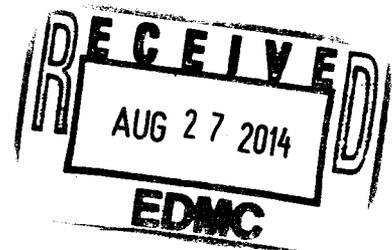


Model Package Report: Vadose Zone Model for the River Corridor

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

Contractor for the U.S. Department of Energy
under Contract DE-AC06-08RL14788

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Model Version 1.0

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River Corridor RI/FS Projects

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Executive Summary

This model package report documents the development of vadose zone (VZ) flow and transport models for the River Corridor portion of the U.S. Department of Energy's Hanford Site, Washington, in support of remedial activities that are currently underway. The results of the flow and transport models are intended for use in evaluating the potential long-term impact of residual VZ contamination on groundwater and surface water quality from waste sites located in various geographic areas in the River Corridor. The modeling results are used in calculating the soil screening levels (SSLs) and preliminary remediation goals (PRGs) for various contaminants to support the clean-up decisions in an effort to protect the groundwater and surface water resources. The goal is to determine and apply these threshold concentrations to a geographic area within the River Corridor without focusing on any given waste site. Because this methodology is designed to be applicable to all waste sites within a given geographic area, the calculations are performed with a conservative set of assumptions. These conservatively determined bounding concentrations provide an efficient way in identifying waste sites, with a high degree of confidence where residual contamination poses acceptable risk, and differentiating them from those waste sites where a more careful evaluation of long-term impacts may be needed.

The report discusses the current understanding of nature and extent of various contaminants of interest in the various geographic areas in the River Corridor, with focus on hexavalent chromium. The term "contaminants of interest" is used to indicate those contaminants considered to aid in the development of this model because of prevalent groundwater contamination. This term is used cautiously because it is not the function of this model package report to identify COPCs or COCs: that will be the function of the RI reports for these OUs. Results from sampling in recent boreholes drilled near high-risk waste sites and potentially contaminated areas are presented as well. The development of representative stratigraphic columns and corresponding one-dimensional numerical models for various geographic areas in the River Corridor is described along with the technical basis for specific model parameters, contamination zone, and boundary conditions. A description of modeling assumptions and modeling conservatism is also provided. The methodology used in predicting the peak concentrations in the groundwater from residual contamination in the VZ and derivation of SSLs and PRGs for protection of groundwater and surface water is described in detail. The overall objective of the modeling effort is to provide a basis for making informed remedial action decisions.

Uncertainty and sensitivity analyses have been conducted to determine the model parameters that impact the prediction of peak concentration. The results indicate that depending upon the vertical extent of contamination, either the vadose zone hydrologic parameters or the hydraulic gradient in the aquifer is important in determining the peak concentrations, if the sorption parameters are held constant.

Contents

1. Introduction.....	1
1.1 Modeling Need.....	2
1.2 Background.....	3
1.3 Document Organization.....	6
2. Model Objectives.....	7
2.1 Soil Screening Levels.....	7
2.2 Preliminary Remediation Goals.....	9
3. Model Conceptualization.....	11
3.1 Geology of River Corridor.....	11
3.1.1 Representative Stratigraphy.....	12
3.2 Modeling Features, Events, Processes, and Assumptions.....	24
3.2.1 Climate and Vegetation.....	24
3.2.2 Recharge and Evapotranspiration.....	29
3.2.3 Columbia River – Aquifer Interactions.....	31
3.2.4 Historical Discharges and Unintended Releases.....	34
3.2.5 Modeling Assumptions.....	48
3.3 Nature and Extent of Contamination.....	49
3.3.1 Geographic Area-specific Distribution of Contaminants in Vadose Zone.....	49
3.3.2 RI/FS Borehole Data.....	52
3.3.3 Cr(VI) Distribution in Vadose Zone and Aquifer.....	58
3.3.4 Cr(VI) Leachability.....	62
4. Model Implementation.....	67
4.1 Governing Equations.....	67
4.1.1 Flow and Solute Transport Equations.....	67
4.1.2 Constitutive Relations.....	69
4.2 Software Used.....	69
4.2.1 STOMP Controlled Calculation Software.....	70
4.2.2 Software Installation and Checkout.....	70
4.2.3 Statement of Valid Software Application.....	71
4.3 Spatial and Temporal Discretization.....	71
4.3.1 Representative Stratigraphic Columns.....	71
4.3.2 Grid and Time-Step Constraints.....	72
4.4 Initial and Boundary Conditions.....	76
4.4.1 Flow and Transport Boundary Conditions.....	76
4.4.2 Flow and Transport Initial Conditions.....	83
4.5 Model Parameterization.....	85
4.5.1 Hydraulic Parameters and Ranges.....	85

4.5.2	Contaminant Transport Parameters and Ranges	101
4.6	Implementation Using STOMP	101
5.	Model Results and Application	103
5.1	Peak Concentration Calculation and Scaling	103
5.2	Soil Screening Level and Preliminary Remediation Level Results	106
5.3	Calculating Dilution Factors	111
5.4	Application	112
6.	Model Sensitivity and Uncertainty	113
6.1	Modeling Conservatism	113
6.2	Sensitivity Analyses	115
6.2.1	Evaluation of K_d Influence on Contaminant Breakthrough	115
6.2.2	Sensitivity to Long Term Recharges	116
6.2.3	Effects of Different Source Distribution	118
6.2.4	Effects of Extending Bare Soil Recharge Period	119
6.2.5	Sensitivity to Solute Transport Solution Methodology	120
6.3	Uncertainty Analyses	121
6.3.1	Contribution to Prediction Uncertainty	122
6.3.2	Model Files and Parameters	123
6.3.3	Results Summary	125
6.3.4	Effect of Gravel Correction	127
7.	Model Configuration Management	129
7.1	Model Version History	129
8.	References	131

Appendices

A	Method for Determining Representative Stratigraphic Columns for Various Geographic Areas	A-i
B	Description of STOMP Input File	B-i
C	CHPRC Fact Sheet STOMP: Validation and Extent of Application	C-i

