an important heat transport mechanism; thus, the capability to accurately simulate heat transport is a prerequisite for modeling flow in non-isothermal systems. To verify the energy component of the STOMP code, diurnal variations in soil temperatures caused by a sinusoidal variation in temperature at the soil surface were simulated. An analytical solution for this type of heat conduction problem has been reported in Campbell (1977). For this heat verification problem, a 1-m (3.3-ft)-deep soil profile consisting of loamy sand is considered. This soil type is representative of many of the near-surface sediments at Hanford, is present in the 300-N Vadose Zone Lysimeter Facility, and is sometimes referred to as the L-soil (PNL-6488). Vapor flow is not included so water contents and thermal conductivities remain constant during the simulation.

Figure 6-9 compares the STOMP-WAE predicted temperature profiles with those predicted by the analytical solution. The agreement between the analytical solution and the simulated temperatures at all depths and times indicates that STOMP-WAE correctly solves the heat conduction equation. More importantly, these results suggest that the use of representative physical, hydraulic, and thermal properties of Hanford Site sediments should allow accurate prediction of the temperature changes as saturation changes.

Figure 6-9. Soil Temperature as a Function of Depth as Determined by the Analytical Solution (*S*ymbols) and STOMP-WAE (*L*ines).



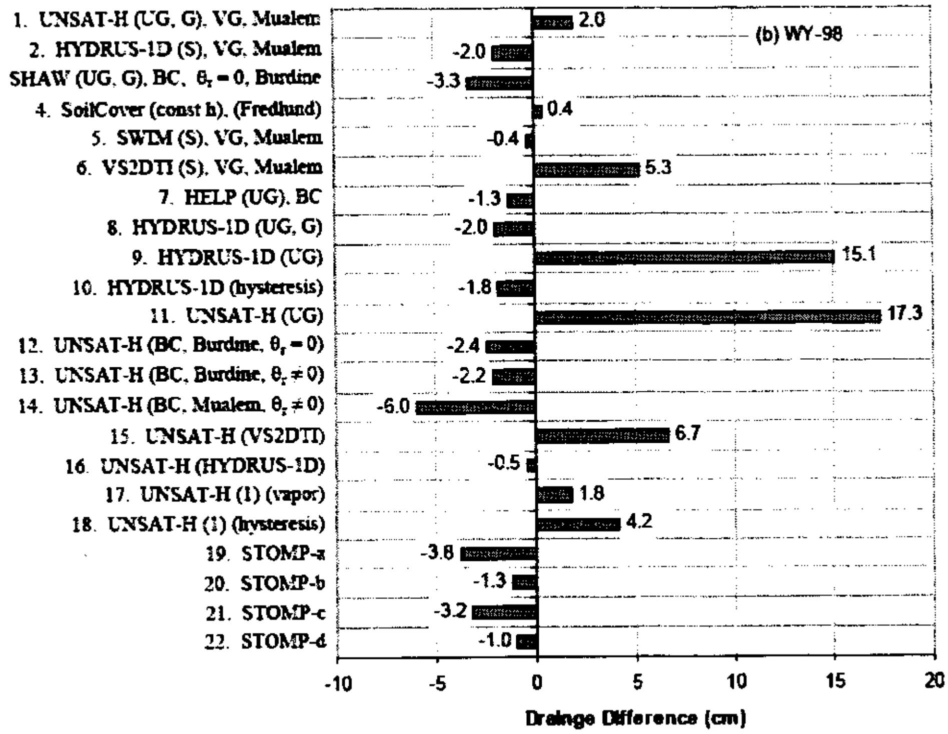
6.3.4 Intercode Comparison

Scanlon et al. (2002) reported on an intercode comparison study aimed at comparing the water-balance simulation results from seven different codes, including HELP, HYDRUS-1D, SHAW, SoilCover, SWIM, UNSAT-H, and VS2DTI. The comparison was based on 1- to 3-year water-balance monitoring data from the Idaho National Engineering and Environmental Laboratory in southeastern Idaho. This example was chosen as a benchmark problem for STOMP in PNNL-15465.

The site and soil information can be found in Scanlon et al. (2002). Details on parameter identification, hourly meteorological data, and problem setup are outlined in PNNL-15465. To perform the verification, four different STOMP simulations were executed with different values of saturated hydraulic conductivity and aerodynamic roughness length. Measured and simulated water balances for the Idaho site were compared for three different time periods. However, only representative results for a single water year and single water-balance component are presented in this document. PNNL-15465 provides descriptions of other components and water years included in the intercode comparison.

Although simulation results from most codes were similar and reasonably approximated measured water-balance components, the STOMP code results were consistently associated with the smallest error. In Figure 6-10, a positive value indicates over-predication while a negative value indicates an under-prediction. For all 22 simulations, these differences vary from -6.0 and 17.3 cm for the water year 1998 (WY98), whereas the results of the four STOMP code simulations were within -3.8 to -1.0 for STOMP code simulations.

Figure 6-10. Differences Between Simulated Drainage and the Measured Values (*in* cm) for Water *in* 1998.



In addition to the QA requirements pertaining to the development and management of the STOMP code at PNNL, there are also QA requirements associated with usage of the code by other Hanford contractors. Example QA (QA plan and testing) and QC (configuration management) requirements for the STOMP code for other Hanford contractors are presented in RPP-18226, RPP-18227, and RPP-18228. In general, these QA requirements are limited to demonstrating the integrity of the executable file after the Fortran source code has been compiled with the commons file and the user-prepared (problem-specific) parameter files on the system operating it. This is accomplished by executing the documented test cases that PNNL used to verify and benchmark the code and comparing the resulting files to files provided by PNNL (e.g., RPP-25859).

6.3.4.1 Hardware Requirements

Written in Fortran with extensions for parallel implementation, the STOMP code has been executed on a variety of platforms at national laboratories, government agencies, private companies, and universities. The STOMP code is a commercial off-the-shelf code (obtainable from PNNL), which requires a compiler to compile the code with a "commons file" and a "problem-specific parameters file." Full optimization of the simulator has been successful on several workstations and mainframe computers. The current configuration management requirements for the STOMP code at CH2M Hill Hanford Group, Inc. limit its operation to stand-alone computers (Intel Xeon Processor, 3.06 GHz, 2GB DDR266 SDRAM memory) with a UNIX® or LINUX® operating system (RPP-18228), which provides an indication of the computer hardware necessary to operate the code practically.

UNIX® is a registered trademark of The Open Group, San Francisco, California.
LINUX® is a registered trademark of Linus Torvalds.

6.3.4.2 Solution Methodology

The STOMP code is a finite-difference code for analyzing multi-phase subsurface flow and transport founded on the conservation of mass and energy equations, with constitutive functions relating the relevant properties to the conservation equations. The fundamental equations are solved using an integral volume finite-difference approach, with the linear systems of equations solved using a direct-banded matrix solver, an unsymmetric pattern, multi-frontal package, or an indirect conjugant gradient-based solver (PNNL-12030). A complete description of the actual equations and the partial differential approximations are contained in the user's guide (PNNL-15782), theory guide (PNNL-12030), and theory guide addendums (PNNL-15465, PNNL-15482).

6.3.4.3 Code Dimensionality

The STOMP code is capable of simulating vadose zone flow and transport in one, two, or three dimensions. The only limitations associated with dimensionality regard the hardware capabilities of the computer system executing the code.

6.3.4.4 Code Output

The STOMP code is capable of generating several types of output to meet any practical output requirements. The STOMP code is capable of generating output files with results of specific variables presented for specific nodes within the model domain identified in the input file by the STOMP code user. The STOMP code is also capable of generating plot files, which contain the results of specific variables for every node in the model domain for a specific time during the execution period. Finally, the STOMP code is capable of generating surface files with flux rate and integral results of specific variables across specific planes within the model domain, including planes across boundary conditions, identified by the code user.

6.4 SUMMARY OF THE STOMP CODE EVALUATION AND ACCEPTABILITY

The STOMP simulator is a robust tool that can be successfully applied at Hanford. However, the validity of STOMP code predictions is highly dependent on the conceptual model and the data available to support its development and incorporation into the numerical modeling framework. Spatial and temporal discretization, appropriate boundary condition assignment, and hydraulic parameter estimates are all examples of factors that impact results independent of any STOMP code capabilities or limitations. Identification of FEPs is a critical step in model development. Because STOMP code developers are located onsite, any FEPs not currently represented in the STOMP simulator can be incorporated into the simulator following strict QA/QC procedures supported by PNNL. Alternatively, any limitations in either the conceptual model or its implementation within the STOMP code may be acceptable for the purposes of risk assessment applications, if simplifying assumptions in the model provide conservative bounding, or limiting conditions, or have risk implications insensitive to the limitations.

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7.0 CONSISTENCY WITH FEDERAL REQUIREMENTS AND GUIDELINES

Consistency with the Federal requirements and guidelines identified in Section 2.0 pertaining to the selection and use of ERMs is achieved by means of the documentation associated with the application of the guidelines. This documentation includes the description of the technical basis, rationale, and processes used in the selection and/or use of an ERM. The general documentation elements recommended by EPA for the selection and use of ERMs (CREM 2003) involve the following general model documentation elements:

- Method/model selection:
  - General management objectives (identification of problem and objectives of the modeling)
  - Conceptual model development
  - Choice of technical approach (method, model, and code selection)
- Model use:
  - Parameter estimation
  - Uncertainty/error evaluation
  - Assumption evaluation
  - Limitations in the applicability of model results
  - Evaluation of model results (conclusions in relationship to management objectives)
  - Recommendations.

These requirements and guidelines are summarized in Table 7-1, where they are divided into two main categories: (1) those pertaining to method, model, and code selection (***green*** headings); and 2) those pertaining to the model use and the use of the results in risk-based applications (***orange*** headings). These requirements are also cross-referenced in Table 7-1, with the specific locations in this document where documentation is provided that pertain to the demonstration and/or support of consistency with the identified Federal ERM documentation elements.

7.1 METHOD/MODEL-TYPE AND CODE SELECTION

The method selection process involved the application of all elements of the Federal guidelines on ERM model selection, which include the following steps:

1. Identify the problem and define the objectives and regulatory purpose of the modeling.
2. Develop a conceptual model and conceptual model components.
3. Determine principal FEPs to be modeled.
4. Identify other factors and requirements to be considered as required model attributes and selection criteria.
5. Select an appropriate model type:
   a. Evaluate candidate methods/models possessing the required attributes for their ability to meet the model criteria.
   b. Select the appropriate ERM model type that possesses the required model attributes and is capable of meeting the modeling objectives.

Table 7-1. Documentation Elements for Consistency with Federal Requirements and Guidelines for the Use of Environmental Regulatory Models.

<table>
<tr><th colspan="4">Federal Compliance Elements and Requirements for the Selection and Use of Environmental Regulatory Models (ERMs) for Risk Based Applications</th><th>Location (Chapter/Section) in this Document</th></tr>
<tr><td rowspan="6">Model/Method Selection</td><td colspan="3">Purpose/Objectives</td><td>1.0, 3.0, 4.1</td></tr>
<tr><td colspan="3">Rationale of need/use for modeling</td><td>2.2</td></tr>
<tr><td colspan="3">Conceptual model(s); description of processes, mechanisms, phenomenon, site and system (i.e., vadose zone) characteristics to be considered</td><td>4.2</td></tr>
<tr><td colspan="3">Determine nature and types of primary system (i.e., vadose zone) FEPs and predictive tasks to be modeled</td><td>4.3</td></tr>
<tr><td colspan="3">Assess/determine other required model requirements/attributes</td><td>4.3</td></tr>
<tr><td colspan="3">Method selection/documentation</td><td>4.3</td></tr>
<tr><td rowspan="2">Code Selection</td><td colspan="3">Evaluation/assessment of adequacy/capabilities of candidate codes (vs. required model attributes)</td><td>6.0</td></tr>
<tr><td colspan="3">Consideration of code-related criteria (characteristics, QA, etc.) and administrative criteria</td><td>6.2, 8.4</td></tr>
<tr><td rowspan="8">Model Use Documentation</td><td rowspan="3">Model Parameterization</td><td colspan="2">Boundary conditions</td><td>Application-Specific</td></tr>
<tr><td colspan="2">Data sources, methods, pedigree</td><td>4.2 + Application-Specific</td></tr>
<tr><td colspan="2">Rationale for parameter estimation & selection</td><td>4.2 + Application-Specific</td></tr>
<tr><td rowspan="5">Evaluation of results</td><td rowspan="3">Uncertainty / Sensitivity Analysis</td><td>Dominant factors, parameters</td><td>5.2 + Application-Specific</td></tr>
<tr><td>Parameter/variable ranges</td><td rowspan="2">4.2, 5.2 + Application-Specific</td></tr>
<tr><td>Magnitude & direction of parameter variability on model results</td></tr>
<tr><td>Model Assumptions Analysis</td><td>Magnitude & direction of effect on model results</td><td>5.3 + Application-Specific</td></tr>
<tr><td colspan="2">Limitations of Modeling & Results</td><td>5.4 + Application-Specific</td></tr>
<tr><td colspan="4">Conclusions, Recommendations</td><td>Application-Specific</td></tr>
</table>

7.1.1 Problem, Objectives and Purpose for the Use of Environmental Regulatory Models at the Hanford Site

The problem (discussed in Sections 1.0 and 4.1) concerns the need for a technically appropriate and regulatory-consistent method of risk characterization associated with vadose zone contaminants at the Hanford Site. The regulatory purpose for the use of an ERM in this capacity concerns the assessment and characterization of the potential risk to groundwater from vadose zone contaminants at Hanford. The use of an ERM for this purpose fulfills the requirements and expectations that the methods and tools used in risk-based applications must be appropriate for addressing the problem to be solved.

7.1.2 Hanford Site-Specific Vadose Zone System Conceptual Model, FEPs, and Model Attributes

Consistency with the Federal requirements concerning the rationale and basis for the development of the conceptual site model includes documentation regarding the conceptual model components, as well as the identification of associated FEPs and model input parameters. The evaluation of these FEPs provides the basis for the identification for use in the evaluation of necessary modeling capabilities. The FEPs for vadose zone modeling at Hanford include consideration of the thick and stratified vadose zone and spatially and temporally varying recharge conditions. The model attributes and criteria for the selection of an appropriate ERM model type were identified by combining the FEPs with other necessary criteria and capabilities, which include consideration of the level of model complexity, dimensionality, and other requirements necessary to achieve the modeling objectives. These other model attributes for Hanford vadose zone modeling include Federal requirements concerning the requirement for the model results to include time (year) of peak concentrations in groundwater, and approximate the spatial movement of contaminants within and between media.

7.1.3 Model Type Selection

As indicated from the application of these Federal guidelines for the model selection process (Section 4.3), two-dimensional fate and transport is the model type identified as necessary to meet the required attributes and criteria. This model type is capable of satisfying the objectives of risk characterization applications at Hanford. The documentation in Section 4.3 provides the information necessary for the demonstration of consistency with the Federal requirements and guidelines for the selection of a method/model appropriate for most vadose zone modeling applications at Hanford.

7.2 CODE SELECTION

Consistency with the Federal guidelines for the code evaluation and selection process is documented in Section 6.0, in the context of the evaluation of a candidate code, STOMP. The code evaluation/selection process involved the determination of the capability of the STOMP code to meet the modeling objectives, the required model attributes, the code-related criteria, and to also be acceptable in the consideration of administrative criteria (EPA 402-R-94-012). The documentation provided in Section 6.0 addresses all aspects of the Federal guideline requirements and expectations. The results of this evaluation indicate that the STOMP code meets all of the required model type attributes and criteria, and it is appropriate for use in conducting vadose zone fate and transport modeling at the Hanford Site at the 200-UW-1 OU waste sites and at other OUs.

7.3 CONSISTENCY WITH FEDERAL REQUIREMENTS FOR THE USE OF ENVIRONMENTAL REGULATORY MODELING AND EVALUATION OF MODEL RESULTS

The documentation provided in Sections 4.2 and 5.0 addresses the aspects of consistency with the Federal guidelines concerning the use of vadose zone fate and transport ERMs at the Hanford Site for risk characterization applications. The information and documentation necessary for complete technical adequacy and regulatory consistency require amending the common elements with waste site- and application-specific information and documentation. This information is intended to serve as a foundation that contributes to the full documentation necessary to demonstrate the technical adequacy and regulatory consistency for most vadose zone modeling efforts at Hanford. The following subsections contain a synopsis of this documentation and its relationship to that required for consistency with these requirements and guidelines.

7.3.1 Model Parameterization

The Federal guidelines for the evaluation and selection of parameter values to be used in ERMs are related to the conceptual site model and uncertainty evaluations. The conceptual model and conceptual model components for the Hanford vadose zone system documented in Section 4.2 provide a starting point and the basis for the selection of model parameters. Input for model parameters (Section 5.1) is obtained from data contained in Hanford Site-specific databases, data packages, and reports. These data provide baseline information on the populations and ranges of parameter values, best-estimate and/or statistical values (e.g., mean and median values), and also information on area and/or waste site-specific sub-populations. This documentation explains how and why the data contained in these documents provide an appropriate basis for assessing the sources, quality, and criteria of the data sets used in the parameterization of vadose zone models at Hanford. This documentation is intended to be augmented by waste site-specific data for application-specific vadose zone ERMs.

7.3.2 Model Use and Evaluation of Model Results, Uncertainties, Assumptions, and Limitations

The remainder of the Federal requirements associated with the use of ERMs concerns documentation pertaining to the evaluation of model results, and the evaluation of model uncertainties, assumptions, and limitations. The documentation presented in Sections 5.2 through 5.4 addresses the extent to which these model use elements can be documented for vadose zone modeling at Hanford in general. Thus, this documentation is intended to provide a fundamental basis and framework that supports the model use documentation necessary for most vadose fate and transport modeling at Hanford. Consistency with the Federal guidelines concerning the evaluation and summary of model results requires application-specific documentation of modeling results, which is not addressed here. Examples of the common limitations in the applicability of vadose modeling at Hanford are documented in Section 5.4. This documentation is also intended to be used as a common basis in the documentation of Hanford vadose zone modeling efforts, but supplemented with application-specific information for the demonstration of consistency with Federal requirements.

7.4 FEDERAL REGULATORY FRAMEWORK

A modified form of the framework for consistency with Federal and state regulations and guidelines (shown in Figure 2-5 and described in Section 2.9) is presented in Figure 2-5. The figure identifies the combined requirements and expectations. The elements of the Federal and state requirements and guidelines (shown in the figure and are color-coded in the same manner used in Table 7-1) are divided between (1) model/method and code selection, and (2) model use and results evaluation. As shown in this figure, the state elements pertaining to the derivation of soil concentrations for groundwater protection have direct and/or indirect counterparts in the Federal requirements and guidelines. Thus, the documentation demonstrating and/or supporting consistency with the Federal guidelines can also serve as the basis for the demonstration of consistency with the corresponding State requirements. A direct comparison of these requirements and locations of documentation concerning consistency and/or relevance to elements is provided in Section 8.6. This comparison illustrates the correspondence between the state and Federal requirements and between the parallel documentation necessary for the demonstration of consistency with both sets of requirements.

7.5 SUMMARY

The summary of documentation presented in this section demonstrates that the elements of the Federal requirements for method, model, and code selection have been addressed. The rationale and technical basis provided in this document are intended to demonstrate consistency with the Federal requirements and guidelines. This documentation addresses the conceptual model, FEPs, and model attributes applicable to the Hanford vadose zone system, and the use of this information in the determination that fate and transport modeling is the most appropriate model type pursuant to risk characterization applications for 200-UW-1 OU waste sites. An evaluation of the adequacy of the STOMP code for implementing vadose zone fate and transport modeling is also documented, which indicates that the STOMP code is appropriate for this vadose zone modeling application.

Many aspects of the elements associated with the Federal guidelines on the of ERMs in the context of vadose zone fate and transport are documented here. This documentation addresses the common background and fundamental information typically associated with vadose zone modeling at Hanford. This documentation provides an important demonstration of and supports consistency with these Federal requirements and guidelines. However, consistency associated with model use is incomplete without site- and application-specific information on model parameterization, and the evaluation of model uncertainties, assumptions, limitations, and model results.

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8.0 DEMONSTRATION OF CONSISTENCY WITH STATE REGULATIONS FOR THE SELECTION AND USE OF A METHOD FOR DERIVING SOIL CONCENTRATIONS FOR GROUND WATER PROTECTION AT THE HANFORD SITE

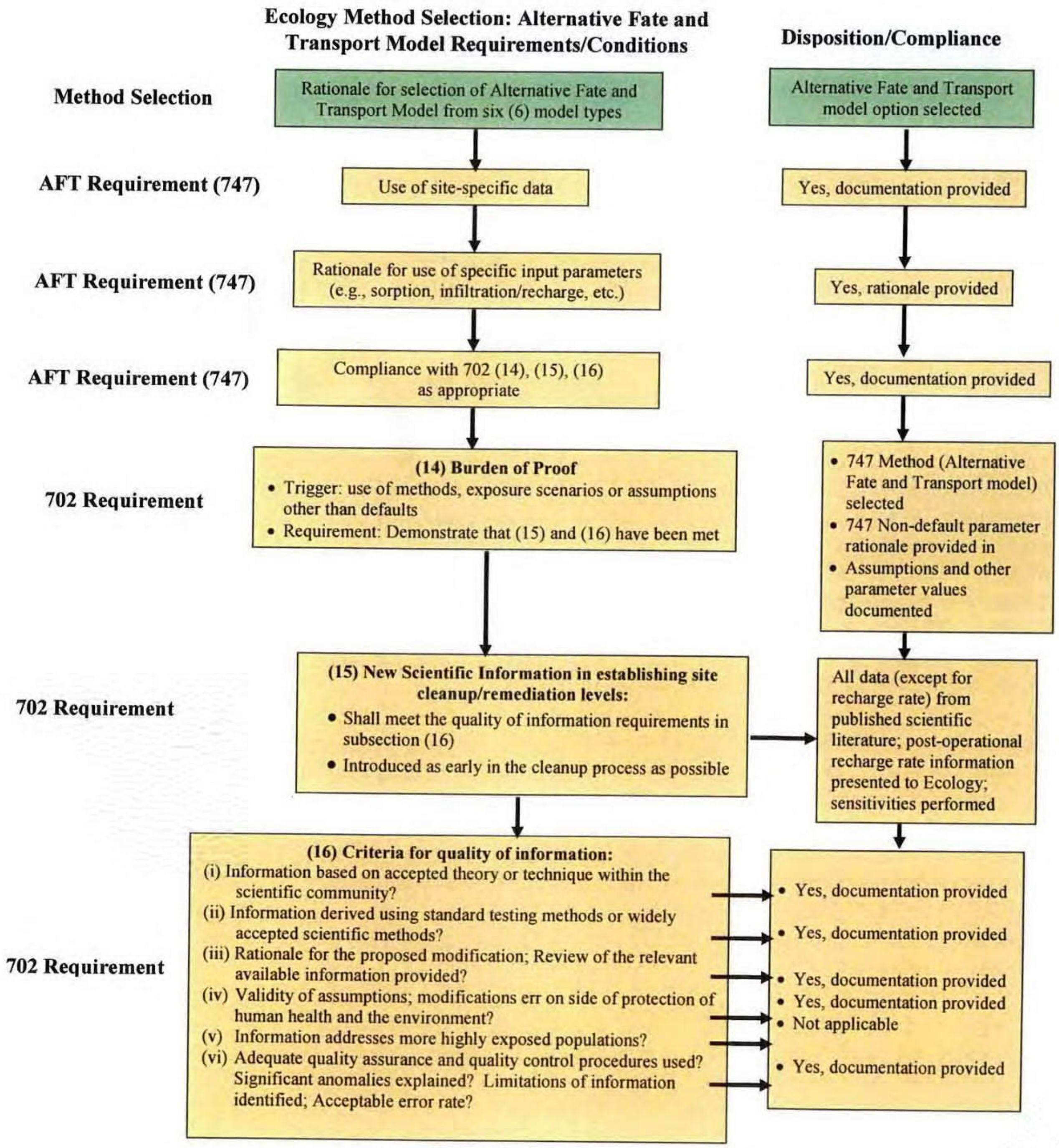
This section addresses consistency with the state regulations most relevant to the use of ERMs for risk characterization applications associated with the Hanford vadose zone system. As discussed in Section 2.8, the requirements of WAC 173-340-747 mandate the selection and use of an appropriate method (ERM) for the purpose of protecting groundwater from vadose zone (soil) contamination. Consistency with the state requirements involves and/or implies the need for documentation of the rationale and technical basis associated with the elements of (1) method selection (WAC 173-340-747), and (2) conditional requirements that accompany the selection of a method. These conditional requirements can include method-specific requirements (e.g., scientific approach and parameterization), and also the WAC 173-340-702(14), (15), and (16) burden of proof requirements. The burden of proof requirements concern the adequacy and quality of information and method/model-specific criteria typically associated with model use (e.g., parameterization, assumptions, uncertainties, limitations, and conservatism).

The evaluation of the state methods described here concerns determination of the extent to which the methods identified in WAC 173-340-747(3) are appropriate and capable of meeting the objectives of vadose zone modeling at the Hanford Site. Based on the application of the ERM selection process described in Section 4.0, it is indicated that fate and transport modeling is the model type most appropriate for meeting the objectives of vadose zone modeling at Hanford. Although this model type is consistent with the "alternative fate and transport modeling" method identified in the WAC 173-340-747(3), all of the identified state methods are evaluated here in the context of their capabilities as appropriate methods/models for meeting the objective of vadose zone modeling at Hanford. The documentation provided here concerning method selection and use demonstrates and/or supports consistency with the requirements and/or intent of state regulations, as illustrated in Figure 8-1. Figure 8-2 illustrates the regulatory consistency framework

The documentation concerning consistency with the State regulations is organized in the following manner. Section 8.1 provides a summary of the information and rationale regarding the selection of "alternative fate and transport" as the most appropriate choice of the state methods. Section 8.2 documents the manner and extent to which this information also demonstrates and/or supports consistency with the conditional state requirements that accompany the selection and use of the "alternative fate and transport modeling" method. The extent to which the rationale, evaluation, and documentation provided on code selection, and the STOMP code in particular, complies with the expectations and/or intent of the WAC 173-340-702(14), (15), and (16) burden of proof requirements is provided in Section 8.4.

Figure 8-1. Summary of WAC 173-340-747 Method Selection Requirements and WAC 173-340-702 Conditions Associated with the Choice of the Alternative Fate and Transport Models.

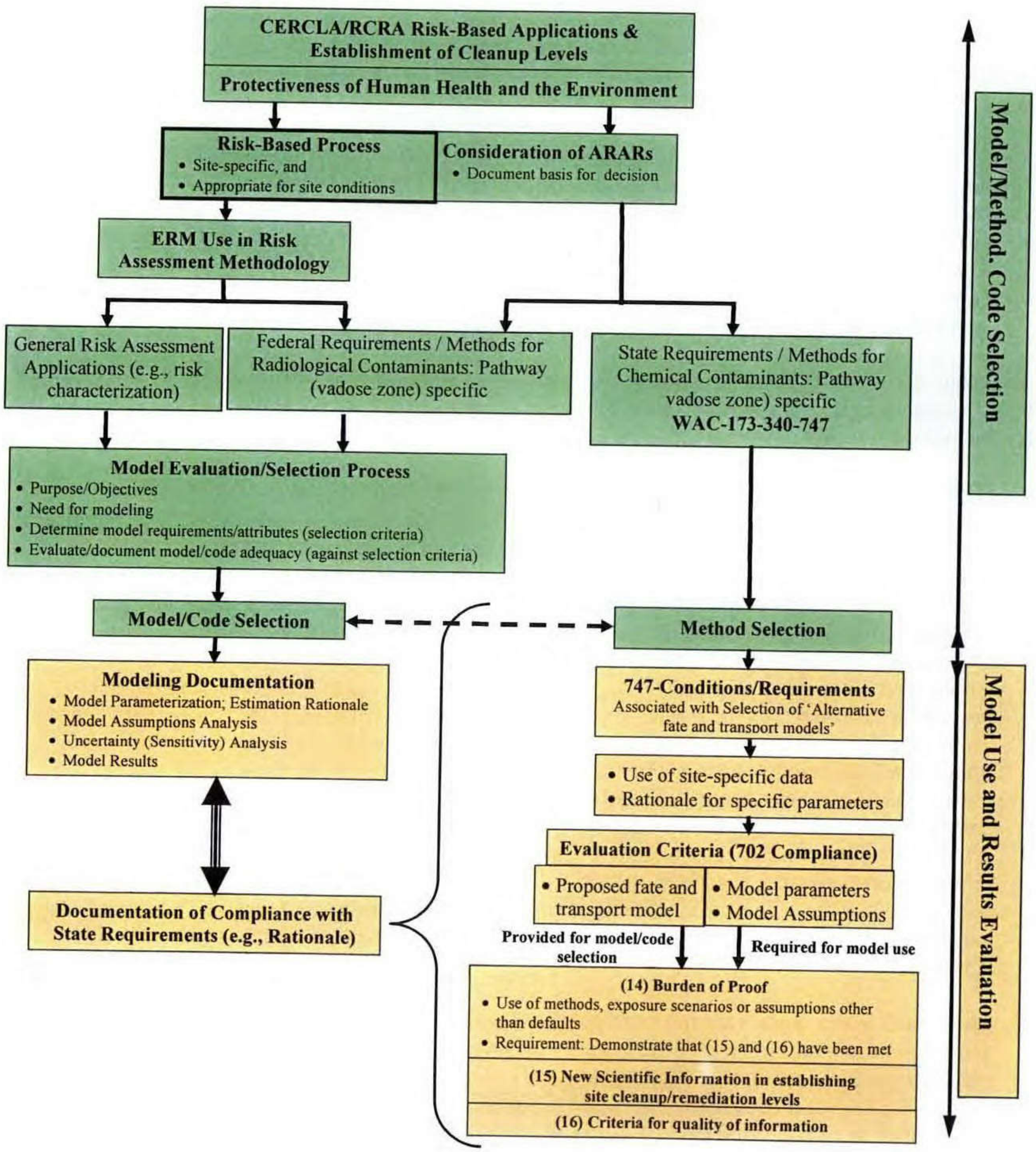
Green highlighted boxes denote requirements associated with method selection. Orange-highlighted boxes denote requirements/conditions associated with method parameterization.



NOTE: Green highlighted boxes denote requirements associated with method selection. Orange-highlighted boxes denote requirements/conditions associated with method parameterization.

Figure 8-2. Regulatory Consistency Framework.

Framework for identifying the processes and requirements for demonstrating consistency with Federal and corresponding state requirements for the use of ERMs. The upper half highlighted in green denotes the requirements and elements associated with the model, method, and code selection process. The lower part, highlighted in orange, denotes the requirements elements associated with model use and model documentation.



8.1 RATIONALE FOR SELECTION OF METHOD FOR THE CALCULATION OF SOIL CONCENTRATIONS FOR GROUNDWATER PROTECTION (WAC 173-340-747)

The WAC regulations address the need for a scientifically valid method for determining cleanup levels protective of groundwater. For the protection of groundwater pathway at Hanford, WAC 173-340-747 is the most pertinent requirement. WAC 173-340-747(2) dictates that one of the methods specified in WAC 173-340-747(4) through (9) shall be used to determine the soil concentration that will not cause an exceedance of the groundwater cleanup level established under WAC 173-340-720.
WAC 173-340-747(3) provides an overview of methods for deriving soil concentrations that meet the criteria specified in WAC 173-343-747(2) and specifies that one of the seven methodologies in WAC 173-340-747(4) through (10), including WAC 173-340-747(8), shall be used. The methods in WAC 173-340-747 include the following:

1. Fixed parameter three-phase partitioning model (WAC 173-340-747[3][a] and [4])
2. Variable parameter three-phase partitioning model (WAC 173-340-747[3][b] and [5])
3. Four-phase partitioning model (WAC 173-340-747[3][c] and [6])
4. Leaching tests (WAC 173-340-747[3][d] and [7])
5. Alternative fate and transport model (WAC 173-340-747[3][e] and [8])
6. Empirical demonstration (WAC 173-340-747[3][f] and [9])
7. Residual saturation (WAC 173-340-747[3][g] and [10]).

The evaluation of the applicability of each methodology to Hanford vadose zone waste sites is presented below along with an associated evaluation of each method documenting the technical basis and rationale for the method selection:

<u>(1) Fixed parameter three-phase partitioning model</u> and <u>(2) Variable parameter three-phase partitioning model</u>: The three-phase partitioning model, either fixed or variable, is a mathematical expression (Equation 747-1 in WAC 170-340-747) used to derive soil concentrations protective of groundwater. Use of the model requires adopting many simplifying assumptions (e.g., constant and uniform recharge conditions) that contamination exists uniformly throughout the vadose zone, that Kd-based partitioning between solid (soil) and liquid (water) phases occurs, and that vadose zone and groundwater dilution may be approximated by an effective dilution factor (DF) that acts as a combined parameter for all vadose zone and groundwater transport processes. This parameter provides a basic and fixed representation of subsurface conditions controlling contaminant transport. These partitioning models/methods (Method 1 and 2) are examples of a simple analytical model. Simple analytical models are typically intended to function as screening tools before the implementation of more complex models (ASTM E 1739-95, EPA 402-R-94-012). Although the partitioning models likely provide conservative estimates of soil concentrations protective of groundwater, the assumptions associated with the model are not representative of dominant processes impacting contaminant transport in the vadose zone at Hanford. Use of such a model is inconsistent with the EPA's stated environmental regulatory policy that identifies and manages uncertainties that compromise the decision-makers' ability to make accurate predictions of risk or risk reduction (Crumbling 2002).

These partitioning models are not capable of representing a dynamic vadose zone system that has fate and transport of contaminants occurring through heterogeneous porous media of variable thickness and hydrogeologic properties. The limitations of simple analytical models include the inability to account for heterogeneous porous medium properties, the inability to account for multiple sources contributing to a plume, and the inability to account for irregular site boundaries. The partitioning models do not account for retardation of contaminants associated with fate and transport processes in natural environments with non-negligible vadose zone thicknesses. The assumptions made in the partitioning model cannot be justified for the Hanford vadose zone system, where the unsaturated zone can extend to over 80 m (262 ft). Empirical data have also confirmed that variable retardation of contaminants occurs in the Hanford vadose zone. The partitioning models also lack the ability to account for retardation and/or sequestration of contaminants associated with fate and transport processes that may change in the system over time. The EPA guidance for the assessment of risk for Superfund Sites (EPA/540-R-92/003, EPA 1995, OSWER Directive 9200.4-18) specifically calls for the assessment of risk/protectiveness over time, in terms of predictions using appropriate models to examine the estimated future threats posed by residual contaminants. These guidelines identify expectations to predict the year of peak concentration and/or dose in groundwater and model the expected movement of contaminants at the site within both the soil and groundwater. The partitioning models, therefore, are not appropriate for applications to the Hanford vadose zone waste sites because they do not adequately incorporate key FEPs required to simulate the system of this complex vadose zone. While acceptable for use as a screening tool, the partitioning model is inadequate for the purpose of risk assessment modeling and establishing appropriate soil contaminant levels protective of groundwater at Hanford vadose zone waste sites.

(3) Four-phase partitioning model: This methodology is a variation of the three-phase partitioning model intended for applications also involving NAPL COCs. This methodology is also not adequate to describe the dominant factors affecting contaminants in the Hanford vadose zone for the same reasons described for the three-phase partitioning methodology.

(4) Leaching tests: The leaching test methodology alone is not a sufficiently robust method to accommodate the FEPS associated with transport and behavior of contaminants in the vadose zone soils at Hanford. Although leaching tests can provide information on contaminant mobility in the context of partitioning between solid (soil) and liquid (water) phases and/or solubility, this is only one aspect of one of the conceptual model components (i.e., geochemistry) concerning contaminant transport and behavior through the vadose zone. While leachability may be a dominant factor in the impact to groundwater for systems where the thickness of the vadose zone is subordinate or inconsequential, it is, by itself, highly inadequate for describing systems with a substantial vadose zone thickness, such as that at the Hanford Site, because this methodology does not accommodate any other key FEPs such as transport-related processes, or other aspects of the vadose system apart from geochemical partitioning. Thus, this methodology, by itself, is incapable of yielding the type of risk characterization information necessary and required for risk-based applications associated with the Hanford vadose zone system.

(5) Alternative fate and transport modeling: This method is the most appropriate model for the derivation of soil concentrations for groundwater protection (WAC 173-340-747[3][e] and [8], "Alternative Fate and Transport Models") for a number of reasons:

- This option provides for the use of site-specific information, data, and model parameters.
- This option provides for the capability to more effectively account for the characteristics and properties of the thick sequences of vadose zone sediments at the Hanford Site that influence contaminant migration.
- This option allows for the use of models capable of simulating the dynamic behavior of contaminants associated with fate and transport associated with unsaturated porous media flow through the Hanford vadose zone much more effectively (i.e., directly) than the other methods.

- This option provides for the capability to simulate the observed attenuation of contaminant flux rates and concentrations through the Hanford vadose zone associated with naturally occurring processes such as tortuosity in the flow paths, anisotropy, dispersion, and contaminant retardation/attenuation.

- This option is the only one of the WAC 173-340-747 methods capable of meeting the EPA criteria of assessment of risk/protectiveness over time, including radioactive decay.

- This option is the most appropriate choice based on the consideration of the assumptions and uncertainties inherent in the method for the intended application.

Overall, this method provides the capabilities necessary to describe the dominant FEPs associated with contaminant behavior in the vadose zone at the Hanford Site.

(6) Empirical demonstration: The empirical demonstration method calls for the use of site-specific soil and groundwater sample data to demonstrate that soil concentrations will not cause an exceedance of the applicable groundwater cleanup level. As stated in WAC 173-340-747(3)(ii), it must be demonstrated that sufficient time has elapsed for the hazardous substances to migrate from the soil (vadose zone) into groundwater. Demonstration of a sufficient lapse of time does not appear to be feasible for certain COCs in the Hanford vadose zone (e.g., significantly retarded COCs). Although measures such as long-term monitoring will have an increasingly important role in assessing vadose zone impacts to groundwater over time, the use of the empirical demonstration method alone is not an adequate method for the purpose of risk characterization concerning groundwater impacts from contamination in vadose zone soils at Hanford.

(7) Residual saturation: This method concerns soil concentrations that do not result in the accumulation of NAPL on or in groundwater. This methodology is not applicable for modeling efforts not involving NAPL COCs.

WAC 173-340-740(c)(ii)(A) and WAC 173-340-745(c)(ii)(A) point to the use of the methods in WAC 173-340-747 to determine soil cleanup levels that are protective of groundwater without providing any indication of preference toward any method. The following is a summary of the limitations of the modeling methods listed in WAC 173-340-747, besides alternative fate and transport models, that prevent these models from adequately simulating contaminant migration in the Hanford Site subsurface:

- The model mathematical expression(s) fails to incorporate the site specific conditions at Hanford such as follows:

  - Arid climate levels of infiltration and recharge
  - Thick vadose zone consisting of heterogeneous units with variable thickness
  - Site-specific geochemistry prone to inhibit the transport of uranium
  - Hydrologic conditions that change over time.

- The expression requires the use of the assumptions of Kd-based partitioning between solid (soil) and liquid (water) phases and an effective DF that cannot be derived from Hanford vadose zone and groundwater mixing dilution effects.

- The expression essentially represents instantaneous, uniform, static equilibrium ratios of vadose zone leachate and volume to groundwater volume, rather than the results of fate and transport through heterogeneous porous media of variable thickness and hydrogeologic properties.

- The expression lacks the ability to account for retardation and/or sequestration of contaminants associated with fate and transport processes in natural environments, or changes in the system over time.

These shortcomings are especially important for applications involving the vadose zone at Hanford, having a thickness that extends over 80 m (260 ft), and/or for empirical data confirming/validating the variable retardation of contaminants in the vadose zone (PNNL-13895, PNNL-13037). The application of inaccurate estimates of potential groundwater contamination can translate to overly conservative risk and cleanup-level estimates.

The WAC 173-340-747(3) directs that a method be chosen that is appropriate for the intended risk assessment application including the determination of cleanup goals. However, this regulation does not identify how method selection should occur, but it does invoke conditional evaluation criteria requirements associated with the selection of "alternative fate and transport models" in WAC 173-340-747(8)(c) and WAC 173-340-702(14), (15), and (16). This evaluation is provided to identify that this method is the only one that is appropriate, relevant, and applicable in terms of its capabilities for meeting all of the required model objectives and attributes for risk assessments and establishing cleanup goals at Hanford (i.e., level of complexity, the use of site specific data, and incorporation of specific information for hazardous and radiological soil contaminants).

As specified in WAC 173-340-747(3), alternative fate and transport models are an acceptable method for calculating soil concentration cleanup levels for any hazardous substance for groundwater protection. Comparison of these methods to the model attributes and FEPs required for vadose zone risk assessment and soil cleanup-level applications is summarized in Table 8-1. It is indicated, from the comparison of the methods identified in WAC 173-340-747(3) to the model attributes and FEPs required for vadose zone modeling at Hanford, that alternative fate and transport models is the only method with the capabilities to meet all of the requirements for risk characterization applications. This method is the most appropriate for the assessment and characterization of risk and the establishment of soil cleanup levels protective of groundwater in the 200 Areas at the Hanford Site. The other methods specified in of WAC 173-340-747(4) through (10) are inadequate for the purposes of risk characterization for the conditions and characteristics of the Hanford vadose zone. The selection of alternative fate and transport modeling for the purposes of risk characterization and the derivation of soil cleanup levels for the protection of groundwater pathway are also consistent with Federal guidelines, which require that models have the capability to incorporate/address the dominant FEPs to be simulated in the natural environment.

8.2 CONDITIONAL REQUIREMENTS ASSOCIATED WITH THE SELECTION OF THE ALTERNATIVE FATE AND TRANSPORT MODELING METHOD

The WAC 173-340-747(8), "Alternative Fate and Transport Model," subsection specifies conditional requirements for establishing soil concentrations through the use of fate and transport models other than those specified in WAC 173-340-747(4) through (6). As specified in subsection (8):

> *"The alternative models may be used to establish a soil concentration for any hazardous substance... Site-specific data are required for use of these models... "Proposed fate and transport models, input parameters, and assumptions shall comply with WAC 173-340-702(14), (15), and (16)."*

Table 8-1. Comparison of the Methods Identified in WAC 173-340-747(3) to Model Attributes and the Features, Events, and Processes Required for Vadose Zone Modeling at the Hanford Site.

Model Attributes and FEPs Required for Vadose Zone Modeling at the Hanford Site	Modified Methods for Fate and Transport Modeling						
	Fixed Parameter Three-Phase Model	Variable Parameter Three-Phase Model	Four-Phase Partitioning Model	Leaching Tests	Alternative Fate and Transport Modeling	Empirical Demonstration	Residual Saturation
Number Associated with Description	1	2	3	4	5	6	7
FEATURES							
Fluid properties				X	X	X	N/A
Hydrogeologic conditions:							
Capillary retention					X		N/A
Fluid pressure and saturation distribution					X		N/A
Geology				X	X	X	N/A
Hydrogeologic material properties:							
Porous media	X	X	X	X	X	X	N/A
Physical characteristics					X		N/A
Vadose zone thickness (depth to groundwater)					X		N/A
EVENTS							
Recharge	X	X	X		X		N/A
Source terms/releases:							
Water					X	X	N/A
Contaminants	X	X	X	X	X	X	N/A
PROCESSES							
Physical transport mechanisms/rates:							
Advection	X	X	X		X		N/A
Vadose zone drainage					X		N/A
Estimating time (year) of peak concentrations in groundwater					X		N/A
Hydrodynamic dispersion					X		N/A
Molecular diffusion					X		N/A
Spatial movement of contaminants within and between media					X		N/A
Physical and chemical interactions:							
Desorption	X	X	X	X	X		N/A
Solubility-based release/precipitate				X	X		N/A
Sorption				X	X		N/A
Capillary fringe:							
Capillary action					X		N/A
Drainage					X	X	N/A
Radioactive decay					X	X	N/A
GROUNDWATER TRANSPORT[a]							
Dilution	X	X	X		X	X	N/A

[a] Groundwater transport is not a vadose zone FEP. It is included in this table because it is an important factor in calculating the contaminant concentration results for the indicated methods.

FEPs = features, events, and processes

Thus, the use of alternative fate and transport modeling invokes conditional requirements associated with WAC 173-340-747(3) and (8) and WAC 173-340-702(14), (15), and (16). The conditional requirements include the use of site-specific data in the models, and demonstration that the fate and transport models, input parameters, and assumptions comply with the burden of proof requirements found in WAC 173-340-702. Some of the conditional requirements associated with the selection of the "alternative fate and transport modeling" method involve model-specific criteria, such as model parameterization and model use requirements (e.g., evaluation of assumptions, uncertainties). These are factors and criteria that are not associated with method, model, or code selection, but rather with ERM use and documentation requirements.

The state conditional requirements that invoke the evaluation criteria for proposed fate and transport models (WAC 173-340-747[8][c] and WAC 173-340-702[14], [15], and [16]) primarily concern the adequacy and quality of data used in the modeling. Elements of WAC 173-340-702(14), (15), and (16) burden of proof requirements are also regarded here as consistent with and contained within elements of the Federal guidelines concerning the acceptability of the model type and code. Demonstration of consistency with these conditional requirements is provided in the following subsections. This documentation provides the basis for demonstrating consistency, and/or support for consistency, with the conditional requirements concerning the selection of the alternative fate and transport models method.

The primary conditions associated with the use of fate and transport models identified by WAC 173-340-747(3) and (8) include the following:

- Use of site specific data
- Documentation concerning the technical basis and rationale for model parameterization and several specific parameters
- Additional evaluation criteria (WAC 173-340-702[14], [15], and [16]) requirements involving documentation of the technical basis and rationale concerning the proposed fate and transport models, input parameters, and model assumptions.

These "burden of proof" conditions associated with WAC 173-340-702 are primarily invoked when one or more of the following is proposed:

- *"Use a reasonable maximum exposure scenario other than the default provided for each medium,"*
- *"Use assumptions other than the default values provided for in this chapter"*
- *"Establish a cleanup level under Method C," or*
- *"Use a conditional point of compliance."*

Most model/code applications at Hanford use a common Hanford Site-specific basis and databases for parameterization of the models. Therefore, the documentation regarding consistency with the WAC 173-340-747(8)(b) conditional requirements is limited to those aspects of the Hanford Site-specific data that are common and applicable for most model applications (e.g., data types, sources, etc.). This documentation concerns these common aspects of parameterization. Waste site-specific applications also require supplemental documentation based on waste site-specific characteristics, conditions, and data for consistency with these requirements.