Figures

Figure 1-1.	River Corridor Area at the Hanford Site	1
Figure 1-2.	Logic Flow Chart for the Graded Approach.....	5
Figure 3-1.	Generalized Geology of the 100 Area	12
Figure 3-2.	Elevation Contours for Top of Ringold E and Water Table	13
Figure 3-3.	Borehole Locations for 100-D and 100-H Areas.....	13
Figure 3-4.	Borehole Locations for 100-B and 100-K Areas.....	14
Figure 3-5.	Borehole Locations for 100-F and 100-IU Areas	14
Figure 3-6.	Borehole Locations for 100-N Area	15
Figure 3-7.	Distribution of Vegetation Types and Areas on the Hanford Site, Washington, before the Year 2000 Fire.....	26
Figure 3-8.	Legend for Figure 3-7.....	27
Figure 3-9.	Extent of Hanford Site, Washington, Burned as a Result of the June 27 to July 2, 2000 Wildfire	28
Figure 3-10.	Relationship of Uranium Concentration to River Stage in the 300 Area Hyporheic Zone.....	32
Figure 3-11.	Cross Section Along a Streamline in the Horn Area Showing Cr(VI) Concentration (upper number) and Specific Conductance (lower number) as Groundwater Discharges to the Columbia River	35
Figure 3-12.	Map of Major 100 B/C Area Liquid Storage and Discharge Locations	37
Figure 3-13.	Map of Major 100 K Area Liquid Storage and Discharge Locations	39
Figure 3-14.	Map of Major 100 D Area Liquid Storage and Discharge Locations.....	42
Figure 3-15.	Map of Major 100 H Area Liquid Storage and Discharge Locations	44
Figure 3-16.	Map of Major 100 F Area Liquid Storage and Discharge Locations	46
Figure 3-17.	Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-BC Geographic Area where a Detectable Concentration was Registered	54
Figure 3-18.	Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-F Geographic Area where a Detectable Concentration was Registered	55
Figure 3-19.	Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-D Geographic Area where a Detectable Concentration was Registered	56
Figure 3-20.	Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-H Geographic Area where a Detectable Concentration was Registered	57
Figure 3-21.	Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-K Geographic Area where a Detectable Concentration was Registered	58
Figure 3-22.	Approximate Location of Fall Chinook Spawning Areas	59
Figure 3-23.	Extent of Cr(VI) Contamination in the 100 Areas.....	61
Figure 3-24.	The Results from Fitting the Two-Site (Two-Region) Model to Experimental Data for Column Experiments 3, 4, 5, and 6	63
Figure 4-1.	Representative Stratigraphic Columns for 100-D, 100-H, and 100-K Geographic Areas.....	73
Figure 4-2.	Representative Stratigraphic Columns for 100-BC, 100-IU-2 and 100-IU-6, and 100-F Geographic Areas.....	74
Figure 4-3.	Representative Stratigraphic Columns for 100-N Geographic Areas.....	75
Figure 4-4.	Flow Boundary Conditions for (a) Water Mass and (b) Solute Mass Conservation Equations.....	77
Figure 4-5.	Recharge Rates Used for Modeling for Undisturbed Soil Conditions.....	81
Figure 4-6.	Initial Contaminant Distribution Models.....	85
Figure 5-1.	Linear Regression Equation for Low K _d Contaminants for 100-D Column 1 and Irrigation Case Recharge with Ephrata Sandy Loam Soil	105
Figure 5-2.	Linear Regression Equation for High K _d Contaminants for 100-D Column 1 and Irrigation Case Recharge with Ephrata Sandy Loam Soil	105
Figure 5-3.	Breakthrough Curves for Different Distribution Coefficients with Native Vegetation Recharge Scenario (Column1 of 100-D OU)	108

SGW-50776, Rev. 3

Figure 5-4.	Dilution Factors for Representative Stratigraphic Columns (lithology in the saturated zone is listed in parenthesis in legend)	111
Figure 6-1.	Breakthrough Curves for Different Distribution Coefficients with Irrigation Recharge Rate	116
Figure 6-2.	Long-Term Recharge Rate for Burbank Sandy Loam: (a) Two-Step Recharge; (b) One- Step Recharge.....	117
Figure 6-3.	Surface Water PRG for Cr(VI) for Different Long-Term Recharge	118
Figure 6-4.	Surface Water PRG for Cr(VI) for Different Source Distributions in Soil	119
Figure 6-5.	Surface water PRG for Cr(VI) for Different Bare Soil Periods under the Base Case Scenario.....	120
Figure 6-6.	Comparison of Non-sorbing Solute Concentration using Patankar and TVD Solution Methodologies for Column 2 of 100-BC Geographic Area with Burbank Sandy Loam recharge and effective 100:0 Contaminant Distribution.....	121
Figure 6-7.	Illustration of how Statistical Distributions for Model Input Parameters and Simulated Predictions can be approached with Similar Methods.....	123
Figure 6-8.	(a) Column 2 of 100-BC Geographic Area and (b) Column 3 of 100-F Geographic Area	124
Figure 6-9.	Relative Contribution of Parameter Groups to Uncertainty of the Peak Concentration Calculation for Column 2 in the 100-BC Geographic Area	127
Figure 6-10.	Relative Contribution of Parameter Groups to Uncertainty of the Peak Concentration Calculation for Column 3 in the 100-F Geographic Area Ringold Units	127

Tables

Table 3-1.	Vadose and Saturated-Zone Thicknesses in the 100 Area Geographic Areas	16
Table 3-2.	Determination of Vadose Zone Thickness and Geology for Geographic Area 100-D.....	17
Table 3-3.	Determination of Vadose Zone Thickness and Geology for Geographic Area 100-H.....	18
Table 3-4.	Determination of Vadose Zone Thickness and Geology for Geographic Area 100-K.....	19
Table 3-5.	Determination of Vadose Zone Thickness and Geology for Geographic Area 100-F.....	20
Table 3-6.	Determination of Vadose Zone Thickness and Geology for Geographic area 100-BC.....	21
Table 3-7.	Determination of Vadose Zone Thickness and Geology for Geographic areas 100-IU-2 and 100-IU-6.....	22
Table 3-8.	Determination of Vadose Zone Thickness and Geology for Geographic Area 100-N.....	23
Table 3-9.	Cumulative Reactor Coolant Volumes and Cr Quantities Used in Single Pass Reactor Operations	35
Table 3-10.	Liquid Discharge Characteristics at the Major 100 B/C Area Sites	38
Table 3-11.	Liquid Discharge Characteristics at the Major 100 K Area Sites	40
Table 3-12.	Characteristics of Significant Liquid Discharges at the 100 D Area Sites	43
Table 3-13.	Characteristics of Significant Liquid Discharges at the 100 H Area Sites	45
Table 3-14.	Liquid Discharge Characteristics at the Major 100 F Area Sites.....	47
Table 3-15.	Contaminants of Interest In the 100 Area Groundwater OUs	53
Table 3-16.	Results from Modeling the Cr(VI) Desorption Data Using a Two-Site Equilibrium and Kinetic Model (Source: PNNL-17674)	63
Table 3-17.	Selected Measured and Calculated Physical Properties in Column Experiments 1, 2, 3, 4, 5, and 6 (Source: PNNL-17674).....	64
Table 4-1.	Recharge Rates for Native Vegetation Recharge Scenario (mm/yr)	79
Table 4-2.	Recharge Rates for Irrigation Recharge Scenario (mm/yr)	80
Table 4-3.	Hydraulic Gradients	82
Table 4-5.	Hydraulic Parameters Used for Geographic Areas 100-D and 100-H.....	92
Table 4-6.	Hydraulic Parameters Used for Geographic Area 100-K.....	94
Table 4-7.	Hydraulic Parameters Used for Geographic Areas 100-F, 100-IU-2 and 100-IU-6.....	95
Table 4-8.	Hydraulic parameters used for Geographic Area 100-BC.....	97
Table 4-9.	Mualem-van Genuchten Hydraulic Parameters for Sandy Gravels in the 100-N Area Vadose Zone.....	98

SGW-50776, Rev. 3

Table 4-10.	Aquifer Horizontal Saturated Hydraulic Conductivity Data Specific to 100-N Area	99
Table 4-11.	Hydraulic Parameters Used for 100-N Source Areas	100
Table 4-12.	Distribution Coefficients (Kd) used in STOMP Simulations	102
Table 5-1.	Specific Activity and Maximum PRG Value for Selected Radionuclides.....	106
Table 5-2.	Representative Soil Column Characteristics and Column Number Used for SSL and PRG Calculation	109
Table 5-3.	Example Groundwater Protection Concentration Results for the First Representative Column in 100-D Geographic Area Using 100:0 Effective Initial Source Distribution.....	110
Table 5-4.	Preliminary Remediation Goal and Soil Screening Level values for 100-K, 100-D, and 100- H Geographic Areas	112
Table 6-1.	Surface Water PRG for Cr(VI) for Two Step vs. One Step Change in Recharge.....	118
Table 6-2.	Model Input Parameters included as Part of the Sensitivity Analysis and their Input Value Ranges and Standard Deviations	126