8.2.1 WAC 173-340-747(8) and (8)(B) – Criteria

WAC 173-340-747(8), "Alternative Fate and Transport Models," specifies the procedures and requirements for establishing soil concentrations through the use of fate and transport models other than those specified in WAC 173-340-747(4) through (6). The assumptions under this subsection further state:

> "*When using alternative models, chemical partitioning and advective flow may be coupled with other processes to predict contaminant fate and transport, provided the following conditions are met:*"

The specific model parameters identified in WAC 173-340-747(8)(b) are as follows:

- Sorption
- Vapor phase partitioning
- Natural biodegradation
- Dispersion
- Decaying source
- Dilution
- Infiltration.

The conditional requirement associated with the selection of the "alternative fate and transport models" method is that specified parameters shall be estimated or derived in accordance with stated conditions. Site-specific data are required for the use of these models. Consistency with this requirement primarily involves documentation of, and demonstration for, the manner in which (1) site data are used in the estimation or derivation of these specified parameters, and (2) specified parameter conditions (e.g., WAC 173-340-747[8][b][v]) are met. The following is a description and/or explanation of the manner in which the conditions for each of these parameters is, or has been, satisfied. The descriptions/explanations, and the information in Table 8-2, serve as documentation and demonstration of consistency with the requirements of WAC 173-340-747(8)(b)(v).

WAC 173-340-747(8)(b)(i), "Sorption"

WAC Condition. "*Sorption values shall be derived in accordance with either subsection (4)(c) of this section or the methods specified in subsection (5)(b) of this section.*"

> **Condition Consistency.** WAC 173-340-747(5)(b) identifies methods for deriving instantaneous equilibrium distribution coefficient (Kd) values from site data, batch tests, and scientific literature. These methods provide the best information currently available. At the Hanford Site, a database of Kd values determined experimentally from site-specific samples for the most common COCs has been assembled. The site-specific database is a compilation of data determined over a period of decades and reported in project-based documents. These data represent laboratory-determined Kd values collected by PNNL and documented in CP-17089, PNNL-13895, PNNL-11800, PNNL-14702, PNNL-14725. These Kd estimates are based on both batch and column tests and have included tests on reaction kinetics, as well as successive water and acid leaching tests in an effort to obtain the most representative, high-quality data for understanding the geochemical processes at Hanford.

Table 8-2. Summary of Specific Model Parameters and Conditions Associated with the Use of Alternative Fate and Transport Models per WAC 173-340-747(8). (2 pages)

Model Parameters Identified in WAC 173-340-747(8)	Requirement/ Condition	Parameter Value(s)	Technical Basis/Rationale; Source	Error on Behalf of Protection of Human Health and the Environment?
Sorption (deriving Kd from site data)	Site-specific measurements (e.g., soils) from same (appropriate) depths and locations. Based on batch equilibrium tests (minimum rigor).	Kd = 0 for Tc-99 and nitrate in all site-specific vadose zone units Kd = 0.6 for uranium in all site-specific vadose zone units except the Cold Creek carbonate Kd = 10 for uranium in the Cold Creek carbonate	Hanford Site-specific laboratory testing results and associated Kd database (PNNL-13895) (see Sections A9.0 through A11.0). "Best-estimate" uranium Kd values from site-specific templates and lithology-specific values; (PNNL-14702b, PNNL-14725b) (for more detail see Sections A9.0 and A12.0). Conservatively biased for uranium Kd determinations in site-specific Cold Creek carbonaceous sediments (Qafoku et al. 2005, Dong et al. 2005) (for more detail see Sections A9.0 and A12.0).	Maximum contaminant mobility. Conservative bias: value for uranium Kd = 25% lower than "best-estimate" value (see Section A12.0). The Kd value of 0.6 mL/g corresponds to a rate of mass transfer 7 to over 80 times greater than for (laboratory) observed desorption kinetic release (see Section A12.1.2 - A12.1.4). The Cold Creek Kd value of 10 mL/g corresponds to a rate of mass transfer up to 5 times greater rate than for (laboratory) observed desorption kinetic release (see Section A12.1.2 - A12.1.4).
Vapor-phase partitioning	Not generally applicable to risk characterization for Hanford Site COCs.	N/A	N/A	N/A
Natural biodegredation	Not generally applicable to risk characterization for Hanford Site COCs.	N/A	N/A	N/A
Dispersion	Estimates of dispersion shall be derived from either site-specific measurements or literature values.	Anisotropy = 10:1; dispersivity values listed in Table 4-2	Based on estimates and calibrations of dispersivity in Hanford-specific sediments from the vadose zone hydrology data package (PNNL-14702a). Anisotropy ratios consistent with moisture-dependent estimations of anisotropy for site-specific sediments types (RPP-17209, Rev. 1, Appendix C).	Conservative bias; based on homogeneous lithology; no consideration of increased dispersion from heterogeneity and greater anisotropy from small-scale, finer-grained facies.
Decaying source	Fate and transport algorithms may be used that account for decay over time.	Tc-99 half-life approximately 210,000 years	N/A	N/A

Table 8-2. Summary of Specific Model Parameters and Conditions Associated with the Use of Alternative Fate and Transport Models per WAC 173-340-747(8). (2 pages)

Model Parameters Identified in WAC 173-340-747(8)	Requirement/ Condition	Parameter Value(s)	Technical Basis/Rationale; Source	Error on Behalf of Protection of Human Health and the Environment?
Dilution	Dilution shall be based on site-specific measurements or estimated using a model incorporating site-specific characteristics.	Based on algorithms integrated into the STOMP code	See STOMP user and theory guides (PNNL-14478 and PNNL-12030, respectively).	Varies with distance downgradient (point of calculation).
Infiltration (site-specific)	Infiltration shall be derived in accordance with subsection (5)(f)(ii)(B): *"Site-specific measurement or estimate of infiltration shall be based on site conditions without surface caps (e.g., pavement) or other structures that would control or impede infiltration, and must comply with WAC 173-340-702(14), (15), and (16)."*	Recharge (pre-Hanford/ undisturbed ground) = 4 mm/yr	Based on conservatively biased recharge measurements and estimates as a function of Hanford Site-specific soil type (Rupert sand) and vegetation condition (PNNL-13033, PNNL-14744) (see Section A1.4).	Best-estimate value = maximum measured value for Rupert sand.
		Recharge (pre-closure operational period) = 63 mm/yr (1944 to 2010)	Based on Hanford Site-specific lysimeter measurements (Gee et al. 2005a, 2005b) (see Sections A6.0 and 7.0).	Conservative bias: based on sorted, medium-grained sand versus natural distribution of grain sizes in site-specific soil.
		Recharge (post-closure) = 8 mm/yr for 30 years then 4 mm/yr thereafter	Best-estimate recharge rates for recovering or young vegetated disturbed soil and long-term based on Hanford Site-specific recharge data (PNNL-14725b)	Conservative upper-bound estimate; 2.5 times maximum measured value for Rupert sand; 10 to 100 times value of undisturbed vegetated soil.

NOTE: See the reference section of this document for the complete citations for the references identified in this table.

COC = contaminant of concern
Kd = instantaneous equilibrium distribution coefficient
N/A = not applicable
STOMP = Subsurface Transport Over Multiple Phases
WAC = *Washington Administrative Code*

Based on the geologic setting conceptual model, the measurement of Kd values from vadose zone samples throughout the Hanford Site can be considered collectively as "site data" because essentially all of the vadose zone (Kd) measurements involved sediments from the Hanford Ringold and Plio-Pleistocene Cold Creek sediments. Waste site-specific Kd values for some COCs, however, are variable as a function of the chemistry of the waste stream. Still, even in these cases, the effects are largely limited to the uppermost portion (up to a few tens of feet) of the vadose zone and for a short time relative to travel time through the vadose zone (up to a few years), because the vadose zone sediments have an intrinsic buffering capacity that tends to neutralize many/most of the these chemical effects for the portions of the vadose zone below/beyond the near-field environment. Where waste stream chemistry does affect solid/liquid partitioning (Kd), the effects appear to be associated with the initial deposition of contaminants in the vadose zone (e.g., initial adsorptive processes) rather than subsequent release (desorption) of contaminants years or decades following cessation of the discharges.

The site data from the Hanford contaminant distribution coefficient (Kd) database that are most representative and appropriate for fate and transport modeling at the various locations and/or waste sites throughout the Hanford Site have been cross-referenced with geographic area, geologic unit, and waste site type and chemistry in the PNNL-14725. The PNNL-14725 guidance document, together with the Hanford Site Kd database (PNNL-13895 and PNNL-4702), provide guidelines for the selection of the most appropriate Kd values for the various stratigraphic units/lithologies in the vadose zone as a function of (1) geographic location at Hanford, (2) underlying vadose zone stratigraphy, (3) waste site operational/process chemistry associated with the waste site; and (4) physical characteristics of the stratigraphic unit (i.e., lithology and grain size).

Result. The WAC criteria have been met. Estimates of K_d values are derived from values available in the Hanford literature cited above, site data, results of batch tests, and other methods of measuring contaminant mobility, partitioning, and geochemical behavior.

WAC 173-340-747(8)(b)(ii), "Vapor Phase Partitioning"

WAC Condition. *"If Henry's Law constant is used to establish vapor-phase partitioning, then the constant shall be derived in accordance with subsection (4)(d) of this section."*

Condition Consistency: Vapor-phase partitioning and multi-phase contaminant transport for individual contaminants are accommodated in the mode/code selection through the use of algorithms that use associated Henry's Law constants (e.g., Sections 4.4 and 8.1 of PNNL-12030). When NAPLs are present, Henry's Law constants are derived according to the regulation for the individual contaminants subject to vapor-phase partitioning or transport.

Result: The WAC criteria are met. Vapor-phase partitioning and multi-phase contaminant transport for individual contaminants are accommodated in the model/code selection through the use of algorithms and associated Henry's Law constants. When applicable, vapor-phase partitioning and Henry's Law constants, derived from site data or scientific literature, may be assigned to individual contaminants.

WAC 173-340-747(8)(b)(iii), "Natural Biodegradation"

WAC Condition. *"Rates of natural biodegradation shall be derived from site-specific measurements."*

Evaluation. Conceptual models of Hanford's waste sites do not typically include contaminants subject to biodegradation. Should this process be specified in a conceptual model, then the method used to approximate the biodegradation rate and data substantiating the rate of natural biodegradation would be provided, evaluated, and subject to review in accordance with WAC 173-340-702(15) and (16).

Results: The WAC criteria are not currently applicable. Should a conceptual model dictate natural biodegradation be implemented, then the method used to approximate the rate biodegradation, and data substantiating the rate of natural biodegradation would be provided, evaluated, and subject to review in accordance with WAC 173-340-702(15) and (16).

WAC 173-340-747(8)(b)(iv), "Dispersion"

WAC Condition. *"Estimates of dispersion shall be derived from either site-specific measurements or literature values."*

Condition Consistency. Mechanical dispersion, as determined by the product of dispersivity and porewater velocity, relates the dispersive solute flux to the solute concentration gradient. Estimates of dispersivity are contained in SAND98-2880 and serve as the basis for the dispersion estimates in PNNL-14702. The use of the estimates of dispersion in SAND98-2880 by composite analysis assumes that these estimates are applicable to soil types located throughout the Hanford Site. Other estimates of dispersivity are contained in RPP-7884 and RPP-10098. Transverse dispersivity values are estimated to be one-tenth of the longitudinal values based on the work of Gelhar et al. (1992).

Result. The WAC criteria have been met. Estimates of dispersion are derived from values available in the Hanford literature.

WAC 173-340-747(8)(b)(v) "Decaying Source"

WAC Condition. *"Fate and transport algorithms may be used that account for decay over time."*

Condition Consistency. Radioactive decay of radionuclides over time is accommodated in model/code selection through the inclusion of appropriate radioactive decay algorithms. The radioactive decay values used in the models use the most current and comprehensive information on radionuclide half-lives (e.g., the comprehensive compilation of half-life for the radioisotopes), which can be found in HNF-EP-0063-3. Radiological decay may be omitted from the fate and transport models when the consideration of radiological decay over the periods modeled has an insignificant impact on model results or conclusions.

Results. The WAC criteria have been met. The fate and transport models include radioactive decay in accordance with the requirements.

WAC 173-340-747(8)(b)(vi), "Dilution"

WAC Condition. *"Dilution shall be based on site-specific measurements or estimated using a model incorporating site-specific characteristics. If detectable concentrations of hazardous substances are present in upgradient groundwater, then the DF may need to be adjusted downward in proportion to the background (upgradient) concentration."*

Condition Consistency. The DFs, per se, are not used in process-, spatial- and temporal-based simulation models. Hence, most models/codes do not include specific DFs, but effective dilution may occur as mass is transported through the system. Model and code selection attributes of the fate and transport models include the capability to output groundwater concentrations (which include the effects of dilution) for COCs at the point of calculation.

The effective dilution associated with fate and transport modeling of the Hanford vadose zone includes consideration of mixing in both the vadose zone and groundwater. Dilution in the vadose zone occurs as recharge interacts with the moisture in the soil and, thus, depends both on the recharge rate and the moisture-retention characteristics of the soil type, as well as all processes that affect the net flux rate of water/leachate to groundwater. Site-specific recharge rates are described in PNNL-14744, whereas vadose zone hydraulic parameters are described in PNNL-14702 and PNNL-14725.

In groundwater, dilution occurs as recharge potentially containing contamination (leachate) enters the aquifer and, thus, depends both on the flux rate of water/leachate to the aquifer and the volume of water flowing through the aquifer. In the aquifer, the volume of water flow is calculated from the hydraulic conductivity, the hydraulic gradient, and the depth of the mixing zone. PNNL-14753 provides estimates for the aquifer properties at various locations beneath the Hanford Site. The hydraulic gradient can also be estimated from the 1944 hind-cast water table map, as reproduced from ERDA-1538 in DOE/ORP-2003-11. Parameters also considered in groundwater dilution effects include an aquifer mixing-zone thickness and, for a two-dimensional model, a unit cross-sectional width of 1 m (3.3 ft), consistent with those identified in WAC 173-340-747 for use in Equation 747-4 (WAC 173-340-747[5][f][i]).

Result. The WAC criteria have been met. Dilution is based on site-specific data for vadose zone and aquifer hydraulic parameters, which include hydraulic properties and recharge rates derived from Hanford studies and databases. Although process-, spatial- and temporal-based simulation models and codes do not include a specific dilution algorithm, effective dilution is determined internally within the fate and transport model during the solution to the mass and solute conservation equations. Dilution can be considered among the model and code selection attributes by requiring the model to have the capability output contaminant groundwater and leachate concentrations.

WAC 173-340-747(8)(b)(vii), "Infiltration"

WAC Condition. *"Infiltration shall be derived in accordance with subsection (5)(f)(ii)(A) or (B) of this section."*

> **Subsection (5)(f)(ii) (B):** *"If a site-specific measurement or estimate of infiltration (Inf) is made, it shall be based on site conditions without surface caps (e.g., pavement) or other structures that would control or impede infiltration. The presence of a cover or cap may be considered when evaluating the protectiveness of a remedy under WAC 173-340-350 through 173-340-360. If a site-specific measurement or estimate of infiltration is made, then it must comply with WAC 173-340-702 (14), (15), and (16)."*

Condition Consistency. Site-specific estimates of infiltration rate for vadose zone fate and transport modeling are based on the site-specific field measurements for the various soil types at Hanford. These measurements have been determined primarily from lysimeter studies specifically designed for the direct measurement of Hanford Site infiltration/recharge rates over periods ranging up to 26 years (e.g., Gee et al. 2005b), and also from isotopic determinations of infiltration (Murphy et al. 1996). These site-specific data have been compiled and evaluated by PNNL in several documents (PNNL-13033; PNNL-14744; PNNL-14702b; Gee et al. 2005a, 2005b), with recommended values for best estimates, reasonable bounding cases, and statistical data identified for the various soil type/class (grain size and pedogenesis) and vegetation conditions. The infiltration/recharge data from these sources are considered in identification of values most appropriate for vadose zone modeling at Hanford. In this analysis, recharge rates are generally determined/estimated for three conditions:

- Natural recharge rate for the undisturbed site-specific soil type
- Recharge for an operational period at unvegetated (bare) and waste sites with disturbed soil conditions
- A post-remedy (e.g., backfilled and revegetated with no surface barrier) recharge rate for the site-specific soil type.

The data collected and analyzed, along with the results of the analyses, satisfy the requirements in WAC 173-340-702(14), (15), and (16). The values used in the model, the basis for the values, and discussion about the variability and uncertainty associated with those values are contained in Sections 4.0 and 5.0 and Appendices A and B. These data and analyses ensure protection of human health and the environment by erring on the side of conservatism (subsection [14]). The estimates are based on published data and information (e.g., reference) and also new scientific information that have been presented as early as possible in the cleanup process (subsection [15]). The information is based on theories and techniques with widespread acceptance in the relevant scientific community (subsection [16][i]), is derived using standard testing methods or other widely accepted scientific methods (subsection [16][ii]), is provided with a review of available information and a rationale explaining the reason for using the information (subsection 16[iii]), the assumptions used in applying the information are valid and err on the side of conservatism to protect human health and the environment (subsection [16][iv]), the information adequately addresses populations likely to be present at the site (subsection [16][v]) (the remedial action goal [RAG] values are based on contaminant levels that do not produce concentrations that exceed maximum contaminant levels [MCLs] in groundwater), and adequate QA/QC procedures have been used, anomalies have been explained, limitations of the information have been identified, and the known or potential rate of error is acceptable (subsection [16][vi]).

Results. The WAC criteria have been met. Estimates of infiltration are derived from Hanford Site data that comply with WAC 173-340-702(14), (15), and (16).

8.2.2 WAC 173-340-747(8)(C) and WAC 173-340-702(14), (15), and (16) – Criteria

WAC 173-340-747(8)(c) identifies "evaluation criteria," which state that "Proposed fate and transport models, input parameters, and assumptions shall comply with WAC 173-340-702(14), (15), and (16)." WAC 173-340-702, "General Polices," includes sections on ***burden of proof*** (subsection [14]), ***new scientific information*** (subsection [15]), and ***criteria for quality of information*** (subsection [16]). The burden of proof subsection calls for demonstration (to the department) that the requirements specified in this section are met for any modification of the default assumptions in the standard Method B and Method C equations (WAC 173-340-740 and WAC 173-340-745, respectively), including modification of the standard reasonable maximum exposures and exposure parameters, or any modification of default assumptions or methods specified in WAC 173-340-747. The "new scientific information" subsection concerns consideration of new scientific information when establishing cleanup levels and remediation levels (for individual sites), in the context of also meeting the quality of information requirements in subsection (16). The documentation requirements pertaining to consistency with WAC 173-340-702(14), (15), and (16) are also regarded as reasonable and appropriate expectations in the context of Federal environmental modeling requirements (CREM 2003).

WAC 173-340-702(14), "Burden of Proof"

> *"Any person responsible for undertaking a cleanup action under this section who proposes to:*
>
> *(a) Use a reasonable maximum exposure scenario other than the default provided for each medium;*
> *(b) Use assumptions other than the default values provided for in this chapter;*
> *(c) Establish a cleanup level under Method C; or*
> *(d) Use a conditional point of compliance,*
>
> *shall have the burden of demonstrating to the department that requirements in this chapter have been met to ensure protection of human health and the environment. The department shall only approve of such proposals when it determines that this burden of proof is met."*

Items (a), (c), and (d) may not be strictly applicable to the Hanford vadose zone modeling because the modeling does not affect the exposure scenario, propose to use a cleanup level under Method C, or use a conditional point of consistency. Item (c) may not be applicable because WAC 173-340-747 does not explicitly state default assumptions and values, except for WAC 173-340-747(4), which prescribes specific assumptions, equations, and parameter values for that particular method. However, model parameterization, assumptions, quality of information, and uncertainties are included in the documentation requirements for model results recommended by the Federal guidelines (e.g., CREM 2003). Thus, for the purpose of completeness, the following subsections intend to demonstrate that requirements of WAC 173-340-702(14), (15), and (16) pertinent to item (c) have been met for Hanford Site-specific vadose zone models. All elements of the recommended elements for model documentation are provided here, and the parts of that documentation that pertain to WAC 173-340-702(14), (15), and (16) are also provided. The following sections demonstrate that the requirements of WAC 173-340-702(14), (15), and (16) have been met with regard to the Hanford Site-specific vadose zone fate and transport model assumptions and input values. The following discussions, in conjunction with information presented in previous sections, demonstrate that the requirements for ensuring protection of human health and the environment in WAC 173-340 have also been met in accordance with WAC 173-340-702(14), (15), and (16).

WAC 173-340-702(15), "New Scientific Information"

> *"The department shall consider new scientific information when establishing cleanup levels and remediation levels for individual sites. In making a determination on how to use this new information, the department shall, as appropriate, consult with the Science Advisory Board, the Department of Health, and the United States Environmental Protection Agency. Any proposal to use new scientific information shall meet the quality of information requirements in subsection (16) of this section. To minimize delay in cleanups, any proposal to use new scientific information should be introduced as early in the cleanup process as possible. Proposals to use new scientific information may be considered up to the time of issuance of the final cleanup action plan governing the cleanup action for a site unless triggered as part of a periodic review under WAC* 173-340-420 *or through a reopener under RCW* 70.105D.040 *(4)(c)."*

Evaluation. Data and inputs used in the Hanford Site-specific fate and transport models are based on values documented in Hanford Site-specific literature. This includes the references to the specific documentation for the data, parameters, and input values. The information is and has been introduced in the form of publicly available government reports and/or scientific literature as early as possible, and the referenced documentation is readily available to the Washington State Department of Ecology (Ecology).

Result. The WAC criteria have been met. The information concerning the data, parameters, and input values used in the Hanford fate and transport models have been introduced as early as possible, and the referenced documentation is available to Ecology.

WAC 173-340-702(16), "Criteria for Quality of Information"

> **WAC 173-340-702(16)(a).** *"The intent of this subsection is to establish minimum criteria to be considered when evaluating information used by or submitted to the department proposing to modify the default methods or assumptions specified in this chapter or proposing methods or assumptions not specified in this chapter for calculating cleanup levels and remediation levels. This subsection does not establish a burden of proof or alter the burden of proof provided for elsewhere in this chapter."*

> **WAC 173-340-702(16)(b).** *"When deciding whether to approve or require modifications to the default methods or assumptions specified in this chapter for establishing cleanup levels and remediation levels, or when deciding whether to approve or require alternative or additional methods or assumptions, the department shall consider information submitted by all interested persons and the quality of that information. When evaluating the quality of the information the department shall consider the following factors, as appropriate, for the type of information submitted:"*

> **WAC 173-340-702(16)(i).** *"Whether the information is based on a theory or technique that has widespread acceptance within the relevant scientific community;"*

Evaluation. The data and inputs described for use in the Hanford fate and transport models are based on values documented in the Hanford-specific literature, most of which is associated with studies undertaken by PNNL, but which also include publicly available government and peer reviewed publications. The methods used to collect, analyze, and interpret the data are identified in these publications. The source references include government documents and journal articles that have undergone peer review inside and outside of the Hanford scientific community. Much of the information has been presented at scientific meetings and symposiums. The information has a demonstrated basis on theories or techniques that have widespread acceptance within the relevant scientific community.

Result. The WAC criteria have been met. The data and inputs used in the Hanford fate and transport models (presented in Section 3.0, with appropriate references) are based on values, theories, and techniques that have widespread acceptance within the relevant scientific community.

> **WAC 173-340-702(16)(ii).** *"Whether the information was derived using standard testing methods or other widely accepted scientific methods;"*

Evaluation. The theories, methods, and techniques used to collect, analyze, and interpret the data used in the Hanford vadose zone fate and transport models are presented in the referenced source material (Section 3.0), much of which have undergone peer review inside and outside of the Hanford scientific community. The theories, methods, and techniques follow accepted standards or establish new standards that the scientific community then implements.

Result. The WAC criteria have been met. The information used in the Hanford fate and transport models were derived or developed using standard testing methods or other widely accepted scientific method.

WAC 173-340-702(16)(iii). *"Whether a review of relevant available information, both in support of and not in support of the proposed modification, has been provided along "with the rationale explaining the reasons for the proposed modification;"*

Evaluation. Section 4.0, as well as Appendices A and B, contain descriptions of and rationale for the data, parameters, and input values commonly used in the Hanford fate and transport models, along with the basis for the values and discussion of the variability, uncertainty, and limitations. These sections and appendixes also contain references to the source material which provides additional information on the data. These sections and appendices also provide the rationale for why default cleanup levels or model parameters, developed for use across the state of Washington, are inconsistent with or do not adequately represent the vadose zone characteristics, conditions, and processes in Hanford's Central Plateau (see Section 4.0). The Central Plateau is characterized by the following conditions and characteristics, which are dissimilar to most other regions in Washington:

- Low annual precipitation and high evapotranspiration rates
- Thick vadose zone (greater that 91.4 m [300 ft] in places)
- Vadose zone made up of multiple layers with varying hydraulic properties conducive to producing lateral flow
- Groundwater velocities that result in dilution factors significantly different than the 20 included in the three-phase models.

Result. The WAC criteria have been met. The rationale for developing model values applicable to Hanford's Central Plateau, the basis for the values used in applicable models, and discussion about the variability and uncertainty associated with those values are contained in Section 3.0.

WAC 173-340-702(16)(iv). *"Whether the assumptions used in applying the information to the facility are valid and would ensure the proposed modification would err on behalf of protection of human health and the environment;"*

Evaluation. Estimated Hanford values for the soil levels that are protective of groundwater are based primarily on conservative assumptions, as well as somewhat conservative parameter values. The validity of assumptions that are part of the conceptual model for Hanford Site modeling, as well as the magnitude and direction of the impact of those assumptions on the model results, are discussed in Sections 5.4 and 5.5. Section 5.5 contains an evaluation of the conservatism associated with the primary vadose zone model assumptions. Over 60% of the nearly 30 assumptions in the model are conservative, most of which have a potentially moderate to high magnitude of impact on contaminant soil concentration values protective of groundwater. Thus, it is indicated that the soil concentration values protective of groundwater are biased low based on a significant amount of compounded conservatism in the model assumptions and parameter selection.

Result. The WAC criteria have been met. The assumptions used in applying the information to the facility are valid and would ensure the proposed modification would err on behalf of protection of human health and the environment.

WAC 173-340-702(16)(v). *"Whether the information adequately addresses populations that are more highly exposed than the population as a whole and are reasonably likely to be present at the site;"*

Evaluation. Hanford vadose zone modeling pertains primarily to the protection of groundwater pathway and uses the MCL as the risk parameter against which groundwater contaminant levels are compared. These efforts do not involve exposure assessments other than those associated with the use of MCLs values for groundwater impacts. In this regard, the soil concentration values protective of groundwater are based on contaminant levels that do not produce concentrations that exceed MCLs in groundwater. The MCLs contain margins to adequately address populations that are more highly exposed than the population as a whole.

Result. The WAC criteria have been met. Risk characterization and remedial action goal values are based on contaminant levels that do not produce concentrations that exceed MCLs in groundwater.

> **WAC 173-340-702(16)(vi).** *"Whether adequate quality assurance and quality control procedures have been used, any significant anomalies are adequately explained, the limitations of the information are identified, and the known or potential rate of error is acceptable."*

Evaluation. Data collected for Hanford vadose zone model parameters and input values used QA and QC procedures. Data associated with parameters and input values for the model derived from Hanford Site-specific scientific literature were determined in conjunction with standard protocols and methods (e.g., as maintained by PNNL). The QA/QC procedures have been vetted in conjunction with the peer-reviewed publication process and document the basis for the parameters and inputs used in Hanford vadose zone model models including descriptions of the QA/QC procedures used to collect the data. Those documents identify and discuss the anomalies and limitations of the data.

Result. The WAC criteria have been met. The QA/QC procedures are contained in the referenced documents and any significant anomalies are adequately explained. The limitations of the information are identified, both in the context of the model input data and the model results. The known or potential rate of error is acceptable.

8.3 DEMONSTRATION OF CONSISTENCY WITH STATE REQUIREMENTS RELATED TO METHOD SELECTION

The consistency documentation presented in Section 8.2 demonstrates that the each of the elements of the state requirements for determining soil cleanup levels for groundwater protection has been addressed. Figure 8-1 provides a schematic compilation of all of the pertinent state requirements associated with the selection of alternative fate and transport modeling and the manner in which they have been addressed. The specific elements identified in the state regulations that pertain to method selection and to the use of alternative fate and transport models are summarized in Table 8-3, which identifies where each element of specific consistency documentation is located.

This documentation also provides the explanation and rationale that support consistency with the conditional requirements in WAC 173-340-747(8)(b) to use site-specific data in the estimation and derivation of selected parameters. Most model/code applications at Hanford use a common basis and databases for parameterization of the models. This documentation concerns these common aspects of parameterization. Waste site-specific applications also require supplemental documentation based on waste site-specific characteristics, conditions, and data for full consistency with these requirements.

Table 8-3. Comparison of the Elements for Federal and State and Requirements Pertaining to the Derivation of Soil RAG Values Protective of Groundwater.

Specific requirements and guidelines are identified in Sections 3.0, and in DOE/RL-2007-34, Section 4.0. The organization of these requirements and consistency documentation references is largely consistent with that of the consistency framework shown in Figure 2-5. The headings for the model, method, and code selection elements of consistency are highlighted in green, and those for the model documentation, parameterization, and evaluation of model results (e.g., uncertainties and assumptions) are highlighted in orange in the same manner as that in Figure 2-5 and Tables 6-1 and 7-1.

Federal Compliance Elements and Requirements for the Selection and Use of Environmental Regulatory Models (ERMs) for Risk Based Applications				Location (Chapter/Section) in this Document
Model/Method Selection	Purpose/Objectives			1.0, 3.0, 4.1
	Rationale of need/use for modeling			2.2
	Conceptual model(s); description of processes, mechanisms, phenomenon, site and system (i.e., vadose zone) characteristics to be considered			4.2
	Determine nature and types of primary system (i.e., vadose zone) FEPs and predictive tasks to be modeled			4.3
	Assess/determine other required model requirements/attributes			4.3
	Method selection/documentation			4.3
Code Selection	Evaluation/assessment of adequacy/capabilities of candidate codes (vs. required model attributes)			6.0
	Consideration of code-related criteria (characteristics, QA, etc.) and administrative criteria			6.2, 8.4
Model Use Documentation	Model Parameterization	Boundary conditions		Application-Specific
		Data sources, methods, pedigree		4.2 + Application-Specific
		Rationale for parameter estimation & selection		4.2 + Application-Specific
	Evaluation of results	Uncertainty / Sensitivity Analysis	Dominant factors, parameters	5.2 + Application-Specific
			Parameter/variable ranges	4.2, 5.2 + Application-Specific
			Magnitude & direction of parameter variability on model results	
		Model Assumptions Analysis	Magnitude & direction of effect on model results	5.3 + Application-Specific
		Limitations of Modeling & Results		5.4 + Application-Specific

State Compliance Elements for the Derivation of Soil Concentrations for Groundwater Protection, and the Selection and Use of Alternative Fate and Transport Models			Location (Chapter/Section) in this Document
Method Selection	Purpose/Objectives		1.0, 3.0, 4.1
	Model (Type) selection; model attributes		4.3
	Method selection/documentation		4.3, 8.1, 8.3
	Code Selection: Demonstration of adequacy, QA/QC		6.0, 8.4
Model Parameterization	Specified parameters		4.2, 8.2.1 + Application-Specific
	Other parameters		4.2 + Application-Specific
Documentation of model application and results	Burden of proof (Asssumptions, RME, point of compliance/calculation)		5.3, 8.2.2, 8.4 + Application-Specific
	(New) Scientific Information		5.0-6.0 + Application-Specific
	Adequacy and Quality of Information	Data/information acceptability, sources, references	8.2.2, 8.4 + Application-Specific
		Accepted methods	
		Assumptions, uncertaintes, conservatism/protectiveness	8.2.2, 8.4 + Application-Specific
		QA/QC, model limitations	8.2.2, 8.4 + Application-Specific

8.4 CONSISTENCY WITH WAC 173-340-747(8)(C) AND WAC 173-340-702(14), (15), AND (16) CONDITIONAL REQUIREMENTS RELEVANT TO CODE SELECTION

The following section addresses the requirements of WAC 173-340-702(14), (15), and (16), as required by WAC 173-340-747(8)(c), as they pertain to the selection and use of a model code. The WAC 173-340-747 and relevant WAC 173-340-702 regulations do not specifically explicate requirements for the selection and demonstration of acceptability of a code used to implement a method/model type. However, elements of the WAC 173-340-702(14), (15), and (16) burden of proof requirements are reasonably consistent with certain elements of the Federal guidelines addressing the selection and acceptability of codes. Documentation pertaining to the fulfillment of these conditional requirements is therefore provided in the following subsections for purpose of demonstrating the completeness of the technical basis used for method and code selection. This documentation provides the basis for demonstrating consistency, and/or support for consistency, with the conditional requirements, and/or intent of the requirements, concerning the selection of the alternative fate and transport models method. This section also addresses the WAC 173-340-702(14), (15), and (16) burden of proof requirements in the context of the acceptability of using the STOMP code. This code, evaluated in Section 6.0 in terms of the Federal guidelines and requirements, was found to be acceptable for implementing vadose zone fate and transport modeling at Hanford.

8.4.1 Criteria

WAC 173-340-747(8)(c) identifies the "evaluation criteria," which state, "Proposed fate and transport models, input parameters, and assumptions shall comply with WAC 173-340-702(14), (15), and (16)." WAC 173-340-702 includes subsections on "burden of proof" (subsection [14]), "new scientific information" (subsection [15]), and "criteria for quality of information" (subsection [16]). The "burden of proof" subsection calls for demonstration (to the department) that the requirements specified in this section are met for any modification of the default assumptions in the standard Method B and Method C equations (WAC 173-340-740 and WAC 173-340-745, respectively), including modification of the standard reasonable maximum exposures and exposure parameters, or any modification of default assumptions or methods specified in WAC 173-340-747. The "new scientific information" subsection concerns consideration of new scientific information when establishing cleanup levels and remediation levels (for individual sites), in the context of also meeting the "criteria for quality of information" requirements in subsection (16).

WAC 173-340-747(3)(e), "Deriving Soil Concentrations for Ground Water Protection," "Overview of Methods," "Alternative Fate and Transport Models," allows the use of fate and transport models as an alternative to the methods described in WAC 173-340-747(4) through (6) to establish soil concentrations that will not cause contamination of groundwater at levels that exceed the groundwater cleanup levels. WAC 173-340-747(8)(a), "Deriving Soil Concentrations for Ground Water Protection," "Alternative Fate and Transport Models," "Overview," specifies the procedures and requirements for using fate and transport models other than those specified in WAC 173-340-747(4) through (6).
WAC 173-340-747(8)(c), "Evaluation Criteria," states that "Proposed fate and transport models, input parameters, and assumptions shall comply with WAC 173-340-702(14), (15) and (16)." Hanford vadose zone fate and transport models, input parameters, and assumptions comply with WAC 173-340-702(14), (15), and (16). This section addresses these requirements as they pertain to the evaluation of a model code, specifically the STOMP code.

WAC 173-340-702(14), "Burden of Proof"

"Any person responsible for undertaking a cleanup action under this chapter who proposes to:

(a) Use a reasonable maximum exposure scenario other than the default provided for each medium;

(b) Use assumptions other than the default values provided in this chapter;

(c) Establish a cleanup level under Method C; or

(d) Use a conditional point of consistency, shall have the burden of demonstrating to the department that requirements in this chapter have been met to ensure protection of human health and the environment. The department shall only approve of such proposals when it determines that this burden of proof is met."

Evaluation. The satisfaction of the WAC 173-340-702(14) "burden of proof" requirements is met through satisfaction of the WAC 173-340-702(15) and (16) requirements with regard to the STOMP code. Therefore, the evaluation of this criterion is deferred until after discussion of consistency with the WAC 173-340-702 (15) and (16) requirements.

Result. Because the evaluation of this criterion is deferred until after discussion of consistency with the WAC 173-340-702(15) and (16) requirements, the result of the evaluation is similarly deferred.

WAC 173-340-702(15), "New Scientific Information"

"The department shall consider new scientific information when establishing cleanup levels and remediation levels for individual sites. In making a determination on how to use this new information, the department shall, as appropriate, consult with the Science Advisory Board, the Department of Health, and the United States Environmental Protection Agency. Any proposal to use new scientific information shall meet the quality of information requirements in subsection (16) of this section. To minimize delay in cleanups, any proposal to use new scientific information should be introduced as early in the cleanup process as possible. Proposals to use new scientific information may be considered up to the time of issuance of the final cleanup action plan governing the cleanup action for a site unless triggered as part of a periodic review under WAC 173-340-420 or through a reopener under RCW 70.105D.040 (4)(c)."

Evaluation. The STOMP code has been routinely used in environmental assessments since before 1997. The scientific theory upon which the code is based is documented in PNNL's STOMP theory guide (PNNL-12030), and guidance for users of the code is presented in PNNL-15782. An application guide (PNNL 11216) is also available. The application guide is organized into several sections that group similar classical vadose zone and groundwater problems and presents their solutions using the STOMP simulator. The examples in the guide were selected to demonstrate the application of the simulator to a variety of thermal and hydrogeologic flow and transport problems while illustrating a range of features available in the simulator. Simultaneously, the application examples serve as verification and benchmark cases wherever possible through comparison to analytic solutions or results reported elsewhere in the literature for similar problems solved using other computer codes. The application guide is available at: http://stomp.pnl.gov/documentation/application_guide.stm.

In addition to the application guide, a STOMP short-course document (PNNL-14440) is available and provides further example problems and exercises. The STOMP short-course documentation was intended to be used as an educational resource; however, the suite of problems (currently over 20 problems) in the short course is also being used in the STOMP QA program.

Result. The WAC criteria have been met. The STOMP code documentation and the referenced documentation about its usage have been introduced as early as possible, and are available to Ecology. Although the STOMP code has been in use for some time and is not necessarily new scientific information, the preceding discussion serves the purpose of fully documenting that STOMP code usage complies with "new scientific information" criteria to "meet the quality of information requirements in subsection (16)." The referenced documents also provide a number of example calculations that demonstrate that the STOMP code provides results that are consistent with other accepted methods for evaluating movement of water and contaminants in the vadose zone. This documentation serves to assist Ecology in their determination on how to use the information.

WAC 173-340-702(16), "Criteria for Quality of Information"

WAC 173-340-702(16)(a). *"The intent of this subsection is to establish minimum criteria to be considered when evaluating information used by or submitted to the department proposing to modify the default methods or assumptions specified in this chapter or proposing methods or assumptions not specified in this chapter for calculating cleanup levels and remediation levels. This subsection does not establish a burden of proof or alter the burden of proof provided for elsewhere in this chapter."*

WAC 173-340-702(16)(b). *"When deciding whether to approve or require modifications to the default methods or assumptions specified in this chapter for establishing cleanup levels and remediation levels, or when deciding whether to approve or require alternative or additional methods or assumptions, the department shall consider information submitted by all interested persons and the quality of that information. When evaluating the quality of the information the department shall consider the following factors, as appropriate, for the type of information submitted:"*

WAC 173-340-702(16)(i). *"Whether the information is based on a theory or technique that has widespread acceptance within the relevant scientific community;"*

Evaluation. The STOMP code's (sequential) and its parallel (scalable) implementation, STOMP SC, are computer codes designed to be general purpose tools for simulating subsurface flow and transport processes. These codes provide scientists and engineers from varied disciplines with multi-dimensional analysis capabilities for modeling subsurface flow and transport phenomena. The original target capabilities for the simulator were guided by proposed or applied remediation activities at Federal sites contaminated with volatile organics and radioactive materials.

The theoretical and numerical approaches applied in the simulator have been documented in a published theory guide (PNNL-12030) and addendums (e.g., PNNL-15465 and PNNL-15482). The simulator has undergone a rigorous validation process against analytical solutions, laboratory-scale experiments, and field-scale demonstrations and currently is maintained under configuration control procedures. Application and use of the simulator have been documented in the STOMP users guide (PNNL-15782) and short-course guide (PNNL-14440).

The STOMP simulator is founded on partial differential equations that describe the conservation of a component mass, thermal energy, or solute mass in variably saturated porous media. These conservation equations, along with a corresponding set of constitutive relations that relate variables within the conservation equations, are solved numerically by employing integrated volume, finite difference discretization to the physical domain and first or second order Euler discretization to the time domain. The resulting equations are non-linear, coupled algebraic equations, which are solved using Newton Raphson iteration.

Each operational mode of the STOMP simulator solves a unique set of conservation equations (e.g., water mass; water and air mass; water, oil, and dissolved oil mass; and water mass, air mass, and thermal energy). Depending on the chosen operational mode, the governing transport equations can be written over multiple phases. Phases relevant to Hanford applications include the aqueous phase and the gas phase. Where organic liquids are present, the simulator may also be configured to simulate NAPLs. Solute transport, radioactive decay, and first order chemical reactions are solved using a direct-solution technique (e.g., Patankar's power law formulation, total variation diminishing) scheme following the solution of the coupled flow equations.

One measure of acceptance of the theory and techniques implemented in the STOMP simulator is its use in subsurface flow and transport investigations within the scientific community. Several groundwater and vadose zone studies have been published in peer reviewed journals that have used the STOMP simulator as a tool to (1) predict laboratory or field results, or (2) perform numerical experiments. These studies have been published by researchers both inside and outside the Hanford community and include investigations of NAPL transport in porous media, as well as two-phase flow and transport. These published studies include the following:

- *Effect of Soil Moisture Dynamics on Dense Nonaqueous Phase Liquid (DNAPL) Spill Zone Architecture in Heterogeneous Porous Media* (Yoon et al. 2007)
- *Three-Dimensional Multifluid Flow and Transport at the Brooklawn Site Near Baton Rouge, LA: A Case Study* (Oostrom et al. 2007)
- *Behavior of a Viscous LNAPL Under Variable Water Table Conditions* (Oostrom et al. 2006)
- *Infiltration and Redistribution of LNAPL into Unsaturated Layered Porous Media* (Wipfler et al. 2004)
- *A Practical Model for Mobile, Residual, and Entrapped NAPL in Water-Wet Porous Media* (White et al. 2004)
- *Flow Behavior and Residual Saturation Formation of Liquid Carbon Tetrachloride in Unsaturated Heterogeneous Porous Media* (Oostrom et al. 2003)
- *Effective Parameters for Two-Phase Flow in a Porous Medium with Periodic Heterogeneities* (Ataie-Ashtiani et al. 2001)
- *Influence of Heterogeneity and Sampling Method on Aqueous Concentrations Associated with NAPL Dissolution* (Brusseau et al. 2000)
- *Movement and Remediation of Trichloroethylene in a Saturated Heterogeneous Porous Medium. 1. Spill Behavior and Initial Dissolution* (Oostrom et al. 1999)
- *Modeling Surfactant-Enhanced Nonaqueous-Phase Liquid Remediation of Porous Media* (White and Oostrom 1998)
- *Infiltration and Redistribution of Perchloroethylene in Partially Saturated Stratified Porous Media* (Hofstee et al. 1998)
- *Multifluid Flow in Bedded Porous Media: Laboratory Experiments and Numerical Simulations* (Schroth et al. 1998)
- *Light Nonaqueous-Phase Liquid Movement in a Variable Saturated Sand* (Oostrom et al. 1997)
- *Assessment of CO2 Injection Potential and Monitoring Well Location at the Mountaineer Power Plant Site* (Bacon et al. 2006)
- *Upscaling Unsaturated Hydraulic Parameters for Flow Through Heterogeneous Anisotropic Sediments* (Ward et al. 2006)
- *A Parameter Scaling Concept for Estimating Field-Scale Hydraulic Functions of Layered Soils* (Zhang et al. 2004)

- *A Numerical Study of Micro-Heterogeneity Effects on Upscaled Properties of Two-Phase Flow in Porous Media* (Das et al. 2004)
- *Transport of Carbon-14 in a Large Unsaturated Soil Column* (Plummer et al. 2004)
- *Estimating Soil Hydraulic Parameters of a Field Drainage Experiment Using Inverse Techniques* (Zhang et al. 2003)
- *A Vadose Zone Water Fluxmeter with Divergence Control* (Gee et al. 2002)
- *Fluid Flow, Heat Transfer, and Solute Transport at Nuclear Waste Storage Tanks in the Hanford Vadose Zone* (Pruess et al. 2002)
- *Oxygenation of Anoxic Water in a Fluctuating Water Table System: An Experimental and Numerical Study* (Williams and Oostrom 2000)
- *Parameterizing Flow and Transport Models for Field-Scale Applications in Heterogeneous, Unsaturated Soils* (Rockhold 1999)
- *PMFCT-2D: A Solute-Transport Simulator for Various Grid Peclet Numbers* (Aimo and Oostrom 1997)
- *Application of Similar Media Scaling and Conditional Simulation for Modeling Water Flow and Tritium Transport at the Las Cruces Trench Site* (Rockhold et al. 1996).

These publications have appeared in a number of peer-reviewed journals that include the following:

- *Advances in Water Resources*
- *Environmental Science & Technology*
- *Ground Water*
- *Journal of Hydraulic Research*
- *Journal of Contaminant Hydrology*
- *Soil and Sediment Contamination*
- *Soil Science Society of America Journal*
- *Transport in Porous Media*
- *Vadose Zone Journal*
- *Water Resources Research.*

Result. The WAC criteria have been met. The STOMP code is based on theory or technique that has widespread acceptance within the relevant scientific community.

> **WAC 173-340-702(16)(ii).** *"Whether the information was derived using standard testing methods or other widely accepted scientific methods;"*

Evaluation. The STOMP simulator has been subjected to a formal verification process that included benchmarking against analytical solutions and independent numerical solutions at both the laboratory and field scales. Initial three-phase verification studies have been published in a peer-reviewed journal (White et al., 1995, Lenhard et al., 1995). Additional verification studies have been formally documented in the STOMP application guide (PNNL-11216), and internal PNNL documents provide further verification studies that compare STOMP numerical solutions against analytical results. In addition, the simulator continues to be evaluated against analytical solutions, numerical solutions, and experimental data when other users conduct independent verification studies. Historically, the best strategy for identifying potential errors has been to build a sizable and diverse user group and encourage the code's application to a variety of problems. The STOMP simulator has a strong user group within the DOE community and academia. Graduate students in both the United States and the European communities have made significant contributions to continued STOMP code development and integrity.