Abbreviations and Acronyms

ACM	alternative conceptual model
amu	atomic mass unit
bgs	below ground surface
CCC	Criterion Continuous Concentration
CERCLA	<i>Comprehensive Environmental Response, Compensation, and Liability Act of 1982</i>
CHPRC	CH2M-HILL Plateau Remediation Company
Ci	curie(s)
cm	centimeter(s)
cm/s	centimeters per second
cm ³ /g	cubic centimeters per gram
COPC	contaminant of potential concern
Cr	chromium
Cr(III)	trivalent chromium
Cr(VI)	hexavalent chromium
DOE	U.S. Department of Energy
DWS	Drinking Water Standards
EPA	U.S. Environmental Protection Agency
EPC	exposure point concentration
ET	evapotranspiration
FEPs	Features, Events, and Processes
FS	Feasibility Study
ft.	feet
FY	fiscal year
g	gram(s)
GA	Graded Approach
h	hour(s)
HEIS	Hanford Environmental Information System (environmental database)
HISI	Hanford Information System Inventory (software database)
HMS	Hanford Meteorology Station
in.	inch
ISRM	In Situ Redox Manipulation
kg	kilogram(s)
km	kilometer(s)
km ²	square kilometer(s)
µg/L	micrograms per liter
m	meter(s)
m/s	meters per second
mg/kg	milligrams per kilogram
mL/g	microliters per gram
mi	mile(s)
mi ²	square mile(s)
mm/yr	millimeters per year
mph	miles per hour
ms/cm	microsiemens per centimeter
NPL	National Priority List
OU	operable unit
pCi/g	picocuries per gram
PNNL	Pacific Northwest National Laboratory
PRG	Preliminary Remediation Goal

QA/QC	quality assurance/quality control
RCVZ	River Corridor Vadose Zone (Models)
RETC	REtention Curve (software)
RI	Remedial Investigation
RPO	Remedial Process Optimization
ROD	Record of Decision
RUM	Ringold upper mud
SSL	soil screening level
STOMP	Subsurface Transport Over Multiple Phases
SZ	saturated zone
TIN	triangulated irregular network
VZ	vadose zone
WCH	Washington Closure Hanford
WQS	water quality standard
yr	year

1. Introduction

Remediation of contaminated waste sites located in the River Corridor of the U.S. Department of Energy's (DOE's) Hanford Site is currently underway. For the purpose of remediation, the River Corridor was divided into different geographic areas (Figure 1-1): 100-BC, 100-K, 100-D, 100-H (managed as 100-D/H), 100-N, 100-F, 100-IU-2, 100-IU-6 (managed as 100-F/IU-2/IU-6), and the 300 Area.

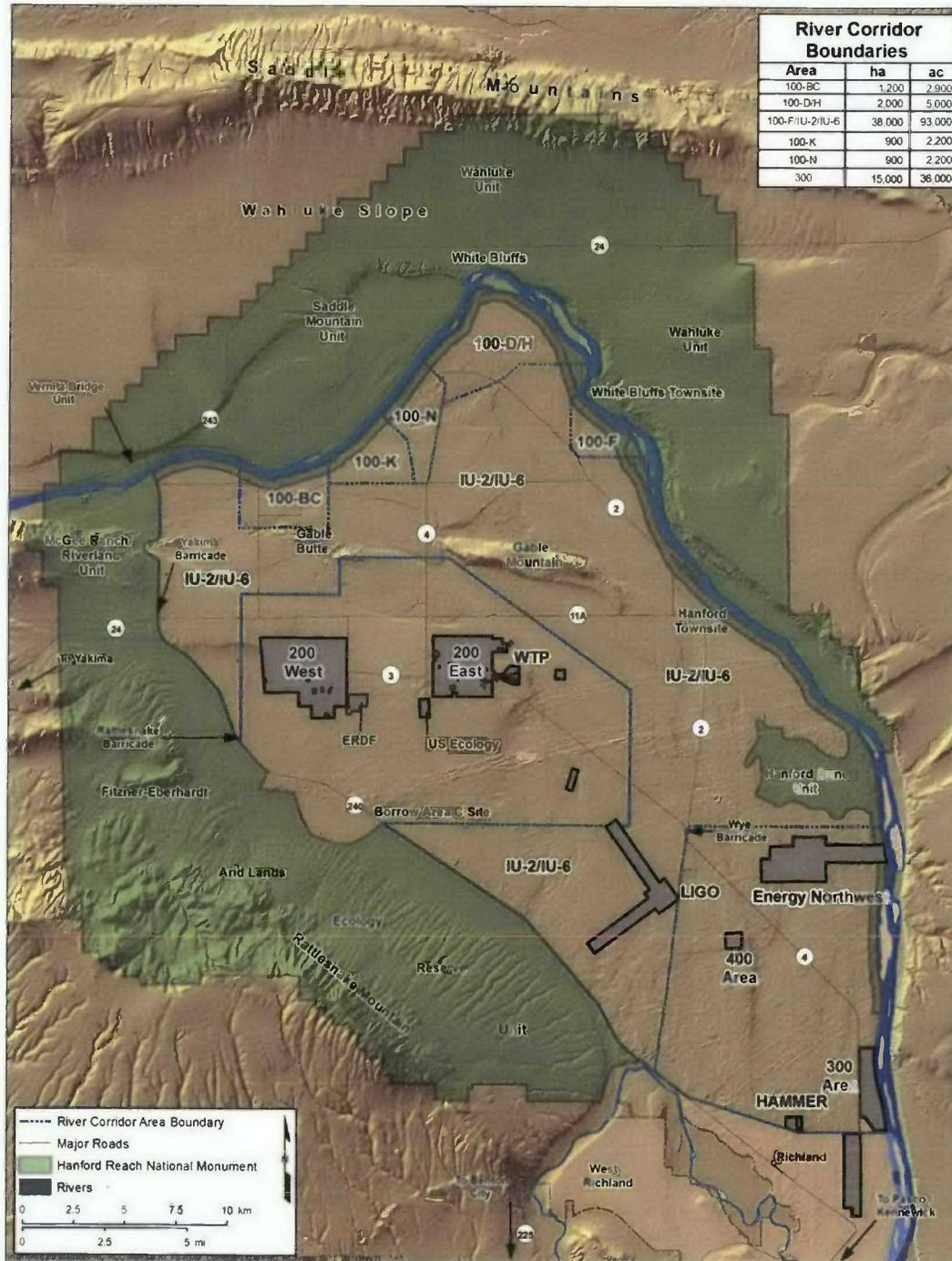


Figure 1-1. River Corridor Area at the Hanford Site

Modeling activities have been undertaken in the River Corridor to support the clean-up process through evaluation of the long-term impact of waste site residual vadose zone (VZ) contamination on groundwater and surface water quality. For purposes of modeling, the waste sites in the River Corridor were sorted into geographic areas and models representative of the generalized geology and surface soil type of each area were developed. In addition to geographic proximity, the nature of waste disposed during waste site operations (e.g., resulting from a nuclear reactor operations) was considered in assigning geographic areas for modeling purposes so that similar remedial action can be considered. The geographic areas are generally large areas and may include groundwater Operable Unit (OU), source OUs, and facilities that encompass the National Priority List (NPL) sites. For example, the 100-BC geographic area consists of the 100-BC-1 and 100-BC-2 Source OUs as well as the 100-BC-5 Groundwater OU. The discussion in this report follows the geographic area nomenclature.

1.1 Modeling Need

Modeling is needed to determine the residual contaminant concentration in the vadose zone that would be protective of groundwater and surface water as defined by the water quality standards (drinking water standards and aquatic water quality standards) in support of risk assessment studies in the River Corridor.

The soil screening levels (SSLs) and preliminary remediation goals (PRGs) provide estimate of the residual contaminant concentration under different set of modeling conditions, which when left behind will not pose unacceptable risk. The goal is to define such threshold concentrations applicable to geographic areas within the River Corridor without attempting to forecast future conditions under any given waste site. This approach provides an efficient way of identifying waste sites, with a high degree of confidence, where residual contamination poses potential risk, and thereby differentiating them from those waste sites where more careful evaluation of long-term impacts are needed. The SSL and PRG calculation is important because separately assessing each of the hundreds of waste sites within River Corridor with detailed characterization and modeling is neither pragmatic nor necessary if the residual contamination in the VZ underneath most of the sites is so small that it will not pose risk to groundwater or surface water quality.

Because this methodology is designed to be applicable to all waste sites within a given geographic area, the calculations are performed with a conservative set of assumptions. These conservative assumptions include:

- Use of a bounding assumption as to the extent of vertical contamination in the vadose zone under the waste site
- Selection of higher recharge rates
- Neglecting dilution and gradient reversals resulting from Columbia River stage fluctuations
- Selection of minimum vadose zone thickness in the soil columns
- Selection of sorption parameter values from the lower end of the empirical distribution functions
- Neglecting attenuation between groundwater under the waste site and the point of discharge in the Columbia River

Furthermore, the calculations are performed in one dimension to maximize the vertical transport rate to the water table, neglecting lateral spreading of contaminants that would serve to attenuate peak groundwater concentration. Because of conservative choices of modeling inputs and boundary conditions,

the resulting SSL and PRG concentrations are deemed to be bounding estimates (i.e., lead to the lowest threshold concentrations). The goal of this calculation is not to accurately predict the contaminant concentrations over time, for which a site-specific model will be required, but rather to estimate a bounding impact from residual contamination that may be left behind under a waste site on groundwater and surface water.

An attempt has also been made to summarize the nature and extent of contamination in various geographic areas in the River Corridor (except for the 100-N and 300 Areas) with particular attention given to chromium (Cr) contamination. Insights gained from Cr leachability tests are presented to support the conceptual model development. The vertical extent of contamination observed in the recently completed remedial investigation (RI) boreholes is also summarized to support the modeling assumptions.

1.2 Background

To manage cleanup activities at the Hanford Site, waste sites are grouped within OUs so that the *Comprehensive Environmental Response, Compensation, and Liability Act of 1982 (CERCLA)* cleanup process can be efficiently implemented. The OUs includes source OUs (i.e., surface and vadose zone areas where waste was disposed) and groundwater OUs (areas in the saturated zone where contamination exists) to perform separate characterization in recognition of the differences between localized contaminants in the soil column at the sources and the more widespread co-mingled contamination in groundwater. Most of the OUs are source OUs. There are five groundwater OUs in the 100 Area, namely, 100-BC-5, 100-KR-4, 100-NR-2, 100-HR-3, and 100-FR-3.

Assessment of potential impacts from soil contamination currently present in the vadose zone (VZ) focuses on the magnitude and timing of solute fluxes to the underlying aquifer and potential migration towards the Columbia River. Migration of VZ contamination towards groundwater and surface water resources is the principal exposure pathway for contaminants deeper than 4.6 meters (m) (15 feet [ft]), the depth to which the contaminated soil from the waste sites is typically removed. The contaminant migration from waste sites through the VZ to the underlying aquifer is controlled by driving forces for water movement in porous media (such as gravity, recharge, and matric potential), interactions between water and sediments, and interactions between the contaminants and the sediment. Because of past waste disposal practices, the type of the contaminant and extent of contamination (spatially and vertically) varies across different geographic areas, and thus calculations specific to each geographic area need to be performed in support of risk assessment studies. The types of sediments and their thicknesses and properties can also vary from one geographic area to another and can affect the rate and direction of solute and water movement to the aquifer. The non-linear physics governing flow and solute transport in the VZ under arid climate conditions can lead to long transport times (hundreds to thousands of years or more) for some contaminants before the contaminant concentration in groundwater approaches or exceeds water quality standards (WQSs). The concentration of contaminant in the groundwater is dependent on a variety of features and processes, such as solute flux from the VZ, aquifer thickness and dilution from mixing with the groundwater, retardation and dispersion in the aquifer, and river water and groundwater interaction.

To evaluate the impact of residual contamination in VZ on groundwater and surface water quality at the waste site boundary, the modeling is conducted using the Graded Approach (GA). The GA allows for evaluating the impact of residual contamination underneath the waste sites in a gradational or stepwise fashion through rapid differentiation of relatively low-risk sites from higher-risk sites so that resources (data-collection related and modeling related) can be focused on the potentially high-risk sites. By

evaluating waste sites in a gradational fashion, the GA assesses sites using the entire range of conservative simplifications to rigorous site specifics. Using soil concentrations obtained by employing very conservative but relatively simple contaminant transport model, the GA first identifies waste sites that are unlikely to constitute a risk to groundwater protection. The remaining waste sites, which pose a greater risk to groundwater and surface water protection, are again evaluated in a stepwise manner that matches the complexity and data needs of the assessment to the risk posed. The GA thus provides efficient, conservative, and rigorous evaluation of sites by allocating evaluation and characterization resources to those sites for which groundwater protection is a significant problem.