Result. The WAC criteria have been met. The STOMP simulator was derived using standard testing methods or other widely accepted scientific methods.

> **WAC 173-340-702(16)(iii).** *"Whether a review of relevant available information, both in support of and not in support of the proposed modification, has been provided along with the rationale explaining the reasons for the proposed modification;"*

Evaluation. Section 6.0 presents the rationale for the model code selection process and includes a description of the STOMP code and its features, capabilities, and limitations. Sections 3.5 through 3.7 present the rationale for determining the necessary complexity of the alternate fate and transport model needed to adequately represent the vadose zone characteristics and conditions. The STOMP code has been selected for vadose zone fate and transport modeling at Hanford because it is capable of simulating the necessary complexity of the vadose zone FEPs. The rationale for using alternate fate and transport models in general includes the evaluation of the methods identified in WAC 173-340- 747, "Deriving Soil Concentrations for Ground Water Protection," which is provided in Section 4.0. The conclusion of the evaluation is that the use of alternate fate and transport models (WAC 173-340-747[8]) is the most appropriate method for Hanford vadose zone modeling. The use of alternate fate and transport models (WAC 173-340-747[8]) is proposed for vadose zone modeling because the other methods proposed by WAC 173-340-747(4) through (10) cannot adequately represent the vadose zone characteristics and conditions in Hanford's Central Plateau, nor do they adequately represent the vadose zone processes at Hanford.

Result. The WAC criteria have been met. The rationale for using the STOMP code is presented in Sections 3.5 through 3.7, which identify the model complexity required to simulate Hanford's Central Plateau FEPs, and Section 6.0, which presents a description of the STOMP code. Review of models proposed by WAC 173-340-747(4) through (6) has been provided and selection of alternate fate and transport models for vadose zone modeling explained in Section 4.0. A description of the STOMP code, its features, capabilities, and limitations are presented in Section 6.0.

> **WAC 173-340-702(16)(iv).** *"Whether the assumptions used in applying the information to the facility are valid and would ensure the proposed modification would err on behalf of protection of human health and the environment;"*

Evaluation. Responses to (i) and (ii) address this requirement for the STOMP code. The validity of assumptions that are part of the conceptual model and that are made as the conceptual model is translated into a numerical model will be addressed when the evaluation of the numerical model is made. Ensuring the proposed modification errors on the behalf of protection of human health and the environment will be addressed with each site-specific assessment.

Result. The WAC criteria have been met for the STOMP code.

> **WAC 173-340-702(16)(v).** *"Whether the information adequately addresses populations that are more highly exposed than the population as a whole and are reasonably likely to be present at the site;"*

Evaluation. This criterion is not applicable to the STOMP code because this code only calculates contaminant distribution in the environment and does not apply exposure scenarios to that contaminant distribution. The contaminant distribution is consistent regardless of population sensitivity to the contaminant. Differences in exposure among elements of a population must be accounted for in the exposure calculation.

Result. Not applicable.

WAC 173-340-702(16)(vi). *"Whether adequate quality assurance and quality control procedures have been used, any significant anomalies are adequately explained, the limitations of the information are identified, and the known or potential rate of error is acceptable."*

Evaluation. The STOMP simulator has been under software configuration management at PNNL since 1997 (PNNL-SA-54023). Currently, concurrent version system (CVS) software (Cederqvist et al. 1993) is used to manage source code updates and provides a means to track versions for both the individual source code files and the STOMP software releases. Formal procedures for software problem reporting and corrective actions for software errors and updates are maintained and rigorously implemented. Production code releases of the STOMP software undergo rigorous testing for both intended and unintended uses (PNNL-SA-54022). Testing is performed on a mode-by-mode basis and is benchmarked against analytical solutions and data. Documentation of all test results is publicly available.

In addition, the STOMP software is supported by software requirement specifications (PNNL-SA-54079) and software design documents (PNNL-SA-54078), maintained by PNNL, which are essential for developing quality software and lifecycle maintenance. In the software design documents, the overall source code structure is described, including a description of the control flow, control logic, and data flow model. In the software requirement documents, user input requirements are outlined with the primary purpose of guiding software testing. Requirements on subsurface flow and transport theory, and the mathematical representations of those theories, are specified in the STOMP theory guide and addendums (e.g., PNNL-12030. PNNL-15465, and PNNL-15482). The user's guide (PNNL-15782) provides support on specific input file requirements.

The STOMP software is compliant with *Quality Assurance Requirements for Nuclear Facility Applications* (NQA-1-2000), and also complies with DOE requirements for safety software (DOE G 414.1-40 and DOE O 414.1C). Under this order, STOMP software has been generically graded as "Class C safety software," but the classification is application dependent and is re-evaluated for each application.

Result. The WAC criteria have been met.

8.5 DOCUMENTATION/DEMONSTRATION OF CONSISTENCY WITH STATE REQUIREMENTS RELATED TO CODE SELECTION

The preceding documentation demonstrates that the primary conditions associated with the use of fate and transport models identified by WAC 173-340-747(3) and (8), including the additional evaluation criteria in WAC 173-340-702(14), (15), and (16) have been met with respect to the selection and use of the STOMP code. Several criteria (e.g., the requirement to use site specific data and provide documentation concerning the technical basis and rationale for model parameterization and several specific parameters) do not pertain directly to the code selection process, other than to the inferred requirement that the code be able to incorporate site specific data. The STOMP theory and user's guides provide thorough description and explanation of how to do that. The satisfaction of the WAC 173-340-702(14) "burden of proof" requirements have been met through the satisfaction of the WAC 173-340-702(15) and (16) requirements Therefore, the evaluation of these criteria demonstrate that the WAC 173-340-747(3) and (8) and WAC 173-340-702 (14) "burden of proof" requirements have been met regarding the selection and use of the STOMP code for fate and transport modeling of Hanford vadose zone system.

8.6 SUMMARY AND CORRESPONDENCE WITH FEDERAL CONSISTENCY DOCUMENTATION

The information presented in Sections 8.1 through 8.5 addresses and meets the specific and conditional WAC 173-340-747(3) requirements concerning method selection. Most elements of the WAC 173-340-702(15) and (16) conditional requirements pertaining the selection and use of the "alternative fate and transport" method (WAC 173-340-747[8]) are also addressed. This documentation supports the demonstration of consistency, for method/model type and code selection, required for site-specific applications of fate and transport modeling at the Hanford Site. A summary of the main elements of these state regulations pertaining to the selection and use of a method for the purpose of deriving soil concentrations protective of groundwater, together with the locations of the documentation that demonstrates the consistency of these elements, is shown in Table 8-3. This table includes the distinction between the state requirements relevant to method/model and code selection and those associated with the use of and ERM, such as fate and transport modeling.

As shown in the framework in Figure 8-1, the state elements pertaining to the derivation of soil concentrations for groundwater protection have direct and/or indirect counterparts in the Federal requirements and guidelines concerning the selection and use of ERMs. The headings for the method, model, and code selection elements of consistency in Table 8-3 are highlighted in green to facilitate comparison to their counterparts in the Federal documentation elements for consistency (see Figure 2-5 and Table 7-1). The headings for the model documentation, parameterization, and evaluation of model results (e.g., uncertainties and assumptions) are highlighted in orange for comparison to their Federal counterparts identified in Table 7-1. A direct comparison of state and Federal requirements, along with the locations of consistency documentation, is summarized in Table 8-3. It is indicated from the summary of consistency with State requirements in this Section, and the summary of consistency with the Federal requirements in Section 7.0, that the documentation provided in Section 7.0 addresses all pertinent elements of both. Therefore, the documentation provided in Section 7.0 regarding consistency with Federal guidelines can also serve to demonstrate of consistency with all of the State requirements, as indicated in Table 8-3.

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9.0 SUMMARY

This document identifies the Federal and state requirements and guidelines pertaining to the selection and use of ERMs, and also documents the application of the processes for method/model selection vadose zone modeling. There are specific requirements and expectations associated with their use in risk characterization applications concerning potential impacts to groundwater from vadose zone contamination at Hanford. Understanding the pertinent requirements, criteria, and expectations concerning the selection and use of ERMs is needed to demonstrate consistency with Federal and/or state requirements.

The Federal and state regulations, requirements, and guidelines that pertain to the selection and use of ERMs in risk assessment applications are summarized and evaluated in Section 2.0. As indicated from this evaluation, the Federal requirements and guidelines identify systematic processes for the selection and use of ERMs. Documentation provided in Sections 3.0 and 4.0, identify information for model selection concerns the common aspects of the FEPs of the vadose zone system at Hanford. Based on the common objectives of most vadose zone modeling and FEPs, the Federal guidelines can be applied to selection of a model type that is most appropriate for vadose zone modeling at Hanford.

A demonstration of the application of the Federal guidelines concerning code selection is also documented. It involves the use of required model type attributes and criteria in evaluating the acceptability of the STOMP code for implementing the model type. It is indicated from this evaluation (Section 6.0) that the STOMP code is acceptable for modeling the fate and transport of the vadose zone at the Hanford Site.

The manner and extent to which this documentation is consistent with the Federal requirements and guidelines concerning the selection and use of ERMs are presented in Section 7.0 for vadose zone modeling applications at Hanford. The manner in which the documentation provided here is consistent with and/or supports consistency with the state requirements that pertain to the selection and use of a method/model for vadose zone risk characterization applications at Hanford (WAC 173-340-747 and WAC 173-340-702[14], [15], and [16]) is presented in Section 8.0. The documentation meets all aspects of the requirements and expectations of Federal and state regulatory consistency concerning the common elements of method/model and code selection.

It is further indicated from the comparison of the Federal and state requirements and guidelines that the Federal requirements and guidelines encompass all aspects of the specific and conditional state requirements, and/or the intent of these requirements. All state requirements are shown to correspond to elements of the processes identified in Federal requirements and guidelines for ERM selection and use, and that documentation of consistency with these Federal guidelines can be used in the demonstration of consistency with the state requirements. Consistency with these Federal guidelines and processes also helps to ensure that the information and rationale necessary for demonstration of the technical adequacy and defensibility are incorporated in modeling documentation.

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10.0 REFERENCES

40 CFR 300, "National Oil and Hazardous Substances Pollution Contingency Plan," *Code of Federal Regulations*.

Aimo, N. J., and M. Oostrom, 1997, "PMFCT-2D: A Solute-Transport Simulator for Various Grid Peclet Numbers," *Ground Water*, 35(1):30–38.

ASTM E 978-92, 1992, *Standard Guide for Evaluating Mathematical Models for the Environmental Fate of Chemicals*, American Society for Testing and Materials, West Conshohocken, Pennsylvania (http://www.astm.org).

ASTM, 1999, *RBCA Fate and Transport Models: Compendium and Selection Guidance*, American Society for Testing and Materials, West Conshohocken, Pennsylvania (http://www.astm.org).

Ataie-Ashtiani B., S. M. Hassanizadeh, M. Oostrom, M. A. Celia, and M. D. White, 2001, "Effective Parameters for Two-Phase Flow in a Porous Medium with Periodic Heterogeneities," in *J. Contam. Hydrol.*, 49(1–2):87–109.

Bacon, D. H., M. D. White, N. Gupta, J. R. Sminchak, and M. E. Kelley, 2006, "Assessment of CO2 Injection Potential and Monitoring Well Location at the Mountaineer Power Plant Site," in *8th International Conference on Greenhouse Gas Control Technologies*, GHGT-8, June 19-22, 2006, Trondheim, Norway, p. 6 pages, Elsevier Amsterdam, Amsterdam, Netherlands.

Bailey, L. E. F., and D. E. Billingham, 1998, *Overview of the FEP Analysis Approach to Model Development*, NIREX Science Report S/98/009, United Kingdom Nirex Limited, Oxfordshire, United Kingdom.

Baker, R. R., B. N. Bjornstad, A. J. Busacca, K. R. Fecht, E. P. Kiver, U. L. Moody, J. G. Rigby, O. F. Stradling, and A. M. Tallman, 1991, "Quaternary Geology of the Columbia Plateau" in *Quaternary Nonglacial Geology; Conterminous U.S., v. K-2 of The Geology of North America*, R. B. Morrison (ed.), Geological Society of America, Boulder Colorado.

Bargar, J., R. Reitmeyer, and J. A. Davis, 1999, "Spectroscopic Confirmation of Uranium(VI)-Carbonato Adsorption Complexes on Hematite," in *Environ. Sci. Technol.*, 33:2481-2484.

Bertsch, P. M., D. B. Hunter, S. R. Sutton, S. Bajt, and M. L. Rivers, 1994, "In Situ Chemical Speciation of Uranium in Soils and Sediments by Micro X-Ray Absorption Spectroscopy," in *Environ. Sci. Technol.*, 28:980-984.

Beyeler, W. E., T. J. Brown, W. A. Hareland, S. Conrad, N. Olague, D. Brosseau, E. Kalinina, D. P. Gallegos, and P. A. Davis, 1998, *Review of Parameter Data for the NUREG/CR-5512 Residential Farmer Scenario and Probability Distributions for the D and D Parameter Analysis*, Letter Report for NRC Project JCN W6227, U.S. Nuclear Regulatory Commission, Washington, D.C.

BHI-00184, 1995, *Miocene- to Pliocene-Aged Suprabasalt Sediments of the Hanford Site, South Central Washington*, Bechtel Hanford, Inc., Richland, Washington.

BHI-01103, 1999, *Clastic Injection Dikes of the Pasco Basin and Vicinity – Geologic Atlas Series*, Rev. 0, Bechtel Hanford, Inc., Richland, Washington.

BHI-01573, 2001, *The Application of Features, Events, and Process Methodology at the Hanford Site*, Rev. 0, Bechtel Hanford, Inc., Richland, Washington.

Bretz, J. H., 1928, "The Channeled Scabland of Eastern Washington," in *Geographical Review*, 18:446-477.

Bretz, J. H., 1969, "The Lake Missoula Floods and the Channeled Scabland," in *Journal of Geology*, 77:505-543.

Brusseau, M. L., N. T. Nelson, M. Oostrom, Z. H. Zhang, G. R. Johnson, and T. W. Wietsma, 2000, "Influence of Heterogeneity and Sampling Method on Aqueous Concentrations Associated with NAPL Dissolution," in *Environ. Sci. Technol.*, 34(17):3657–3664.

Buck, E. C., N. R. Brown, and N. L. Dietz, 1994, "Distribution of Uranium-Bearing Phases in Soils from Fernald," in *Scientific Basis for Nuclear Waste Management XVII*, A. Barkatt and R. A. Van Konynenburg (eds.), pp. 437-444. Materials Research Society Symposium Proceedings, Volume 333, Materials Research Society, Pittsburgh, Pennsylvania.

Burns, P. C., and R. J. Finch, 1999, "Wyartite: Crystallographic Evidence for the First Pentavalent-Uranium Mineral," in *American Mineralogist* (in press).

Campbell, G. S., 1977, *An Introduction to Environmental Biophysics*, Springer-Verlag, New York, New York.

Catalano, J. G., S. M. Heald, J. M. Zachara, and G. E. Brown Jr., 2004, "Spectroscopic and Diffraction Study of Uranium Speciation in Contaminated Vadose Zone Sediments from the Hanford Site, Washington State," in *Environ. Sci. Technol.*, 38(10):2822-2828.

Cederqvist et al., 1993, *Version Management with CVS for CVS 1.10.8*, available on the Internet at http://www.wincvs.org/howto/cvscod/cvs_1.htm#SEC1.

Cleary, R. W., and M. J. Ungs, 1978, *Groundwater Pollution and Hydrology*, Report 78-WR-15, Department of Civil Engineering, Princeton University, Princeton, New Jersey.

Comprehensive Environmental Response, Compensation, and Liability Act of 1980, Public Law 96-510, as amended, 94 Stat. 2767, 42 U.S.C. 9601, et seq.

CREM, 2001, *Proposed Agency Strategy for the Development of Guidance on Recommended Practices in Environmental Modeling*, prepared by Model Evaluation Action Team, The Council on Regulatory Environmental Modeling for the U.S. Environmental Protection Agency, Washington, D.C.

CREM, 2003, *Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models*, prepared by The Council for Regulatory Environmental Modeling for the U.S. Environmental Protection Agency, Office of Science Policy, Office of Research and Development, Washington, D.C.

Crumbling, D. M., 2002, "In Search of Representativeness: Evolving the Environmental Data Quality Model," *Quality Assurance: Good Practice, Regulation and Law*, 9:3&4 pp. 179-190, July-December 2002 (available online at http://cluin.org/download/char/dataquality/dcrumbling.pdf).

Das, D. B., S. M. Hassanizadeh, B. E. Rotter, and B. Atale-Ashtiani, 2004, "A Numerical Study of Micro-Heterogeneity Effects on Upscaled Properties of Two-Phase Flow in Porous Media," in *Transport in Porous Media*, 56(3):329–350.

Delegard, C. H., R. L. Weiss, R. T. Kimura, A. G. Law, and R. C. Routson, 1986, "Characterization and Anion Exchange Removal of Uranium from Hanford Ground Water," in *Waste Management '86, Volume 1*, R. G. Post (ed.), pp. 545-550, Arizona Board of Regents, Arizona.

DOE, 2005, *Technical Guidance Document for Tank Closure Environmental Impact Statement Vadose Zone and Groundwater Revised Analysis*, Rev. 0, dated March 25, 2005, U.S. Department of Energy, Washington, D.C.

DOE/EH-0484, 1995, *CERCLA Baseline Risk Assessment Reference Manual for Toxicity & Exposure Assessment and Risk Characterization*, U.S. Department of Energy, Washington, D.C.

DOE G 414.1-4, *Safety Software Guide for Use with 10 CFR 830 Subpart A, Quality Assurance Requirements*, U.S. Department of Energy, Washington, D.C.

DOE O 414.1C, *Quality Assurance*, U.S. Department of Energy, Washington, D.C.

DOE/ORP-2000-24, 2001, *Hanford Immobilized Low Activity Waste (ILAW) Performance Assessment 2000 Version*, Rev. 0, U.S. Department of Energy, Office of River Protection, Richland, Washington.

DOE/ORP-2003-11, 2003, *Preliminary Performance Assessment for Waste Management Area C at the Hanford Site Washington*, Rev. 0, U.S. Department of Energy, Office of River Protection, Richland, Washington.

DOE/ORP-2005-01, 2006, *Initial Single Shell Tank System Performance Assessment for the Hanford Site*, Rev. 0, U.S. Department of Energy, Office of River Protection, Richland, Washington.

DOE/RL-88-30, 2003, *Hanford Site Waste Management Units Report*, Rev. 12, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-91-44, 1991, *Description of Codes and Models to be Used in Risk Assessment*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-92-23, 1992, *Hanford Site Background: Part 1, Soil Background for Nonradioactive Analytes*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-92-24, 1994, *Hanford Site Background: Part 1, Soil Background for Nonradioactive Analytes*, Rev. 2, Vol. 1 of 2, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-96-61, 1996, *Hanford Site Background: Part 3, Groundwater Background*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-98-48, 1999, *Groundwater/Vadose Zone Integration Project Background Information and State of Knowledge.*, Vol. II, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-2002-39, 2002, *Standardized Stratigraphic Nomenclature for the Post-Ringold-Formation Sediments Within the Central Pasco Basin*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-2003-23, 2005, *Focused Feasibility. Study for the U Plant Closure Area Waste Sites*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-2005-01, 2005, *Hanford Site Air Operating Permit Semiannual Report for the Period July 1, 2004, through December 31, 2004*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RL-2007-35, 2008, *200-UW-1 Operable Unit Remedial Action Goals for Removal/Treatment/ Disposal Waste Sites*, Rev. 0, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

DOE/RW-0164, 1988, *Consultation Draft Site Characterization Plan. Reference Repository Location, Hanford Site, Washington,* U.S. Department of Energy, Office of Civilian Radioactive Waste Management, Washington, D.C.

Dong, W., W. P. Ball, C. Liu, Z. Wang, A. T. Stone, J. Bail, and J. Zachara, 2005, "Influence of Calcite and Dissolved Calcium on U(VI) Sorption to a Hanford Subsurface Sediment," in *Environ. Sci. Technol.*, 39(20):7949-7955.

Duff, M. C., and C. Amrhein, 1996, "Uranium(VI) Adsorption on Goethite and Soil in Carbonate Solutions," in *Soil Sci. Soc. Am. J.*, 60:1393-1400.

Ecology 94-145, 2001, *Model Toxics Control Act Cleanup Levels & Risk Calculations (CLARC), Version 3.1*, Washington State Department of Ecology, Olympia, Washington.

Ecology, EPA, and DOE, 2003, *Hanford Federal Facility Agreement and Consent Order* (Tri-Party Agreement), 2003, 2 vols., as amended, 89-10, Rev. 6, Washington State Department of Ecology, U.S. Environmental Protection Agency, and U.S. Department of Energy, Olympia, Washington.

EPA, 1985, *Methodology for Characterization of Uncertainty in Exposure Assessments*, prepared by Research Triangle Institute, NTIS PB85-240455, U.S. Environmental Protection Agency, Washington, D.C.

EPA, 1992, *Supplemental Guidance to RAGS: Calculating the Concentration Term,* U.S. Environmental Protection Agency, Washington, D.C.

EPA, 1995, *Guidance for Risk Characterization,* dated February 1995, U.S. Environmental Protection Agency, Washington, D.C.

EPA, 1999, *White Paper on the Nature and Scope of Issues on Adoption of Model Use Acceptability Guidance*, Science Policy Council, Model Acceptance Criteria and Peer Review, U.S. Environmental Protection Agency, Washington, D.C.

EPA, 2001, *Proposed Agency Strategy for the Development of Guidance on Recommended Practices in Environmental Modeling,* Model Evaluation Action Team, Council for Regulatory Environmental Modeling, U.S. Environmental Protection Agency, Washington, D.C.

EPA, 2003a, *Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models*, U.S. Environmental Protection Agency, Office of Science Policy, Office of Research and Development, Washington, D.C.

EPA, 2003b, *A Summary of General Assessment Factors for Evaluating the Quality of Scientific and Technical Information*, U.S. Environmental Protection Agency, Science Policy Council, Washington, D.C.

EPA 402-R-04-002C, 2004, *Understanding Variation in Partition coefficient, Kd, Values, Volume III: Review of Geochemistry and Available Kd Values for Americium, Arsenic, Curium, Iodine, Neptunium, Radium, and Technetium*, U.S. Environmental Protection Agency, Washington, D.C.

EPA 402-R-93-005, 1993, *Establishment of Cleanup Levels for CERCLA Sites with Radioactive Contamination (Computer Models Used to Support Cleanup Decision-Making at Hazardous and Radioactive Waste Sites)*, NTIS PB93-183333/XAB, U.S. Environmental Protection Agency, Office of Air and Radiation, Washington, D.C.

EPA 402-R-93-009, 1993, *Environmental Pathway Models-Groundwater Monitoring in Support of Remedial Decisions-Making at Sites Contaminated with Radioactive Material*, U.S. Environmental Protection Agency, Washington, D.C.

EPA 402-R-94-012, 1994, *Technical Guide to Ground-Water Model Selection at Sties Contaminated with Radioactive Substances*, NTIS PB-205804/XAB, U.S. Environmental Protection Agency, Washington, D.C.

EPA 500-R-94-001, 1994, *Report of Agency Task Force on Environmental Regulatory Modeling: Guidance, Support Needs, Draft Criteria and Charter*, U.S. Environmental Protection Agency, Washington, D.C.

EPA 540-F-96/002, 1996, *Fact Sheet: Documenting Ground-Water Modeling at Sites Contaminated with Radioactive Substance*, U.S. Environmental Protection Agency, Washington, D.C.

EPA 540-R-02-002, 2001, *Risk Assessment Guidance for superfund: Volume III – Part A, Process for Conducting Probabilistic Risk Assessment*, OSWER Directive 9285.7-45, NTIS PB202 963302, U.S. Environmental Protection Agency, Washington, D.C.

EPA, 1985, *Methodology for Characterization of Uncertainty in Exposure Assessments*, prepared by Research *to Guideline on Air Quality Models: Adoption of a Preferred Long Range Transport Model and Other Revisions*, U.S. Environmental Protection Agency, Washington, D.C.

EPA/100/B-04/001, 2004, *An Examination of EPA Risk Assessment Principles and Practices*, U.S. Environmental Protection Agency, Washington, D.C.

EPA/540/1-89/002, 1989, *Risk Assessment Guidance for Superfund Volume I, Human Health Evaluation Manual (Part A)*, U.S. Environmental Protection Agency, Washington D.C.

EPA/540/R-92/003, 1991, *Risk Assessment Guidance for Superfund Volume I, Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Remediation Goals)*, U.S. Environmental Protection Agency, Washington D.C.

EPA/540/R-96-003, 1996, *Documenting Groundwater Modeling at Sites Contaminated with Radioactive Substances*, U.S. Environmental Protection Agency, Washington, D.C.

EPA/600, 1989, *Exposure Assessment Methods Handbook*, U.S. Environmental Protection Agency, Exposure Assessment Group, Office of Health and Environmental Assessment, Washington, D.C.

EPA/600Z-92/001, 1992, *Guidelines for Exposure Assessment*, U.S. Environmental Protection Agency, Risk Assessment Forum, Washington, D.C.

EPA-SAB-06-009, 2006, *Review of Agency Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models* and *Models Knowledge Base*, by Regulatory Environmental Modeling Guidance Review Panel of the EPA Science Advisory Board, Office of the Administrator Science Advisory Board, U.S. Environmental Protection Agency, Washington, D.C.

EPA-SAB-EEC-89-012, 1989, *Resolution on the Use of Mathematical Models by EPA for Regulatory Assessment and Decision-Making*, U.S. Environmental Protection Agency, Science Advisory Board, Washington, D.C.

Fecht, K., S. Reidel, and A. Tallman, 1987, "Paleodrainage of the Columbia River on the Columbia Plateau of Washington State – A Summary," in *Washington Division of Geology and Earth Resources Bulletin*, 77:219-248, Washington Department of Resources, Olympia, Washington.

Freehley, C. E., C. Zheng, and F. Molz, 2000, "A Dual-Domain Mass Transfer Approach for Modeling Solute Transport in Heterogeneous Aquifers: Application to the Macrodispersion Experiment (MADE) Site," in *Water Resources Research*, Vol., 36, No. 9, 2501-2515.

Gee, G. W., M .J. Fayer, M. L. Rockhold, and M. D. Campbell, 1992, "Variations in Recharge at the Hanford Site," in *Northwest Sci.*, 66:237-250.

Gee, G. W., A. L. Ward, T. G. Caldwell, and J. C. Ritter, 2002, "A Vadose Zone Water Fluxmeter with Divergence Control," in *Water Resources Research*, 38(8): Article No. 1141.

Gee, G. W., J. M. Keller, and A. L. Ward, 2005a, "Measurement and Prediction of Deep Drainage from Bare Sediments at a Semiarid Site," in *Vadose Zone Journal*, 4 (1):32-40

Gee, G. W., Z. F. Zhang, S. W. Tyler, W. H. Albright, and M. J. Singleton, 2005b, "Chloride Mass Balance: Cautions in Predicting Increased Recharge Rates," in *Vadose Zone Journal*, 4:72-78.

Gelhar, L. W., C. Welty, and K. R. Rehfeldt, 1992, "A Critical Review of Data on Field-Scale Dispersion in Aquifers," in *Water Resources Research*, 28:1955-1974.

Hanke, C., B. Jahrling, and K. H. Lieser, 1986, "Properties and Solubility of Technetium Dioxide," in *Technetium in the Environment*, G. Desmetand and C. Myttenaere (eds.), Elsevier Applied Science Publishers, pp. 179-187.

Haverkamp, R., M. Vauclin, J. Touma, P. J. Wierenga, and G. Vachaud, 1977, "Comparison of Numerical Simulation Models for One-Dimensional Infiltration," in *Soil Sci. Am. J.*, 41:285-294.

Hills, R. G., I. Porro, D. B. Hudson, and P. J. Wierenga, 1989, "Modeling One-Dimensional Infiltration into Very Dry Soils, 1 – Model Development and Evaluation," in *Water Resources Research*, 25(6):1259-1269.

HNF-5294, 1999, *Computer Code Selection Criteria for Flow and Transport Code(s) to Be Used in Vadose Zone Calculations for Environmental Analyses in the Hanford Site's Central Plateau*, CH2M Hill Hanford Group, Inc., Richland, Washington.

HNF-EP-0063-3, 1991, *Hanford Site Solid Waste Acceptance Criteria*, Fluor Hanford, Inc., Richland, Washington.

Hofstee, C., M. Oostrom, J. H. Dane, and R. C. Walker, 1998, "Infiltration and Redistribution of Perchloroethylene in Patrially Saturated Stratified Porous Media, " in *J. Contam. Hydrol.*, 34(4):293–313.

Hunter, D. B., and P. M. Bertsch, 1998, "In Situ Examination of Uranium Contaminated Soil Particles by Micro-X-Ray Absorption and Micro-Fluorescence Spectroscopies," in *J. of Rad. Nucl. Chem.*, 234:237-242.

HW-9671, 1948, *Underground Waste Disposal at Hanford Works*, General Electric Hanford Company, Richland, Washington.

HW-43149, 1957, *Earth Sciences' Waste Disposal Monitoring Activities Summary, January, 1956*, General Electric Company, Hanford Atomic Products Operation, Richland, Washington.

HW-60601, 1959, *Aquifer Characteristics and Ground-Water Movement at Hanford*, General Electric Company, Richland, Washington.

Kaluarachchi, J. J., and J. C Parker, 1989, "An Efficient Finite Element Method for Modeling Multiphase Flow," in *Water Resources Research*, 25 (1):43-54.

Kool, J. B., J. C. Parker, and M. T. van Genuchten, 1985, "Determining Soil Hydraulic Properties from One Step Outflow Experiments by Parameter Estimation: 1. Theory and Numerical Studies," in *Soil Sci. Soc. Am. J.*, 49:1348-1354.

Langmuir, D., 1978, "Uranium Solution-Mineral Equilibria at Low Temperatures with Applications to Sedimentary Ore Deposits," in *Geochimica et Cosmochimica Acta*, 42:547-569.

Langmuir, D., 1997, *Aqueous Environmental Geochemistry*, Prentice Hall, Upper Saddle River, New Jersey.

Lenhard, R. J., M. Oostrom, and M. D. White, 1995, "Modeling Fluid-Flow and Transport in Variably Saturated Porous-Media with the STOMP Simulator. 2. Verification and Validation Exercises," in *Advances in Water Resources*, 18(6)365–373.

Lindsey, K., and D. Gaylord, 1990, "Lithofacies and Sedimentology of the Miocene-Pliocene Ringold Formation, Hanford Site, South-Central Washington," in *Northwest Sci.*, 4:165-180.

Liu., C., J. M. Zachara, O. Qafoku, J. P. McKinley, S. M. Heald, and Z. Wang, 2004, "Dissolution of Uranyl Microprecipitates in Subsurface Sediments at Hanford Site," in *Geochimica et Cosmochimica Acta*, 68(22):4519-4537.

Morris, D. E., P. G Allen, J. M. Berg, C. J. Chisholm-Brause, S. D. Conradson, R. J. Donohoe, N. J. Hess, J. A. Musgrave and C. D. Tait, 1996, "Speciation of Uranium in Fernald Soils by Molecular Spectroscopic Methods: Characterization of Untreated Soils," in *Environ. Sci. Technol.*, 30:2322-2331

Murphy, E. M., T. R. Ginn, and J. L. Phillips, 1996, "Geochemical Estimates of Paleorecharge in the Pasco Basin: Evaluation of the Chloride Mass-Balance Technique," in *Water Resources Research*, 32(9):2853-2868.

National Research Council, 1983, *Risk Assessment in the Federal Government –Managing the Process*, National Academy Press, Washington, D.C.

National Research Council, 1994, *Science and Judgment in Risk Assessment*, National Academy Press, Washington, D.C.

NEA, 2000, *Features, Events and Processes (FEPs) for Geologic Disposal of Radioactive Waste, an International Database*, Organization for Economic Co-Operation and Development (OECD) Publications, France.

Newcomb, R., J. Strand, and F. Frank, 1972, *Geology and Ground-Water Characteristics of the Hanford Reservation of the U.S. Atomic Energy Commission, Washington*, Professional Paper 717, U.S. Geological Survey, Washington, D.C.

NQA-1-2000, 2000, *Quality Assurance Requirements for Nuclear Facility Applications*, American Society of Mechanical Engineers, New York, New York.

NUREG/CR-5621, 1998, *Groundwater Models in Support of NUREG/CR-5512*, U.S. Nuclear Regulatory Commission, Washington, D.C.

NUREG/CR-6565, 1997, *Uncertainty Analyses of Infiltration and Subsurface Flow and Transport for SDMP Sites*, U.S. Nuclear Regulatory Commission, Washington, D.C.

Oostrom, M., R. J. Lenhard, and M. D. White, 1995, "Infiltration and Redistribution of Dense and Light Nonaqueous Phase Liquids in Partly Saturated Sand Columns," in *Proceedings of Fifteenth Annual American Geophysical Union Hydrology Days*, Fort Collins, Colorado, pp. 215-226.

Oostrom, M., C. Hofstee, and J. H. Dane, 1997, "Light Nonaqueous-Phase Liquid Movement in a Variable Saturated Sand," in *Soil Sci. Soc. America J.*, 61(6):1547–1554.

Oostrom, M., C. Hofstee, R. C. Walker, and J. H. Dane, 1999, "Movement and Remediation of Trichloroethylene in a Saturated Heterogeneous Porous Medium. 1. Spill Behavior and Initial Dissolution," in *J. Contam. Hydrol.*, 37(1–2):159–178.

Oostrom, M., C. Hofstee, R. J. Lenhard, and T. W. Wietsma, 2003, "Flow Behavior and Residual Saturation Formation of Liquid Carbon Tetrachloride in Unsaturated Heterogeneous Porous Media," in *J. Contam. Hydrol.*, 64:93–112.

Oostrom, M., C. Hofstee, and T. W. Wietsma, 2006, "Behavior of a Viscous LNAPL Under Variable Water Table Conditions," in *Soil & Sediment Contamination*, 15(6):543–564.

Oostrom, M., M. J. Truex, P. D. Thorne, and T. W. Wietsma, 2007, "Three-Dimensional Multifluid Flow and Transport at the Brooklawn Site Near Baton Rouge, LA: A Case Study," in *Soil & Sediment Contamination*, 16(2):109–141.

OSWER Directive 9200.4-18, 1997, *Establishment of Cleanup Levels for CERCLA Sites with Radioactive Contamination*, NTIS PB97 963210, U.S. Environmental Protection Agency, Washington, D.C.

Plummer, M.A., L. C. Hull, and D. T. Fox, 2004, "Transport of Carbon-14 in a Large Unsaturated Soil Column," in *Vadose Zone Journal*, 3(1):109–121.

PNL-6488, 1988, *Characterization of Unsaturated Hydraulic Conductivity at the Hanford Site*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-7296, 1990, *Multimedia Environmental Pollutant Assessment System (MEPAS) Sensitivity Analysis of Computer Codes*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-8597, 1993, *Refined Conceptual Model for the Volatile Organic Compounds-Arid Integrated Demonstration and 200 West Area Carbon Tetrachloride Expedited Response Action*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-8889, 1993, *Solid-Waste Leach Characteristics and Contaminant-Sediment Interactions, Volume 1: Batch Leach and Adsorption Tests and Sediment Characterization*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-10195, 1994, *Three-Dimensional Conceptual Model for the Hanford Site Unconfined Aquifer System, FY 1994 Status Report*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-10379, 1995, *Distribution Coefficient Values Describing Iodine, Neptunium, Selenium, Technetium, and Uranium Sorption to Hanford Sediments*, Supplement 1, Pacific Northwest Laboratory, Richland, Washington.

PNL-10722, 1995, *Solid Waste Leach Characteristics and Contaminant-Sediment Interactions Volume 2: Contaminant Transport Under Unsaturated Moisture Contents*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNL-SA-10390, 1982, *Energy Transport in Condensed Phase*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

PNNL-10886, 1995, *Development of a Three-Dimensional Ground-Water Model of the Hanford Site Unconfined Aquifer System: FY 1995 Status Report*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-11216, 1997, *STOMP Subsurface Transport Over Multiple Phases Application Guide*, Rev. 0, UC-2010, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-11217, 1996, *STOMP Subsurface Transport Over Multiple Phases Application Guide*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-11310, 1996, *Gas Release During Salt Well Pumping: Model Predictions and Comparisons to Laboratory Experiments*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-11485, 1996, *Radionuclide Adsorption Distribution Coefficients Measured in Hanford Sediments for the Low-Level Waste Performance Assessment Project*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-11966, 1998, *Radionuclide Distribution Coefficients for Sediments Collected from Borehole 299-E17-21: Final Report for Subtask 1a*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-12030, 2000, *STOMP Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide*, Rev. 0, UC-2010, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-12192, 1999, *Anoxic Plume Attenuation in a Fluctuating Water Table System: Impact of 100-D Area In Situ Redox Manipulation on Downgradient Dissolved Oxygen Concentrations*, Rev. 0, UC-2000, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13033, 1999, *Recharge Data Package for the Immobilized Low-Activity Waste 2001 Performance Assessment*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13037, 2000, *Geochemical Data Package for the Hanford Immobilized Low-Activity Tank Waste Performance Assessment (ILAW PA)*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL- 13037, 2004, *Geochemical Data Package for the 2005 Hanford Integrated Disposal Facility Performance Assessment*, Rev. 2, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13091, 1999, *Information on Hydrologic Conceptual Models, Parameters, Uncertainty Analysis and Data Sources for Dose Assessments at Decommissioning Sites*, Rev. 0, NUREG/CR-6656, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13249, 2000, *UNSAT-H Version 3.0: Unsaturated Soil Water and Heat Flow Model—Theory, User Manual, and Examples*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13672, 2001, *A Catalog of Vadose Zone Hydraulic Properties for the Hanford Site*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-13895, 2003, *Hanford Contaminant Distribution Coefficient Database and Users Guide*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14022, 2002, *300 Area Uranium Leach and Adsorption Project*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14115, 2003, *Hydrologic Characterizations Using Vadose Zone Monitoring Tools: Status Report*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14440, 2003, *STOMP Subsurface Transport Over Multiple Phases Version 3.0 An Introductory Short Course*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14594, 2004, *Characterization of Vadose Zone Sediments Below the TX Tank Farm: Probe Holes C3830, C3831, C3832 and 299-W10-27*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14702a, 2004, *Vadose Zone Hydrogeology Data Package for the 2004 Composite Analysis*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14702b, 2006, *Vadose Zone Hydrogeology Data Package for the 2004 Composite Analysis*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14725, 2004, *Geographic and Operational Site Parameters List (GOSPL) for the 2004 Composite Analysis*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14725, 2006, *Geographic and Operational Site Parameters List (GOSPL) for Hanford Assessments*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14744, 2004, *Recharge Data Package for the 2005 Integrated Disposal Facility Performance Assessment*, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14753, 2006, *Groundwater Data Package for Hanford Assessments*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14907, 2004, *Vadose Zone Contaminant Fate-and-Transport Analysis for the 216-B-26 Trench*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15121, 2005, *Uranium Geochemistry in Vadose Zone and Aquifer Sediments from the 300 Area Uranium Plume*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15443, 2006, *Vadose Zone Transport Field Study: Summary Report*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15465, 2005, *STOMP Subsurface Transport Over Multiple Phases Version 1.0 Addendum: Sparse Vegetation Evapotranspirational Model for the Water-Air-Energy Operational Mode*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15482, 2005, *STOMP Subsurface Transport Over Multiple Phases Version 1.0 Addendum: ECKEChem Equilibrium-Conservation-Kinetic Equation Chemistry and Reactive Transport*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15502, *Characterization of 200-UP-1 Aquifer Sediments and Results of Sorption-Desorption Tests Using Spiked Uncontaminated Groundwater*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15782, 2006, *STOMP Subsurface Transport Over Multiple Phases Version 4.0 Users Guide*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15955, 2007, *Geology Data Package for the Single-Shell Tank Waste Management Areas at the Hanford Site*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-16198, 2006, *Carbon Tetrachloride Flow and Transport in the Subsurface of the 216-Z-18 Crib and 216-Z-1A Tile Field at the Hanford Site: Multifluid Flow Simulations and Conceptual Model Update*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-65410, 2001, *Rapid Migration of Radionuclides Leaked from High-Level Water Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-SA-34515, 2004, *Use of Process Relationship Diagrams in Development of Conceptual Models*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-SA-54022, 2007, *STOMP Software Test Plan*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-SA-54023, 2007, *STOMP Software Configuration Management Plan*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-SA-54078, 2007, *Software Design Description for Subsurface Transport Over Multiple Phases (STOMP) Software*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-SA-54079, 2007, *Requirements for STOMP Subsurface Transport Over Multiple Phases*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNWD-3111, 2001, *Initial Assessments for S-SX Field Investigation Report (FIR): Simulations of Contaminant Migration with Surface Barriers*, Rev. 0, Pacific Northwest Laboratory, Richland, Washington.

Pruess K., S. Yabusaki, C. Steefel, and P. Lichtner, 2002, "Fluid Flow, Heat Transfer, and Solute Transport at Nuclear Waste Storage Tanks in the Hanford Vadose Zone," in *Vadose Zone Journal*, 1(1):68–88

Qafoku, N., J. M. Zachara, C. Liu, P. L. Gassman, O. Qasfoku, and S. C. Smith, 2005, "Kinetic Desorption and Sorption of U(VI) During Reactive Transport in a Contaminated Hanford Sediment," in *Environ. Sci. Technol.*, 39(9):3157-3165.

RCW 70.105, "Hazardous Waste Management Act," *Revised Code of Washington.*

Resource Conservation and Recovery Act of 1976, Public Law 94-580, 42 U.S.C. 6901, et seq.

RHO-BWI-ST-14, 1981, "Suprabasalt Sediment of the Cold Creek Syncline Area" in C. W. Myers and S. M. Price (eds.), *Subsurface Geology of the Cold Creek Syncline*, pp. 1-2, Rockwell Hanford Operations, Richland, Washington.

RHO-ST-23, 1979, *Geology of the Separation Areas, Hanford Site, South-Central Washington*, Rockwell Hanford Operations, Richland, Washington.

RHO-ST-46-P, 1984, *Field Calibration of Computer Models for Application to Buried Liquid Discharges: A Status Report*, Rockwell Hanford Operations, Richland, Washington.

Rockhold, M. L, 1999, "Parameterizing Flow and Transport Models for Field-Scale Applications in Heterogeneous, Unsaturated Soils," in *Geophysical Monograph*, 108:243–260.

Rockhold, M. L., R. E. Rossi, and R. G. Hills, 1996, "Application of Similar Media Scaling and Conditional Simulation for Modeling Water Flow and Tritium Transport at the Las Cruces Trench Site," in *Water Resources Research*, 32(3):595-609.

Roh, Y., S. R. Lee, S. K. Choi, M .P. Elless, and S. Y. Lee, 2000, "Physicochemical and Mineralogical Characterization of Uranium-Contaminated Soils," in *Soil and Sed. Contam.*, 9:463-486.

RPP-7884, 2002, *Field Investigation Report for Waste Management Area S-SX*, Rev. 0, CH2M Hill Hanford Group, Inc., Richland, Washington.

RPP-10098, 2002, *Field Investigation Report for Waste Management Area B-BX-BY*, Rev. 0, CH2M Hill Hanford Group, Inc., Richland, Washington.

RPP-17209, 2006, *Modeling Data Package for an Initial Assessment of Closure of the S and SX Tank Farms*, Rev. 1, CH2M Hill Hanford Group, Inc. Richland, Washington.

RPP-18226, 2005, *CH2M HILL_STOMP Test Plan*, Rev. 0, CH2M Hill Hanford Group Inc., Richland, Washington.

RPP-18227, 2005, *CH2M HILL_STOMP Software Quality Assurance Plan*, Rev. 0, CH2M Hill Hanford Group Inc., Richland, Washington.

RPP-18228, 2005, *CH2M HILL_STOMP Configuration Management Plan*, Rev. 0, CH2M Hill Hanford Group Inc., Richland, Washington.

RPP-23405, 2005, *Tank Farm Vadose Zone Contamination: Volume Estimates for Risk Assessments*, Rev. 1, CH2M Hill Hanford Group, Inc., Richland, Washington.

RPP-23748, 2006, *Geology, Hydrogeology, Geochemistry, and Mineralogy Data Package for the Single-Shell Tank Waste Management Areas at the Hanford Site*, Rev. 0, CH2M Hill Hanford Group, Inc. Richland, Washington.

RPP-23752, 2005, *Field Investigation Report for Waste Management Areas T and TX-TY*, Rev. 0, CH2M Hill Hanford Group, Richland, Washington.

RPP-25859, 2005, *CH2M HILL_STOMP Quality Assurance Test Results*, Rev. 0, CH2M Hill Hanford Group Inc., Richland, Washington.

RPP-26744, 2005, *Hanford Soil Inventory Model*, Rev. 1, CH2M Hill Hanford Group, Inc., Richland, Washington.

SAND98-2880, 1999, *Stochastic Parameter Development for PORFLOW Simulations of the Hanford AX Tank Farm,* Sandia National Laboratories, Albuquerque, New Mexico.

Scanlon, B. R., M. Christmans, R. C. Reedy, I. Porro, J. Simunek, and G. N. Flerchinger, 2002, "Intercode Comparisons for Simulating Water Balance of Surfacial Sediments in Semiarid Regions," in *Water Resour. Res.*, 38 (2):1323.

Schroth, M. H., J. D. Istok, J. S. Selker, M. Oostrom, and M. D. White, 1998, "Multifluid Flow in Bedded Porous Media: Laboratory Experiments and Numerical Simulations," in *Advances in Water Resources*, 22(2):169–183.

SD-BWI-DP-039, 1984, *Suprabasalt Stratigraphy Within and Adjacent to the Reference Repository Location*, Rockwell Hanford Operations, Richland, Washington.

Ségol, G., 1994, *Classic Groundwater Simulations: Proving and Improving Numerical Models*, Prentice-Hall, Englewood Cliffs, New Jersey.