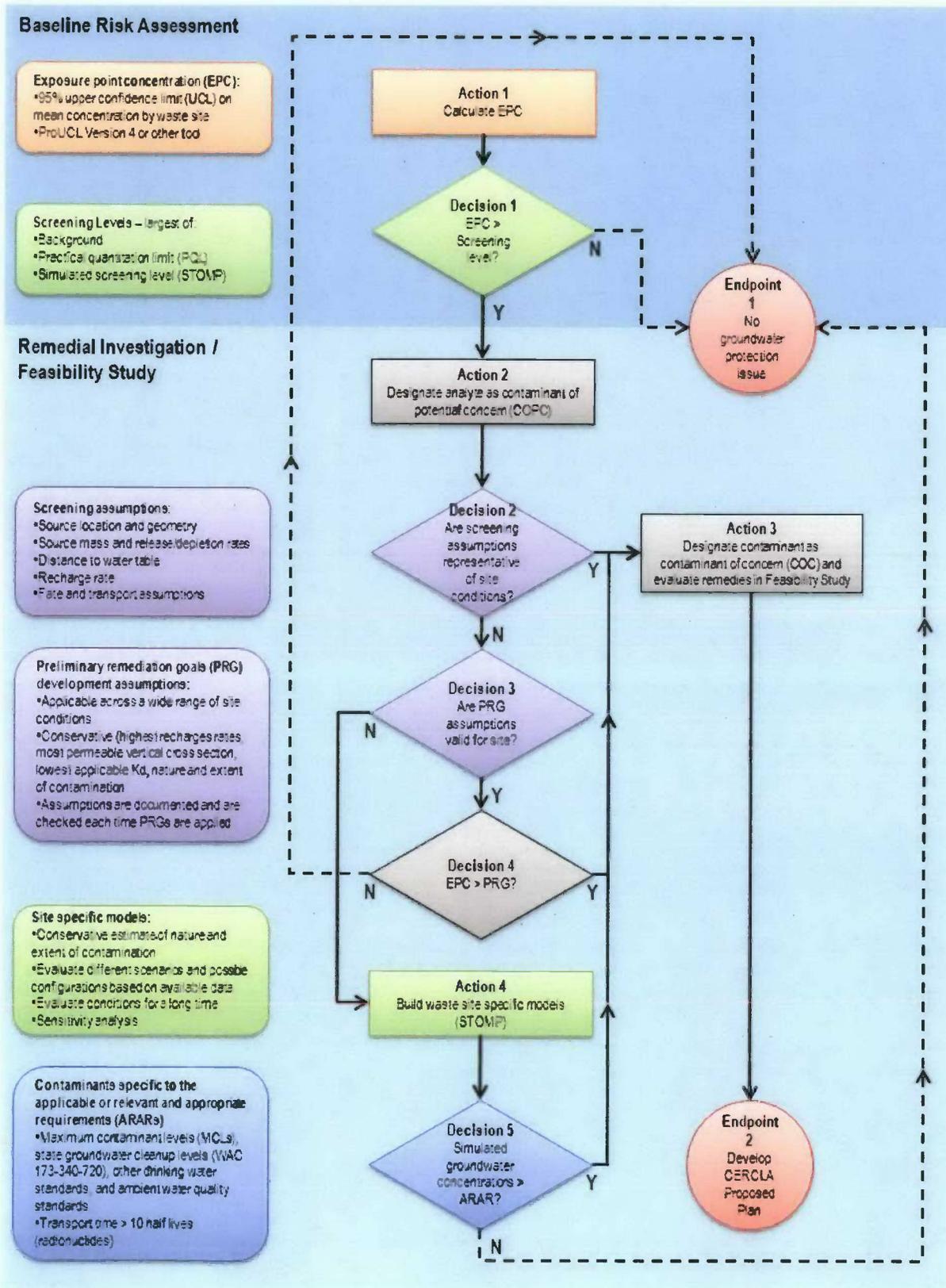
Figure 1-2 shows the logic flow chart for the GA (DOE/RL-2011-50, *Regulatory Basis and Implementation of a Graded Approach to Evaluation of Groundwater Protection*). The decisions are shown as diamonds and actions as rectangles. Boxes with rounded corners provide descriptive information for the various decisions and actions. The first action in the GA is to compare the exposure point concentration (EPC) of an analyte at the site with a SSL to determine if it should be designated as a contaminant of potential concern (COPC). If the EPC for a given analyte is less than or equal to the SSL, then that analyte does not pose a significant risk to groundwater and passes the screen. However, if the EPC exceeds its SSL, it fails the screen and is designated a COPC. The SSL calculation is important because separately assessing each of the hundreds of waste sites within River Corridor with individual models is neither pragmatic nor necessary if the residual contamination in the VZ underneath most of the sites is so small that it will not pose risk to groundwater or surface water quality. The SSL for each contaminant is defined as the larger of: 1) a background level, 2) a practical quantification limit, or 3) a calculated SSL computed using the Subsurface Transport Over Multiple Phases (STOMP) code (PNNL-12030, *STOMP Subsurface Transport Over Multiple Phases Version 2.0 Theory Guide*; PNNL-11216, *STOMP Subsurface Transport Over Multiple Phases: Application Guide*; PNNL-15782, *STOMP Subsurface Transport Over Multiple Phases Version 4.0 User's Guide*) using a conservative set of assumptions for the site vicinity (see Section 2.1 for more details).

Although the assumptions that underlie the SSL calculation are deliberately highly conservative and typically are not representative of site conditions, the site of each contaminant that fails the screening assumptions is further evaluated in Decision 2 based on additional information:

- If the screening assumptions represent site conditions, or if available site data and information are not sufficient to modify the assumptions used to develop the screening values, then the site is directly carried into the Feasibility Study (FS) (Action 4).
- If sufficient information is available to use a more site specific representative calculation, then the COPC is evaluated using PRGs, which are the initial or proposed cleanup goals developed in the CERCLA process to provide risk reduction targets or candidate cleanup levels (see Section 2.2) (Decisions 3 and 4).

It is more likely that all of the COPCs that fail screening will be carried into the site assessment using the PRG evaluation step rather than be directly carried into the FS because the highly conservative assumptions underpinning the SSLs are not expected to be representative of conditions at many waste sites. Furthermore, if a site shows concentration levels that are higher than the screening levels, additional information is typically gathered at the site to assist in the risk evaluation. This information is what enables the evaluation against the screening assumptions.

For the Hanford Site, PRGs will be calculated with the assumption that once the remedial actions are completed, native xerophytic vegetation will be re-established as the land cover. PRGs for other remedial alternatives, such as an evapotranspiration barrier, can be calculated as well.



Source: DOE/RL-2011-50

Figure 1-2. Logic Flow Chart for the Graded Approach

Transitioning a site from any given step of the GA to another can occur with the addition of new information, such as additional data, analyses, and modeling. A more thorough discussion of the GA is given in DOE/RL-2011-50.

1.3 Document Organization

The document is organized into three basic parts: (1) basis for development of the model; (2) model implementation and modeling results; and (3) uncertainty and sensitivity analyses. Section 2 presents the modeling objectives. Section 3 presents the geology of the River Corridor and the relevant Features, Events, and Processes (FEPs) that affect flow and transport in the 100 Area, along with the modeling assumptions and the nature and extent of contamination. Because contamination of hexavalent chromium [Cr(VI)] is prevalent but varies among the geographic areas in the 100 Area, a more detailed discussion of Cr(VI) contamination is presented with discussion of desorption test results based on leachability experiments. Section 4 describes the modeling implementation details, initial conditions, boundary conditions, and parameter values. Modeling results are presented in Section 5 for both the SSL and PRG calculations for each geographic area, while Section 6 discusses the sensitivity and uncertainty analyses. Section 7 provides the details related to configuration management of the model inputs and outputs including the software used.

2. Model Objectives

The purpose of modeling is to develop bounding residual contaminant concentration levels in the VZ rock matrix, underneath the waste sites located in the River Corridor, such that the effluent concentrations resulting from the residual contamination would not exceed the surface water and groundwater quality standards. Two separate calculations are performed to determine the residual contaminant concentration level in the VZ. The first calculation is a geographic area-specific screening level calculation where modeling is performed using a conservative set of parameter values and modeling assumptions of fully contaminated VZ and maximum possible recharge rate (irrigation scenario) to determine the minimum residual contaminant concentration values in the rock matrix that would be protective of surface water and groundwater quality standards. If the VZ contaminant concentrations underneath the waste sites are found to be below the screening level then no remedial action is needed. The second calculation is geographic area specific PRG calculation where modeling is performed using assumption of fully contaminated VZ but with base (expected) recharge rates that are consistent with the soil type. Both calculations are performed for 192 non-radionuclides and 28 radionuclides in groundwater and 192 non-radionuclides in surface water (specifically, the Columbia River).