USGS-WP-7, 1949, *Geologic and Hydrologic Features of the Richland Area, Washington, Relevant to Disposal of Waste at the Hanford Operations Office of the Atomic Energy Commission*, U.S. Government Printing Office, Washington, D.C.

WAC 173-340, "Model Toxics Control Act – Cleanup," *Washington Administrative Code*.

WAC 173-340-702, "General Policies," *Washington Administrative Code*.

WAC 173-340-704, "Use of Method A," *Washington Administrative Code*.

WAC 173-340-705, "Use of Method B," *Washington Administrative Code*.

WAC 173-340-706, "Use of Method C," *Washington Administrative Code*.

WAC 173-340-740, "Unrestricted Land Use Soil Cleanup Standards," *Washington Administrative Code*.

WAC 173-340-745, "Soil Cleanup Standards for Industrial Properties," *Washington Administrative Code*.

WAC 173-340-745(7), "Soil Cleanup Standards for Industrial Properties; Point of Compliance," *Washington Administrative Code*.

WAC 173-340-747, "Deriving Soil Concentrations for Ground Water Protection," *Washington Administrative Code*.

Ward, A. L, Z. F. Zhang, and G. W. Gee, 2006, "Upscaling Unsaturated Hydraulic Parameters for Flow Through Heterogeneous Anisotropic Sediments," in *Advances in Water Resources*, 29(2):268-280.

WHC-MR-0206, 1990, *Borehole Completion Data Package for the 216-S-10 Ditch and Pond*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-EE-004, 1991, *Revised Stratigraphy for the Ringold Formation, Hanford Site, South-Central Washington*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-EV-027, 1993, *Hydrogeology of the 100-N Area, Hanford Site, Washington*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-008, 1992, *Geologic Setting of the 200 West Area: An Update*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-011, 1992, *Geology of the Northern Part of the Hanford Site: An Outline of Data Sources and Geologic Setting of the 100 Areas*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-012, 1992, *Geologic Setting of the 200 East Area: An Update*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-014, 1992, *Hydrogeologic Model for the 200 West Area Groundwater Aggregate Area*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-019, 1992, *Hydrogeologic Model for the 200 East Groundwater Aggregate Area*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-052, 1992, *Phase I Hydrogeologic Summary of the 300-FF-5 Operable Unit, 300 Area*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-132, 1993, *Geologic Setting of the 100-HR-3 Operable Unit, Hanford Site, South-Central Washington*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-133, 1993, *Geology of the 100-B/C Area, Hanford Site, South-Central Washington*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

WHC-SD-EN-TI-155, 1993, *Geology of the 100-K Area, Hanford Site, South-Central Washington*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

White, M. D., M. Oostrom, and R. J. Lenhard, 1995, "Modeling Fluid Flow and Transport in Variably Saturated Porous Media with the STOMP Simulator 1, Nonvolatile Three-Phase Model Description," in *Advances in Water Resour.* 18(6):353-364.

White, M. D., and M. Oostrom, 1998, "Modeling Surfactant-Enhanced Nonaqueous-Phase Liquid Remedation of Porous Media," in *Soil Sci.*, 163(12):931–940.

White, M. D., M. Oostrom, and R. J. Lenhard, 2004, "A Practical Model for Mobile, Residual, and Entrapped NAPL in Water-Wet Porous Media," in *Ground Water*, 42(5):734–746.

Williams, M. D., and M. Oostrom, 2000, "Oxygenation of Anoxic Water in a Fluctuating Water Table System: An Experimental and Numerical Study," in *J. of Hydrol.*, 230:70–85.

Wipfler, E. L., M. Ness, G. D. Breedveld, A. Marsman, and S. van der Zee, 2004, "Infiltration and Redistribution of LNAPL into Unsaturated Layered Porous Media," in *J. of Contam. Hydrol.*, 71(1–4):47–66.

Yeh, T.-C. J., M. Ye, and R. Khaleel, 2005, "Estimation of Effective Unsaturated Hydraulic Conductivity Tensor Using Spatial Moments of Observed Moisture Plume," in *Water Resour. Res.* 41, W03014, doi:10.1029/2004WR003736.

Yoon, H. K., A. J. Valocchi, and C. J. Werth, 2007, "Effect of Soil Moisture Dynamics on Dense Nonaqueous Phase Liquid (DNAPL) Spill Zone Architecture in Heterogeneous Porous Media," in *J. of Contam. Hydrol.*, 90(3–4):159–183.

Zhang, Z. F., A. L. Ward, and G. W. Gee, 2003, "Estimating Soil Hydraulic Parameters of a Field Drainage Experiment Using Inverse Techniques," in *Vadose Zone Journal*, 2(2):201–211.

Zhang, Z. F., A. L. Ward, and G. W. Gee, 2004, "A Parameter Scaling Concept for Estimating Field-Scale Hydraulic Functions of Layered Soils, " in *J. of Hydrol. Res.*, 42:93–103.

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APPENDIX A

PREFERENTIAL PATHWAYS

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APPENDIX A

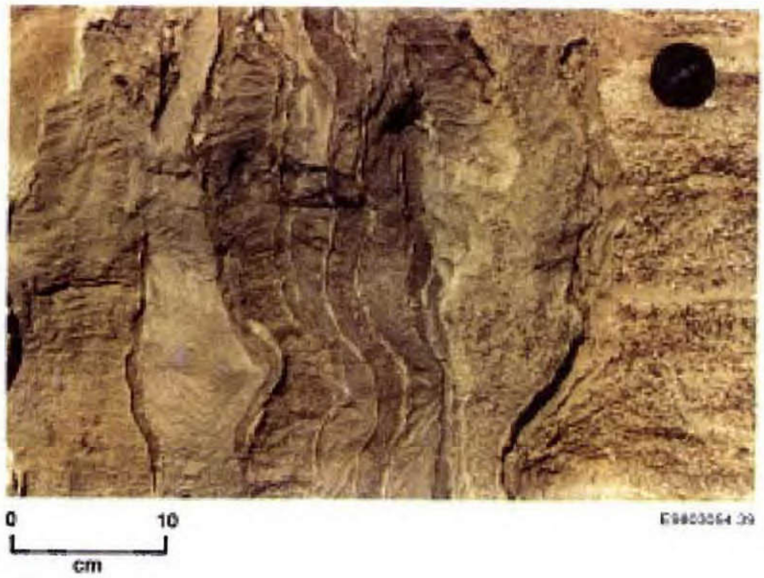
PREFERENTIAL PATHWAYS

Preferential pathways are not the most common transport-related mechanism in the Hanford vadose zone. They are of particular interest because of their potential for allowing fluid to bypass normal vadose zone fate and transport processes and impact groundwater sooner than otherwise possible. Preferential flow has been recognized and widely studied under saturated or near-saturated flow conditions (Nkedi-Kizza et al. 1983, De Smedt and Wierenga 1984), but there is little evidence of it occurring in arid and semi-arid climates or under low-water fluxes, particularly where soils are coarse-grained (Scanlon et al. 1997), such as in the Hanford formation. Water infiltration at arid sites, particularly ones with interfluvial settings with unconsolidated sediments, appears to occur mostly as piston-like flow rather than in preferential flow paths. Capillary and adsorptive forces greatly exceed gravitational forces, so instability along the wetting front does not appear to occur under low infiltration rates (Scanlon et al. 1997).

The most likely preferential flow paths in Hanford sediments are unsealed well boreholes and clastic dikes (Figure A-1). Poorly sealed or compromised well boreholes may provide preferential flow conduits for uncharacteristically rapid transport of subsurface water and contamination to the water table, but only under saturated or near-saturated conditions. The groundwater contamination plume(s) in the vicinity of the 216-U-1 and U-2 Cribs is/are believed to be evidence of this. During 1984-1985, high-volume discharges of contaminated water into the 216-U-16 Crib (located about 100 m [328 ft] to the south of the 216-U-1 and U-2 Cribs) perched on the Cold Creek Unit and migrated northward along a sedimentary structure contact. It is believed to have then intersected the outer casings of wells in the vicinity of 216-U-1 and U-2 Cribs (many of the wells near the 216-U-1 and U-2 Cribs were drilled prior to the initiation of *Washington Administrative Code* [WAC] standards to seal boreholes). These unsealed boreholes likely served as conduits for the contamination observed in groundwater there in the 1980s (WHC-EP-0133).

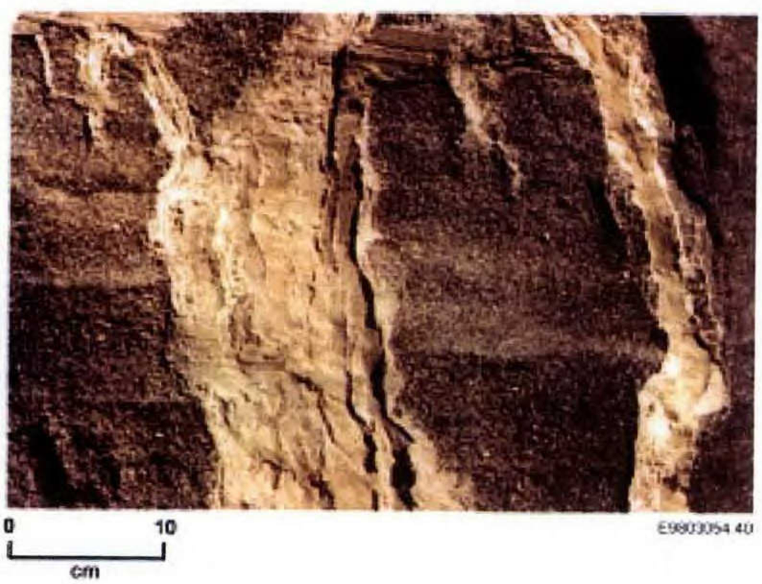
Clastic dikes and sills are ubiquitous sedimentary structures in the Hanford vadose zone, especially in the Hanford formation in the 200 Areas (BHI-01103). Clastic dikes are discordant sedimentary structures that occur as near-vertical tabular bodies filled with multiple layers of unconsolidated sediments. There is very little evidence, however, to indicate that they extend all the way from near the ground surface to the water table. In general, the hydraulic properties of clastic dikes can be considered as a subset of the porous matrix properties for the Hanford sediments (PNNL-14224). This is based on laboratory measurements of clastic dike samples. Clastic dikes are typically composed of fine-silt to very fine-grained, sand-sized material with vertically laminated orientations. When water is introduced into these fine-grained discordant structures, vertical flow is significantly retarded due to the high matric potential in these units, compared to vertical flow within coarser adjacent sediments. In general, clastic dike sediments represent properties of fine sediments (e.g., fine sand, silt, and clay) and can, therefore, represent regions of high moisture content (PNNL-14224).

Figure A-1. Infilled Sediments within Clastic Dikes.



(From BHI-01103.)

The middle portion of the two photographs shows the infilled sediments within a dike. The host sediments are shown on the left and right edges of the two photographs.



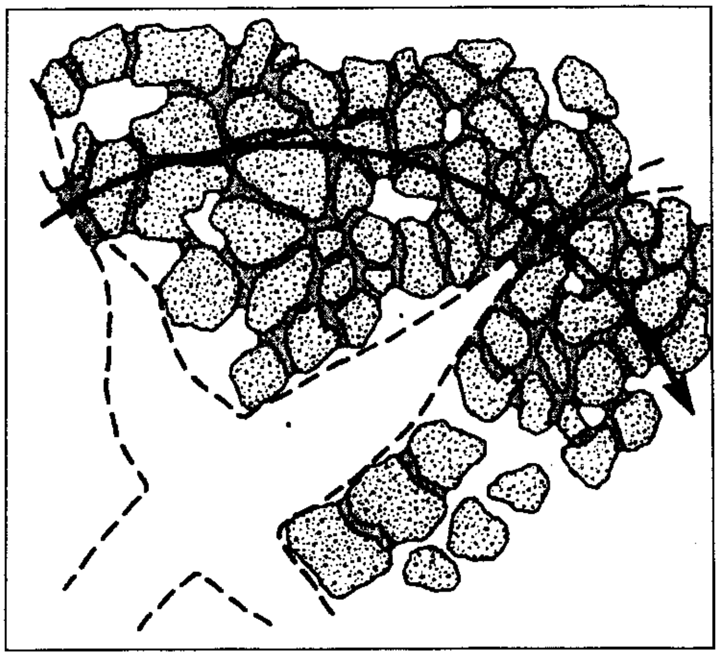
(From *Hydrologic Mechanisms Governing Fluid Flow in Saturated, Fractured, Porous Media* [Wang and Narasimhan 1985])

Although these features may act as preferentially faster flow pathways under saturated conditions, under unsaturated flow conditions, these features tend to act as barriers to transport rather than preferential, fast-flow channels. For example, if the area between the sediments and the outer well casing contained large void spaces, or the clastic dikes were filled with gravelly sediments (with large pore sizes), the bulk of laterally migrating water does not divert downward along the casing or within the dike under unsaturated conditions for the following reasons:

- The porous matrix has a much smaller average pore size than the gravelly media within the clastic dike.
- Under low recharge, unsaturated conditions, material with larger pore spaces or voids will contain or attract less moisture than finer-grained porous sediments because of the greater matric potential of the finer-grained material.

Under natural recharge conditions, precipitation at arid sites is usually too low (in relation to saturated hydraulic conductivity) to invoke preferential flow. Much of the water in the dry soils is simply adsorbed onto the grain surfaces and cannot move along preferred pathways. A conceptual model component for this phenomenon is illustrated schematically in Figure A-2. The expanded vertical slice illustrates the manner in which bulk flow, under unsaturated conditions and low recharge, bypasses the pathway formed by larger pore sizes and essentially follows the pathway formed by smaller pore size network. The large, open spaces in the figure mimic large pores, such as those in a gravelly medium. Under unsaturated conditions, the bulk of the flow is shown to be prevented from entering the media with large pore sizes. The flow bypasses them along routes composed of finer-grained material and smaller pore spaces.

Figure A-2. Conceptualization of Fracture Flow under Unsaturated Conditions (from Wang and Narasimhan 1985).



REFERENCES

BHI-01103, 1999, *Clastic Injection Dikes of the Pasco Basin and Vicinity – Geologic Atlas Series,* Rev. 0, Bechtel Hanford, Inc., Richland, Washington.

De Smedt, F., and P. J. Wierenga, 1984, "Solute Transfer through Columns of Glass Beads," in *Water Resources Res.*, 20:225-232.

Nkedi-Kizza, P., J. W. Biggar, M. T. van Genuchten, P. J. Wierenga, H. M. Selim, J. M. Davidson, and D. R. Nielsen, 1983, "Modeling Tritium and Chloride 36 Transport Through an Aggregated Oxisol," in *Water Resources Res.*, 19:691-700.

PNNL-14224, 2003, *Influence of Clastic Dikes on Vertical Migration of Contaminants in the Vadose Zone at Hanford*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

Scanlon, B. R., S. W .Tyler, and P. J. Wierenga, 1997, "Hydrologic Issues in Arid, Unsaturated Systems and Implications for Contaminant Transport," in *Reviews of Geophysics*, 35(4):461-490.

Wang, J. S., and T. N. Narasimhan, 1985, "Hydrologic Mechanisms Governing Fluid Flow in Saturated, Fractured Porous Media," in *Water Resources Res.*, 21:1861-74.

WHC-EP-0133, 1988, *U1/U2 Uranium Plume Characterization, Remedial Action Review and Recommendation for Future Action*, Rev. 0, Westinghouse Hanford Company, Richland, Washington.

APPENDIX B

HANFORD SITE-SPECIFIC GUIDELINES FOR SELECTION OF APPROPRIATE KD VALUES

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APPENDIX B

HANFORD SITE-SPECIFIC GUIDELINES FOR SELECTION OF APPROPRIATE KD VALUES

ROADMAP FOR SELECTION OF HANFORD SPECIFIC KDs FOR VADOSE ZONE ANALYSIS

These guidelines have been developed to assist operable unit managers in the selection of Hanford Site-specific instantaneous equilibrium distribution coefficients (Kds) from data compiled in the PNNL-14702.

1. Identify the appropriate geographical area for the waste site(s) of interest (e.g., letter designations keyed to geographic areas map) (Figure B-1) (PNNL-14702, Figure 3.1) AND/OR from geographic area designations (Table B-1) (PNNL-14702, Table 3.2).
2. Identify the appropriate site-specific area designation for the area of interest from Table B-2 (PNNL-14702, Table 3.3).
3. Identify the appropriate group of hydrostratigraphic templates for the waste site(s) and/or geographic area of interest (Table B-3 or Table B-4) (PNNL-14702, Table 3.1 or Table 3.6).
4. Identify appropriate waste site type and waste chemistry information using the PNNL-14725 appendix: "Simplified Rendition of the Geographic and Operational Site Parameters List for Waste Sites to be Simulated in Hanford Assessments."
   a. Identify appropriate waste site identifier:
      i. By geographic area designation
      ii. By Waste Information Data System (WIDS) database identifier:
         1. WIDS site code (e.g., 216-U-1/2)
         2. Site type
   b. Identify key information pertaining to Kd selection:
      i. Site hydrostratigraphic template (e.g., 216S_U_N-4) (Table B-5) (PNNL-14702, Table 3.7)
      ii. Waste chemistry group (numbered 1 through 6, as described in PNNL-14702, Section 3.2.3, and Table B-6 [PNNL-14702, Table 3.5], e.g., 2 for very high salt/very basic or 4 for low salt/near neutral waste chemistries)
      iii. Impact zone (e.g., "H" for high or near-field; "I1" and "I2" for intermediate or far-field vadose zone sand and gravel, respectively; "G" for very far-field vadose zone or groundwater impact zones)
   c. Identify Kd class for each stratigraphic unit within the appropriate site-specific waste chemistry/source category (e.g., 2H, 4I1, 4I2):
      i. 2H = Very high salt/very basic waste chemistry in the high or near-field impact zone
      ii. 4I1 = Low salt/near neutral waste chemistry in the intermediate or far-field impact zone sand

iii. 4I2 = Low salt/near neutral waste chemistry in the intermediate or far-field impact zone gravel

5. Select appropriate K_d value(s) (e.g., best, minimum, maximum) for the analyte of interest from Table B-7 (Kd ranges by waste chemistry/source category) (PNNL-14702, Table 4.11):

Individual reports will need to identify whether Kd data are from the existing database and/or include new sources (e.g., laboratory measurements) that exist for the specific contaminants, waste chemistry types, or vadose zone geochemistry at the site(s):

- Specific vadose zone unit or contaminant measurements (particularly for deeper vadose zone units)
- The number of and representativeness of the measurements
- Analogous or comparable vadose zone unit, waste chemistry, and/or contaminant measurements
- Technical basis for the use and/or extrapolation of specific vadose zone unit or contaminant measurements and/or analogous or comparable data.

REFERENCES

PNNL-14702, 2006, *Vadose Zone Hydrogeology Data Package for Hanford Assessments*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-14725, 2006, *Geographic and Operational Site Parameters List (GOSPL) for Hanford Assessments*, Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

Figure B-1. Location of Geographic Areas Represented by a Single Generalized Stratigraphic Column (PNNL-14702, Figure 3.1).

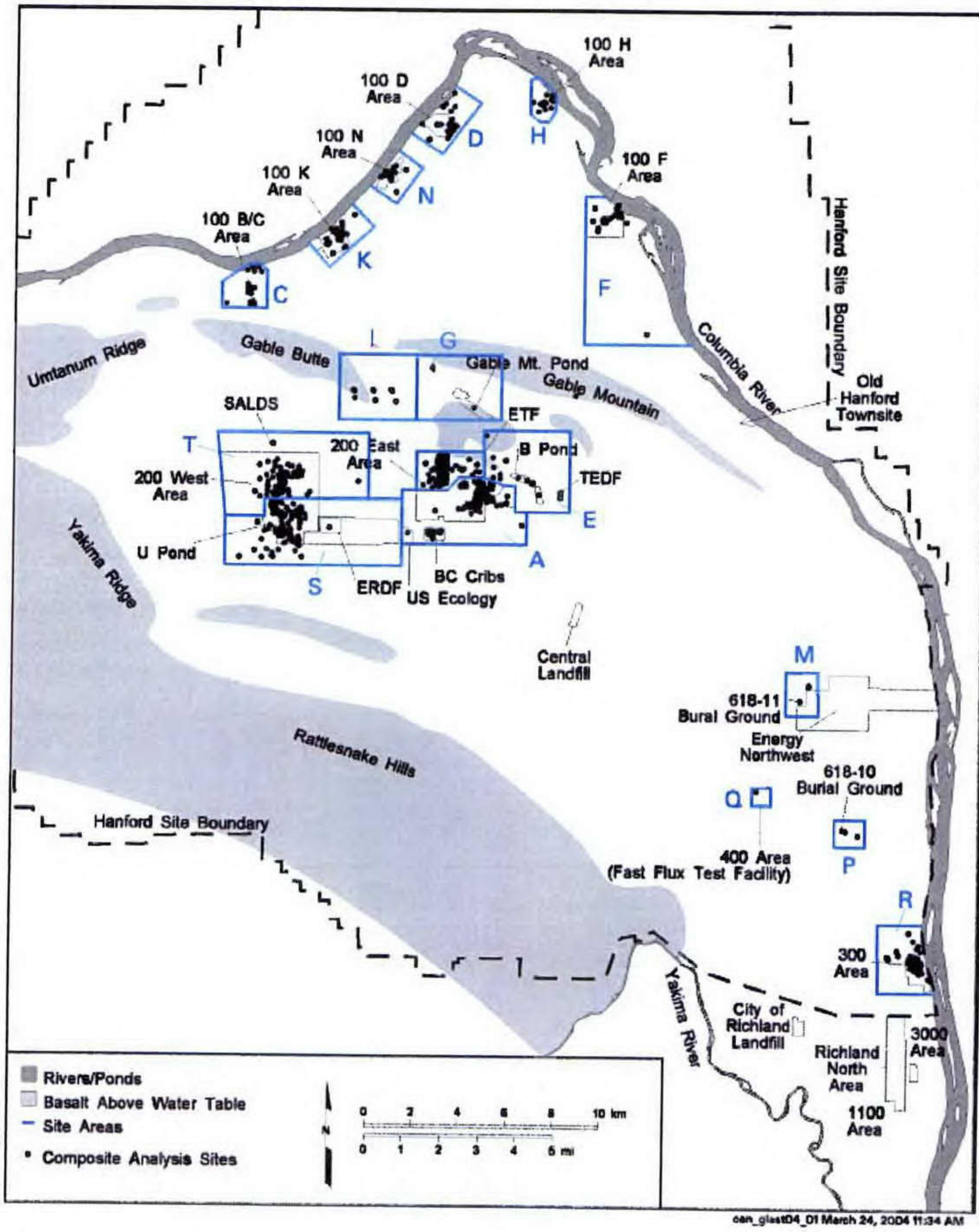

Table B-1. Geographic Area Designations Used in the Hydrostratigraphic Template Codes.