The calculations are performed using a conservative set of assumptions, such as:

- Extended vertical zone of contamination under the waste site
- Higher recharge rates
- Ignoring dilution and gradient reversals due to Columbia River stage fluctuations
- Choosing minimum vadose zone thickness in the soil columns
- Choosing sorption parameter values from lower end of the empirical distribution functions
- Ignoring attenuation between groundwater under the waste site and the point of discharge in the Columbia River or mixing within the surface water body

Furthermore, the calculations are performed in one-dimension to maximize the vertical transport to the water table thereby ignoring any lateral spreading of contaminants. Due to conservative choice of modeling inputs and boundary conditions, the SSL and PRG concentrations are deemed to be bounding estimates (i.e., lead to the lowest threshold concentrations).

In the calculation methodology, the saturated zone is assumed initially uncontaminated, which may not always be true since plumes can migrate from upgradient locations over time. However, due to several in-built modeling conservatisms mentioned above, the SSL and PRG calculations are deemed to remain bounding when compared to the results derived from a more sophisticated site-specific predictive model that incorporates all the features and processes relevant at the scale of the model, including any contaminant migration from upgradient locations.

2.1 Soil Screening Levels

SSLs are not cleanup standards, nor are they definitions of “unacceptable” levels of soil contaminants (EPA/540/R-95/128, *Soil Screening Guidance: Technical Background Document*). Rather, SSLs are used to separate contaminants from COPCs and distinguish which COPCs warrant further evaluation or investigation (EPA/540/R-96/018, *Soil Screening Guidance: Users Guide*; EPA/540/R-95/128;

DOE-STD-1153-2002, *A Graded Approach for Evaluating Radiation Doses to Aquatic and Terrestrial Biota*).

The calculation of peak values of groundwater concentration with STOMP provides the first, forward calculation step to deriving SSL and PRG values. STOMP is used in the forward calculation step to compute peak groundwater concentrations that result from a unit initial source concentration (1.0 mg/kg for nonradionuclide COPCs, or 1.0pCi/kg for radionuclide COPCs), uniformly applied over the assumed contaminated thickness of the vadose zone. The resulting peak groundwater concentration is then used in the second, back-calculation step to determine SSL and PRG values. This second, back-calculation step involves scaling the peak groundwater concentration against the appropriate regulatory compliance criteria to back-calculate the maximum initial soil concentration that would not result in an exceedance. The maximum value obtained from this back-calculation step is assigned as the SSL or PRG value (depending on the recharge scenario used). The unit concentration therefore is not to be confused as constituting an actual observed waste site residual soil concentration. As a measure of maximum allowable contaminant concentration in the soil, SSLs and PRGs are expressed as contaminant mass per mass of soil for non-radionuclides (e.g., mg/kg) and as contaminant activity per mass of soil for radionuclides (e.g., pCi/kg).

The SSL is defined as the largest of the following:

- A statistically defined upper bound on the range of background values (e.g., 90th percentile)
- A practical limit for measuring the contaminant's concentration or activity (if radionuclide)
- A simulated minimum amount of material (concentration or activity) that will not cause groundwater cleanup standards to be exceeded, even under conservative assumptions within an extended time frame (e.g., 1,000 years)

The calculated SSL for any contaminant is simply the ratio of the applicable WQS to the simulated peak groundwater concentration (or radioisotope activity) for a unit initial contaminant source concentration (or radioisotope activity). It is calculated by the following equation in a back-calculation as:

$$SSL = aC_I \frac{WQS}{CPK} \quad \text{Eqn. 2-1}$$

where:

- SSL* = calculated soil screening level (contaminant mass or activity per unit mass of soil, typically expressed as mg/kg for mass or pCi/kg for activity)
- a* = a constant selected to balance units
- C_I* = the initial contaminant concentration associated with the rock matrix in the VZ (contaminant mass or activity per unit mass of soil, typically expressed as mg/kg for mass or pCi/kg for activity) applied in the STOMP forward calculation over the appropriate depth range of the vadose zone (see Section 4.4.2).
- WQS* = water quality standard (contaminant mass or activity per unit volume of water, typically expressed as mg/L for mass or pCi/L for activity)
- CPK* = peak groundwater concentration caused by *C_I* (contaminant mass or activity per unit volume of water, typically expressed as mg/L for mass or pCi/L for activity) result obtained from the STOMP forward calculation

The surface WQs were utilized to compute SSLs protective of surface water, whereas the groundwater WQs were used to compute SSLs protective of groundwater.

The simulations were run using the STOMP code (PNNL-12030) to yield a peak groundwater concentration for each contaminant within the uppermost 5 m of the aquifer, representing the screened interval of a water table monitoring well. Simulations for calculating the SSLs for the waste sites in the 100 Area for protection of surface water and groundwater were carried out separately for each geographic area with highly conservative assumptions to maximize the peak concentration in the aquifer. A conservative sets of hydraulic and transport properties related to saturated hydraulic conductivity, saturated volumetric water content, residual volumetric water content, dispersivity, van Genuchten α and n parameters, and bulk density was assumed for SSL calculations. Distribution of contaminants in the soil column (i.e., fully or partially contaminated), an important driving force for SSL calculations, was assumed based on the distribution coefficients of the contaminants. The details on this assumption are described in Section 5 of this document. Other conservative assumptions used to calculate SSLs focused on the driving forces, specifically, relatively large recharge through the VZ under irrigation scenario and lower aquifer flux rate to minimize dilution. However, it is crucial that assumptions are selected to balance conservatism with site appropriate conditions. For example, selecting a lowest-observed hydraulic gradient value that applies to only one of many sites is not warranted if this low value is well outside the range of values observed for similar aquifer formations.

2.2 Preliminary Remediation Goals

PRGs are residual contaminant concentration in the soil that will be protective of groundwater and surface water under specific site conditions. The PRGs represent the maximum quantity of contaminant concentration or radioisotope activity in the rock matrix that can remain in the VZ without causing an exceedance of applicable water quality standards (the federal and/or state drinking water standards and aquatic water quality standards). The PRGs can be defined for protection of groundwater or for protection of surface water simply by the choice of the applicable standard used in the calculation. They are developed to guide risk assessment decisions and evaluate selected remedies.

The value of a 100 Area PRG for a particular contaminant depends on a number of key factors. Waste site characteristics, specifically, source mass distribution and distance to the water table, are key factors. Another key factor is land cover condition and the associated recharge rate. The interactions between the VZ geology and water movement and between VZ geology and contaminant chemistry are the two remaining key factors. PRGs were calculated assuming that the entire VZ thickness is fully or partially contaminated based on the distribution coefficients of the contaminants (See Section 5 for details) and that ambient recharge rate is a function of natural land cover and varies over time (as opposed to irrigation based recharge for the SSL calculations). PRGs were calculated with the assumption that once the remedial actions are completed, native land cover vegetation will be reestablished after 30 years. The recharge rate associated with this land cover varies over time as the land cover transitions from bare soil (highest recharge rate), to grasses and immature shrub steppe (reduced recharge rate), to mature shrub steppe (lowest recharge rate).

Variability in hydraulic properties was incorporated into PRG development by selection of conservative values. Hydraulic properties include saturated hydraulic conductivity, porosity, and unsaturated flow parameters such as the Mualem-van Genuchten α , n , and residual water content parameters (Mualem [1976], "A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media"; van Genuchten [1980], "A Closed-Form Solution for Predicting the Conductivity of Unsaturated Soils"). PRG

values can be relatively sensitive to the saturated hydraulic conductivity values for the aquifer, so values from the lower end of the range were chosen, yielding a more conservative PRG value. PRG development captures the effects of geologic variability by simulating flow and transport through a set of representative stratigraphic columns for each geographic area. Peak groundwater concentrations are simulated for each representative column and PRGs are calculated for each column. The minimum value is adopted as the final PRG for each geographic area for each contaminant.

The PRG calculation for each contaminant is performed using the same equation (Equation 2-1) as that for the SSL except that the inputs are different as mentioned above.

3. Model Conceptualization

The VZ models for the River Corridor consider porous media flow and transport through the unsaturated portion of the various geographic areas. The stratigraphy and thickness of the vadose and saturated zone plays an important role in determining the peak concentration of contaminants in the groundwater. This section provides an overview of the conceptual model development based on the geology in the 100 Area and the thickness of vadose and saturated zone. Modeling relevant Features, Events, and Processes (FEPs) are also presented to help in developing the flow and transport models. The nature and extent of contamination in the geographic areas is also presented to aid model development for SSL and PRG calculations.

3.1 Geology of River Corridor

There are two distinct hydrostratigraphic units present in the VZ and upper unconfined aquifer of the 100 Area: the younger is known as the Hanford formation and the older as the E unit of the Ringold Formation. Overlying the Hanford formation is a thin cover of more recent Holocene alluvium and eolian deposits.

Composed of silt, sand, and gravel, the recent Holocene surficial sediments were deposited by a combination of aeolian and alluvial processes. These deposits are observed as a thin layer (2 m or less) across the 100 Area where the surface has not been disturbed or altered by construction, and are treated as part of the Hanford formation for this study.

The Hanford formation is characterized by mostly unconsolidated coarse and fine-grained sediments including large to very large cobble-boulder fragments, sand, silt, and gravel. Three facies of the Hanford formation have been identified in the 100 Area: (1) gravel-dominated facies, (2) sand-dominated facies, and (3) interbedded sand to silt-dominated facies (DOE/RL-2002-39, *Standardized Stratigraphic Nomenclature for Post-Ringold-Formation Sediments within the Central Pasco Basin*). Within the 100 Area, the coarse-grained unconsolidated sand and gravel-dominated facies are most common, the result of high-energy fluvial deposition processes caused by the cataclysmic Missoula Floods (SGW-44022, *Geologic Data Package in Support of 100-BC-5 Modeling*). For this reason, the Hanford formation in the 100 Area tends to be coarser and contain a larger gravel component than other areas of the Hanford Site.

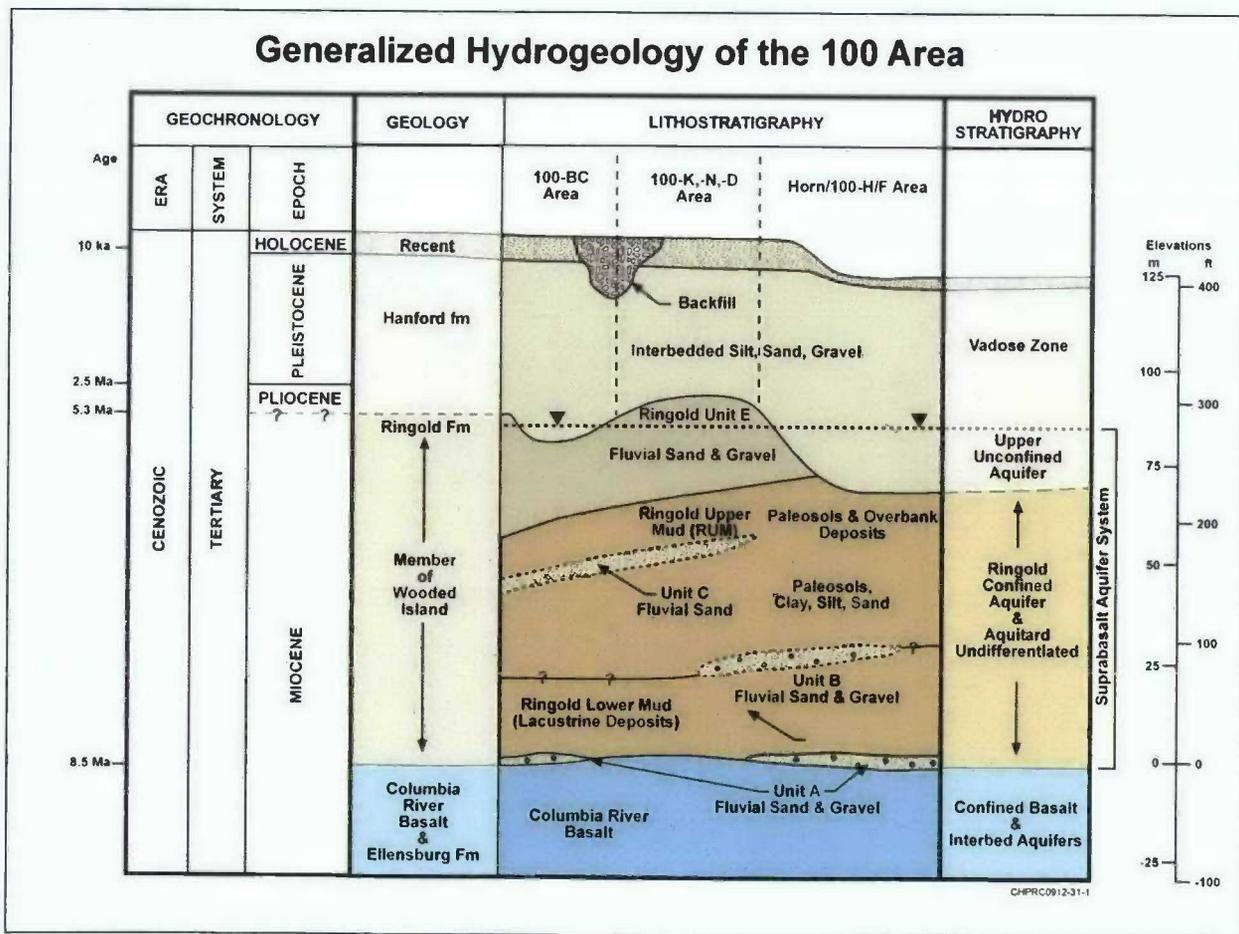
Below the Hanford formation, the Ringold Formation contains two units: one is fluvial gravel referred to as the Ringold Unit E, and the other is lower-energy sand, silt, and a clay interval referred to as the Ringold upper mud (RUM). The saturated hydraulic conductivity of the Ringold E is several orders of magnitude lower than that of the Hanford formation, whereas the RUM, an aquitard that is the base of the unconfined aquifer, has the lowest hydraulic conductivity of all hydrostratigraphic units in the 100 Area. The RUM directly underlies the Hanford formation where Ringold E was removed by the Missoula Floods (SGW-40781, *100-HR-3 Remedial Process Optimization Modeling Data Package*).