Designation	Geographic Area Description
A	Southern 200 East Area - encompassing the PUREX (A plant), hot semi-works (C-Plant), associated facilities (including PUREX tunnels), BC cribs, US Ecology, and the A, AN, AP, AW, AX, AY, AZ, C Tank Farms
B	Northwestern 200 East Area - encompassing the B-plant, associated waste disposal facilities, and the B, BX, BY Tank Farms
C	100-B/C Area
D	100-D/DR Area
E	East of 200 East – B Pond
F	100-F Area
G	Gable Mountain Pond Areas
H	100-H Area
I	200 North
K	100-KE/KW Area
M	600 Area near Energy Northwest and the 618-11 burial ground
N	100-N Area
P	600 Area southwest of the 400 area near the 618-10 burial ground
Q	400 Area
R	300 Area (and a few isolated facilities in and near the 400 Area)
S	Southern 200 West Area - encompassing the REDOX (S-Plant), U-plant, Z-plant associated facilities, ERDF, and the S, SX, SY, U Tank Farms
T	Northern 200 West Area - encompassing T Plant , associated facilities, and the T, TX, TY Tank Farms

(PNNL-14702, Table 3.2)

Table B-2. Site-Specific Area Designations Used in the Hydrostratigraphic Template Codes.

Designation	Site-Specific Area Description
A_BC_W	Southern 200 East Area – representing the western portion of the BC cribs area
A_BC_E	Southern 200 East Area – representing the eastern portion of the BC cribs area
A_BCT_N	Southern 200 East Area – representing the northern portion of the BC trench area
A_BCT_S	Southern 200 East Area – representing the southern portion of the BC trench area
A_BCT_W	Southern 200 East Area – representing the western portion of the BC trench area
A_C	Southern 200 East Area – representing the 241-C Tank Farm
A_ILAW_C	Southern 200 East Area – representing the central portion of the ILAW site
S_ERDF_E	Southern 200 West Area – representing the eastern half of ERDF
S_ERDF_W	Southern 200 West Area – representing the western half of ERDF
S_U	Southern 200 West Area – representing the 241-U Tank Farm
S_U_N	Southern 200 West Area – representing the northern portion of the 216-U-1&2 crib area
S_U_S	Southern 200 West Area – representing the southern portion of the 216-U-1&2 crib area
S_Z9	Southern 200 West Area – representing the 216-Z-9 trench area

(PNNL-14702, Table 3.3)

Table B-3. Waste Site Type Designations Used in the Hydrostratigraphic Template Codes.

Site Type Code[a]	Relative Depth of Waste Release	Representative WIDS Site Types
100, 200, 300, 400	Ground Surface (generally less that 3 m deep).	Surface and/or near surface facilities (e.g., process sewers, reactor buildings,[b] laboratory buildings, storage, stacks, ponds, ditches, valve pits, process unit/plants,[b] unplanned releases except tank leaks).
116, 216, 316, 616	Shallow Subsurface (generally 3-15 m below ground surface)	Shallow liquid and/or dry waste disposal facilities (e.g., cribs, burial grounds, retention basins, trenches, French drains, storage tunnels, drain/tile fields, pipelines, sewers).
241	Intermediate Subsurface (generally 9 to 17 m below ground surface)	High level waste tanks, settling tanks, diversion boxes, catch tanks, tank leak unplanned releases.
166, 266	Deep Subsurface (generally greater than 18 m below ground surface)	Deep injection sites (e.g., reverse [injection] wells)
276	Very Deep Subsurface (generally near or into the water table)	Very deep injection sites (e.g., very deep reverse [injection] wells)
River[c]	River Level	River outfalls and associated pipelines
Pump[d]	Not Applicable	Water supply wells

(a) First digit represents the area: 1 = 100 Area, 2 = 200 Area, 3 = 300 Area, 4 = 400 Area, 6 = 600 Area. Second and third digits indicate the general facility type and relative release depth.
(b) Some reactors and process unit/plants (such as canyon buildings) have basements and/or fairly deep foundations, however for the ease of simulation, all above ground structures are treated the same.
(c) River outfall discharged waste directly to the river, thus there is no vadose zone flow and transport component for these sites.
(d) Water supply wells withdraw water from the aquifer, thus there is no waste released, and no vadose zone flow and transport component for these sites.
WIDS = Waste Information Data System.

(PNNL-14702, Table 3.1)

Table B-4. General Hydrostratigraphic Templates for Each Geographic Area. (2 pages)

Template Designation	Geographic Area		Waste Site Types		Waste Chemistry Designation[d]
	Area	Designation[a]	Description	Designation[b]	
100C-4	100 B/C	C	Surface Facilities	100	4
116C-4			Near Surface Facilities	116	4
100D-4	100 D	D	Surface Facilities	100	4
116D-4			Near Surface Facilities	116	4
100F-4	100 F	F	Surface Facilities	100	4
116F-4			Near Surface Facilities	116	4
100H-4	100 H	H	Surface Facilities	100	4
116H-4			Near Surface Facilities	116	4
100K-4	100 K	K	Surface Facilities	100	4
116K-4			Near Surface Facilities	116	4
166K-4			Reverse (Injection) Wells	166	4
100N-4	100 N	N	Surface Facilities	100	4
116N-4			Near Surface Facilities	116	4
200G-4	Gable Mtn.	G	Surface Facilities	200	4
200I-4	200N	I	Surface Facilities	200	4
200E-4	E 200 E (B-Pond)	E	Surface Facilities	200	4
216E-4			Near Surface Facilities	216	4
200B-2	N 200 E (B-Plant)	B	Surface Facilities	200	2
200B-4					4
216B-2			Near Surface Facilities	216	2
216B-3					3
216B-4					4
241B-2			Tanks	241	2
266B-4			Reverse (Injection) Wells	266	4
267B-2				267[c]	2
200A-2	S 200 E (PUREX, BC Cribs)	A	Surface Facilities	200	2
200A-4					4
216A-2			Near Surface Facilities	216	2
216A-4					4
241A-2			Tanks	241	2
241A-3					3
266A-4			Reverse (Injection) Wells	266	4
200S-2	S 200 W (Redox, U-Plant, Z-Plant)	S	Surface Facilities	200	2
200S-4					4

Table B-4. General Hydrostratigraphic Templates for Each Geographic Area. (2 pages)

Template Designation	Geographic Area		Waste Site Types		Waste Chemistry Designation[d]
216S-1	S 200 W (Redox, U-Plant, Z-Plant)	S	Near Surface Facilities	216	1
216S-2					2
216S-4					4
241S-2			Tanks	241	2
241S-3					3
241S-4					4
266S-4			Reverse (Injection) Wells	266	4
200T-2	N 200 W (T Plant)	T	Surface Facilities	200	2
200T-4					4
216T-2			Near Surface Facilities	216	2
216T-3					3
216T-4					4
241T-2			Tanks	241	2
266T-2			Reverse (Injection) Wells	266	2
266T-4					4
300R-4	300 Area (North Richland	R	Surface Facilities	300	4
316R-4			Near Surface Facilities	316	4
400Q-4	400	Q	Surface Facilities	400	4
616M-4	600	M	Near Surface Facilities	616	4
616P-4	600	P	Near Surface Facilities	616	4
Pump	-	-	Water Supply Wells	Pump	-
River	-	-	River outfalls	River	-

(a) Assigned letter designation for geographic area.
(b) Assigned number designation for waste site type: First number designates traditional Hanford Site area (i.e., 100, 200, 300, 400, 600 Areas); last two numbers designate waste site type (00 = surface facilities, 16 = near surface facilities, 41 = tanks, 66/67 = reverse wells).
(c) Two designations are used for reverse (injection) wells that have very different depths within a single geographic area. The "67" designation distinguishes the very deep reverse (injection) wells from those at a more intermediate depth (66).
(d) Assigned number designation for waste chemistry type (see Table 3.5).

(PNNL-14702, Table 3.6)

Table B-5. Site-Specific Templates Established for a Few Key Facilities.

Template Designation	Site-Specific Area		Waste Site Types		Waste Chemistry Designation[c]
	Area	Designation[a]	Description	Designation[b]	
216A_BC_W-3	S 200 E, BC Cribs, Western Portion	A_BC_W	Near Surface Facilities	216	3
216A_BC_E-3	S 200 E, BC Cribs, Eastern Portion	A_BC_E	Near Surface Facilities	216	3
216A_BCT_N-3	S 200 E, BC Trenches, Northern Portion	A_BT_N	Near Surface Facilities	216	3
216A_BCT_N-4					4
216A_BCT_S-3	S 200 E, BC Trenches, Southern Portion	A_BT_S	Near Surface Facilities	216	3
216A_BCT_W-3	S 200 E, BC Trenches, Western Portion	A_BT_W	Near Surface Facilities	216	3
216A_ILAW_C-5	S 200 E, ILAW Site, Central Portion	A_ILAW_C	Near Surface Facilities	216	5
216A_ILAW_C-6					6
216S_ERDF_E-4	S 200 W, ERDF, eastern half	S_ERDF_E	Near Surface Facilities	216	4
216S_ERDF_W-4	S 200 W, ERDF, western half	S_ERDF_W	Near Surface Facilities	216	4
216S_U_N-4	S 200 W, 216-U-1&2 Area, Northern Portion	S_U_N	Near Surface Facilities	216	4
216S_U_S-4	S 200 W, 216-U-1&2 Area, Northern Portion	S_U_S	Near Surface Facilities	216	4
216S_Z9-1	S 200 W, 216-U-1&2 Area, Northern Portion	S_Z9	Near Surface Facilities	216	1
241A_C-2	S 200 E, 241-C Tank Farm	A_C	Tanks	241	2
241A_C-3					3
241S_U-2	S 200 W, 241-U Tank Farm	S_U	Tanks	241	2

(a) Assigned letter designation for geographic area.
(b) Assigned number designation for waste site type: First number designates traditional Hanford Site area (i.e., 100, 200, 300, 400, 600 Areas); last two numbers designate waste site type (00 = surface facilities, 16 = near surface facilities, 41 = tanks, 66/67 = reverse [injection] wells).
(c) Assigned number designation for waste chemistry type (see Table 3.5).

(PNNL-14702, Table 3.7)

Table B-6. Waste Chemistry Designations Used in the Base Template Codes.

Waste Chemistry Designation	Waste Stream Description
1	Very Acidic
2	High Salt/Very Basic
3	Chelates/High Salt
4	Low Salt/Near Neutral
5	IDF Vitrified Waste
6	IDF Cementitious Waste
IDF = Integrated Disposal Facility.	

(PNNL-14702, Table 3.5)

Geographic and Operational Site Parameters List (GOSPL) for Hanford Assessments

July 2006
PNNL-14725, Rev.1

Appendix

Simplified Rendition of the Geographic and Operational Site Parameters List for Waste Sites to Be Simulated in Hanford Assessments

Appendix A
Hydrostratigraphic Templates (PNNL-14702)

VZ Base Templates - U Cribs

U Cribs (216-U-1, -2 and -16)

Notes/Assumptions:

1) Surface elevation ranges from 211.0 m (692.3 ft) near 216-U-16 to 212.5 m (697.2 ft) MSL near the 216-U-1 and -2 Cribs as taken from the Hanford Site Atlas (BHI 1996).
2) Ground surface and water-table elevations from the HYDRODAT database managed by the Pacific Northwest National Laboratory.
3) The pre-Hanford water table (January 1944) is estimated to have been at an elevation of 406 MSL (based on Kipp and Mudd 1974).
4) The site depth to bottom of the 216-U-1 and -2 Cribs is reported to be 24 ft/min (7.3 m) based on Maxfield (1979). No bottom is reported for the 216-U-16 Crib. Thus, the backfill is assumed to be 24 ft deep for all three cribs.

Template 216S_U_N-x for the area N-NE of the 216-U-1&2 Cribs, based on well 299-W19-16 (N 135029.21, E 567270.68) located 24 m (80 ft) north of 216-U-1 Crib. **216S_U_N-4**

Estimated Thickness (ft)***	Adjusted Thickness (ft)	Bottom Depth (ft)	Bottom Elevation (ft)	Geologic Unit	Description	Hydraulic Property Type *	SAC Soil Type	K_d Zone**		K_d Class
		0	695.157	Surface	NA	NA	NA	NA		NA
24	24	24	671	Backfill	Backfill	B	B	HI		4H
67	67	91	604	Hanford H1	Interbedded layers of fine to coarse sand and sandy gravel	S	Hcs_2W	HI		4H
56	55	146	549	Hanford H2	Interbedded layers of silty to fine, medium, and coarse sand	S	Hfs_U	II		4I1
19	19	165	530	CCU-upper	Silt and fine sand	SS	PPlz_U	II		4I1
2	2	167	528	CCU-lower	Calcium-carbonate cemented sand, silt and clay (caliche)	SS	PPlc	II		4I1
83	83	250	445	Ringold Unit E	Sandy gravel	SG2	Rg_U	II		4I2
		250.59	444.57	Water Table	NA	NA	NA	NA		NA

Template 216S_U_S-x for the southern portion of the 216-U-1& 2 crib area, based on well 299-W19-14 (N 134831.14, E 567267.99), located 9 m (30 ft) from SE edge of 216-U-16 Crib. **216S_U_S-4**

Estimated Thickness (ft)***	Adjusted Thickness (ft)	Bottom Depth (ft)	Bottom Elevation (ft)	Geologic Unit	Description	Hydraulic Property Type *	SAC Soil Type	K_d Zone**		K_d Class
		0	693.44	Surface	NA	NA	NA	NA		NA
24	24	24	669	Backfill	Backfill	B	B	4H		4H
86	86	110	583	Hanford H1	Interbedded layers of fine to coarse sand and sandy gravel	S	Hcs_2W	4H		4H
42	42	152	541	Hanford H2	Interbedded layers of silty to fine, medium, and coarse sand	S	Hfs_U	4I1		4I1
14	14	166	527	CCU-upper	Silt and fine sand	SS	PPlz_U	4I1		4I1
4	4	170	523	CCU-lower	Calcium-carbonate cemented sand, silt and clay (caliche)	SS	PPlc	4I1		4I1
78	78	248	445	Ringold Unit E	Sandy gravel	SG2	Rg_U	4I2		4I2
		248.02	445.42	Water Table	NA	NA	NA	NA		NA

* After Khaleel and Freeman (1996), per white paper by Khaleel (September 2000).

** HI=high impact, II=Intermediate Impact (after Kincaid et al. 1996).

BLUE = Injection/release point.

Appendix A
Hydrostratigraphic Templates (PNNL-14702)

VZ Base Templates S

South 200 West Area (S, U [except U-1&2], Z Areas [except 216-Z-9]) Stratigraphic Columns

Template 2418-X for intermediate depth disposal sites (e.g., high-level waste tanks) (modified after Reidel et al. 2006)

Average Thickness (ft)	Adjusted Average Thickness (ft)	Depth (ft)	Elevation (ft)	Geologic Unit	Description	Hydraulic Property Type *	SAC Soil Type	K_d Zone**			2418-2 K_d Class	2418-3 K_d Class	2418-4 K_d Class
		0	680	Surface	NA	NA	NA	NA			NA	NA	NA
50	50	50	630	Backfill	Medium sands and silt with poorly sorted gravel evolved from Hanford formation	S	S	HI			2H	3H	4H
28.7	29	79	580	H1-b	Upper gravel dominated unit, gravelly sand	SG1	Hg_2W	HI			2H	3H	4H
25.1	25	104	576	H1-a	Upper sand dominated unit, slightly silty	S	Hfs_2W	HI			2H	3H	4H
13.1	13	117	563	H1	Slightly silty coarse to very fine sand	S	Hfs_2W	II			2I1	3I1	4I1
58.2	58	175	505	H2	Slightly silty medium to very fine sand to silty medium to very fine sand	S	Hss_2W	II			2I1	3I1	4I1
33	33	208	472	Old Hanford/Cold Creek silt ("Early Palouse")	Silty fine to very fine sand	SS	PPlz	II			2I1	3I1	4I1
7.4	7	215	465	Cold Creek Carbonate	Pebbly silty coarse to very fine sand to silty medium to very fine sand	SS	PPlc	II			2I1	3I1	4I1
9.2	9	224	456	Taylor flat member, Upper Ringold	Interstratified, well-bedded fine to coarse sand to silt	SS	PPlz	II			2I1	3I1	4I1
92.8	49	273	407	Ringold (Unit E)	Silty Sandy Medium to fine pebble to sandy very coarse to fine pebble (semi-indurated)	SG2	Rg_2W	II			2I2	3I2	4I2
		273	407	Water Table	NA	NA	NA				NA	NA	NA

Template 2668-X for deep injection sites (e.g., reverse wells [e.g., 216-Z-10 (a)])

Average Thickness (ft)	Adjusted Average Thickness (ft)	Depth (ft)	Elevation (ft)	Geologic Unit	Description	Hydraulic Property Type *	SAC Soil Type	K_d Zone**					2668-4 K_d Class
		0	680	Surface	NA	NA	NA	NA					NA
2.5	5	5	675	Eolian	Sand and silt	Hs	Hss	II					4I1
60	65	70	610	Hanford Gravel	Pebbly very coarse to medium sand to silty sandy medium to fine pebble	Hg	Hg_2W	II					4I2
30	30	100	580	Hanford Sand	Slightly silty coarse to very fine sand	S	Hfs_2W	II					4I1
30	30	130	550	Hanford Silty Sand	Slightly silty medium to very fine sand to silty medium to very fine sand	S	Hss_2W	II					4I1
15	20	150	530	Old Hanford/Cold Creek silt ("Early Palouse")	Silty fine to very fine sand	PP	PPlz	HI					4H
20	20	170	510	Cold Creek Carbonate	Pebbly silty coarse to very fine sand to silty medium to very fine sand	PP	PPlc	HI					4H
	103	273	407	Ringold (Unit E)	Silty Sandy Medium to fine pebble to sandy very coarse to fine pebble (semi-indurated)	Rg	Rg_2W	II					4I2
		273	407	Water Table	NA	NA	NA	NA					NA

* After Khaleel and Freeman (1995), per white paper by Khaleel (September 2000).
** HI=high impact, II=intermediate impact (after Kincaid et al. 1998).
BLUE = injection/release point.
(a) Note: Injection well 216-Z-10 is screened from 118-150 ft. Well 216-U-4 is screened from 50-75 ft.

Table B-7. Contaminant Distribution Coefficient Estimates by Waste Chemistry Type. (2 pages)

Waste Chemistry/Source Category 1: Very Acidic									
	High Impact (1H)			Intermediate Impact – Sand (1I1)			Intermediate Impact – Gravel (1I2)		
	Kd Estimate (mL/g)			Kd Estimate (mL/g)			Kd Estimate (mL/g)		
Analyte	Best	Min	Max	Best	Min	Max	Best	Min	Max
Non-Adsorbing Radionuclides									
H3	0	0	0	0	0	0	0	0	0
Tc99	0	0	0.1	0	0	0.1	0	0	0.01
Cl36	0	0	0	0	0	0	0	0	0
Moderately Adsorbing									
I129	4	0	15	0.2	0	2	0.02	0	0.2
U238	0.2	0	4	0.8	0.2	4	0.08	0.02	0.4
Se79	5	3	10	5	3	10	0.5	0.3	1
Np237	0	0	2	10	2	30	1	0.2	3
C14	0	0	0	0	0	100	0	0	100
Highly Adsorbing									
Sr90	10	5	15	22	10	50	6.8	3.1	15.5
Cs137	1000	200	10000	2000	200	10000	620	62	3100
Pu239	0.4	0.1	1	600	200	2000	186	62	620
Eu152	20	1	100	200	10	1000	62	3.1	310

Waste Chemistry/Source Category 2: Very High Salt/Very Basic									
	High Impact (2H)			Intermediate Impact - Sand (2I1)			Intermediate Impact – Gravel (2I2)		
	Kd Estimate (mL/g)			Kd Estimate (mL/g)			Kd Estimate (mL/g)		
Analyte	Best	Min	Max	Best	Min	Max	Best	Min	Max
Non-Adsorbing Radionuclides									
H3	0	0	0	0	0	0	0	0	0
Tc99	0	0	0.1	0	0	0.1	0	0	0.01
Cl36	0	0	0	0	0	0	0	0	0
Moderately Adsorbing									
I129	0.02	0	0.2	0.1	0	0.2	0.01	0	0.02
U238	0.8	0.2	4	0.8	0.2	4	0.08	0.02	0.4
Se79	0	0	0.1	0	0	1	0	0	0.1
Np237	200	100	500	200	100	500	200	100	500
C14	100	0	100	7	0	100	7	0	100
Highly Adsorbing									
Sr90	22	10	50	22	10	50	6.8	3.1	15.5
Cs137	10	0	500	100	10	1000	31	3.1	310
Pu239	200	70	600	600	200	2000	190	62	620
Eu152	200	10	1000	200	10	1000	62	3.1	310

Table B-7. Contaminant Distribution Coefficient Estimates by Waste Chemistry Type. (2 pages)

Waste Chemistry/Source Category 3: Chelates/High Salts									
	High Impact (3H)			Intermediate Impact – Sand (3I1)			Intermediate Impact – Gravel (3I2)		
	Kd Estimate (mL/g)			Kd Estimate (mL/g)			Kd Estimate (mL/g)		
Analyte	Best	Min	Max	Best	Min	Max	Best	Min	Max
Highly Mobile Elements									
H3	0	0	0	0	0	0	0	0	0
Tc99	0	0	0.1	0	0	0.1	0	0	0.01
Cl36	0	0	0	0	0	0	0	0	0
Somewhat Mobile Elements									
I129	0.2	0	2	0.2	0	2	0.02	0	0.2
U238	0.2	0	4	0.8	0.2	4	0.08	0.02	0.4
Se79	0	0	0.1	0	0	1	0	0	0.1
Np237	2	1	15	5	2	30	0.5	0.2	3
C14	0	0	100	0	0	100	0	0	100
Moderately Immobile Elements									
Sr90	1	0.2	20	10	5	20	3.1	1.6	6.2
Cs137	10	0	500	100	10	1000	31	3.1	310
Pu239	10	1	100	600	200	2000	190	62	620
Eu152	20	1	100	200	10	1000	62	3.1	310

Waste Chemistry/Source Category 4: Low Organic/Low Salt/Near Neutral												
	High Impact (4H)			Intermediate Impact – Sand (4I1)			Intermediate Impact – Gravel (4I2)			Groundwater (4G)		
	Kd Estimate (mL/g)			Kd Estimate (mL/g)			Kd Estimate (mL/g)			Kd Estimate (mL/g)		
Analyte	Best	Min	Max	Best	Min	Max	Best	Min	Max	Best	Min	Max
Highly Mobile Elements												
H3	0	0	0	0	0	0	0	0	0	0	0	0
Tc99	0	0	0.1	0	0	0.1	0	0	0.01	0	0	0.1
Cl36	0	0	0	0	0	0	0	0	0	0	0	0
Somewhat Mobile Elements												
I129	0.2	0	2	0.2	0	2	0.02	0	0.2	0.2	0	2
U238	0.8	0.2	4	0.8	0.2	4	0.08	0.02	0.4	0.8	0.2	4
Se79	5	3	10	5	3	10	0.5	0.3	1	5	3	10
Np237	10	2	30	10	2	30	1	0.2	3	10	2	30
C14	0	0	100	0	0	100	0	0	10	0	0	100
Moderately Immobile Elements												
Sr90	22	10	50	22	10	50	7	3	16	22	10	50
Cs137	2000	200	10000	2000	200	10000	620	62	3100	2000	200	10000
Pu239	600	200	2000	600	200	2000	190	62	620	600	200	2000
Eu152	200	10	1000	200	10	1000	62	3.1	310	200	10	1000

(PNNL-14702, Table 4.11)

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