The Hanford-Ringold contact was formed by cataclysmic paleo-floods that first reworked the Ringold Formation surface by eroding into the older sediments and creating paleochannels constrained by uplifted basalt (the bedrock in the region). Hanford formation sediments were subsequently deposited over this reworked Ringold surface (SGW-41213, *100-KR-4 Remedial Process Optimization Modeling Data Package*). Given the large differences in saturated hydraulic conductivity values for the two formations, the location of the Hanford-Ringold contact relative to the water table is important to predicting contaminant migration in the unconfined aquifer. Where the Hanford-Ringold contact occurs below the

water table, water and solute fluxes toward the Columbia River can be orders of magnitude larger than those when the contact is located above the water table (PNNL-14702, *Vadose Zone Hydrogeology Data Package for Hanford Assessments*). Figure 3-1 depicts the generalized geology of the 100 Area. Figure 3-2 presents the top of the Ringold E surface (the Hanford-Ringold E contact) in plan view.

3.1.1 Representative Stratigraphy

Although the stratigraphy of the VZ and the unconfined aquifer within the 100 Area are limited to the Hanford formation and the Ringold E unit, their presence and thicknesses vary within and between each of the geographic areas. These variations can in turn cause important variations in solute fluxes and peak concentrations for contaminants, thereby leading to a range of potential PRG values among various geographic areas. Because of natural variability in the thickness of various hydrostratigraphic units, it is not practical to calculate PRG for all possible variations in thicknesses observed in the various boreholes. Instead, representative stratigraphic columns were identified for each geographic area: D/H, K, BC, F, IU-2, and IU-6. Figure 3-3 through Figure 3-6 illustrate the borehole locations used for each geographic area to produce representative soil columns for modeling purposes.



Source: SGW-44022

Figure 3-1. Generalized Geology of the 100 Area

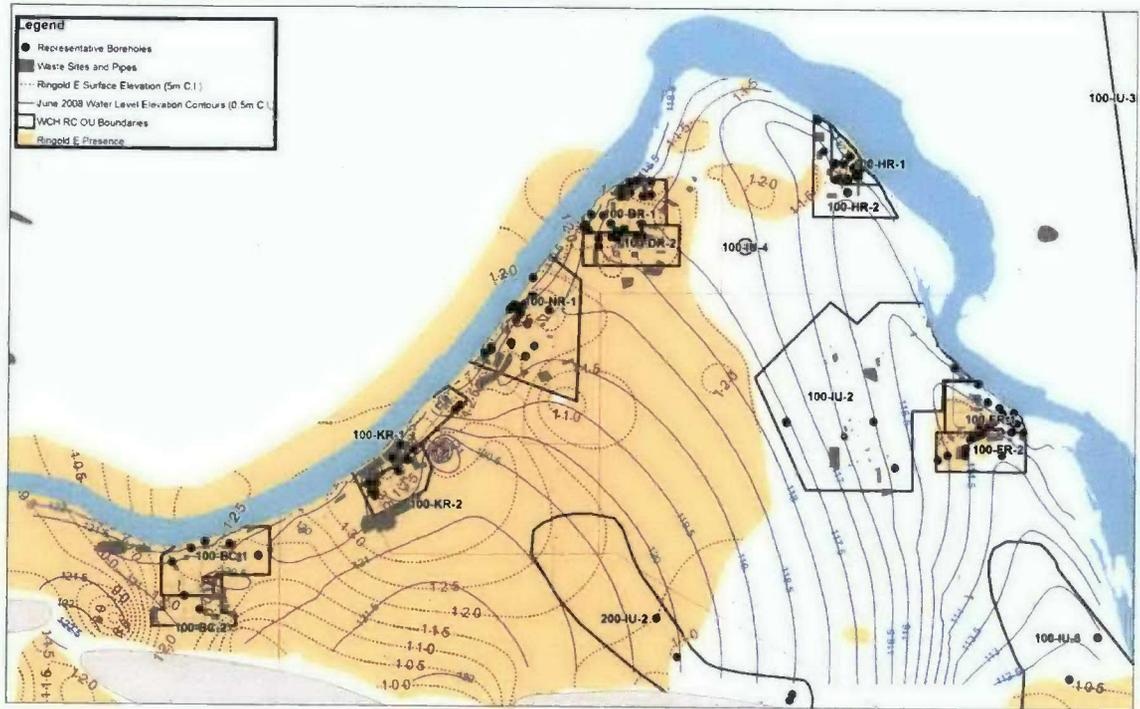


Figure 3-2. Elevation Contours for Top of Ringold E and Water Table

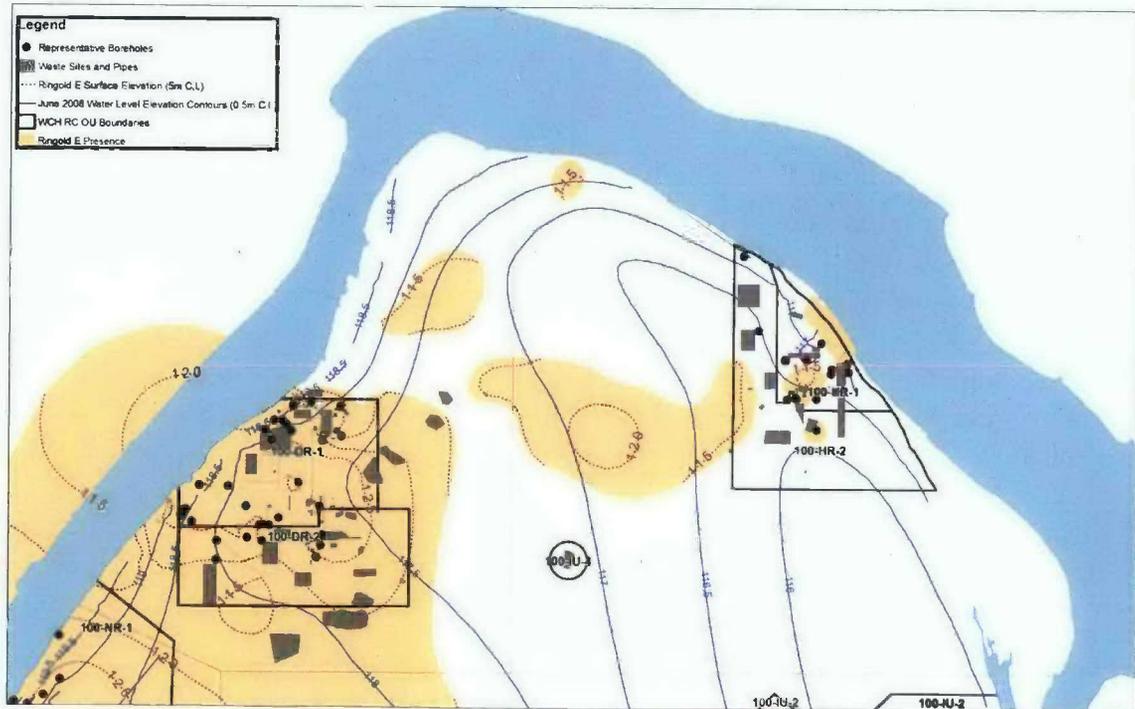


Figure 3-3. Borehole Locations for 100-D and 100-H Areas

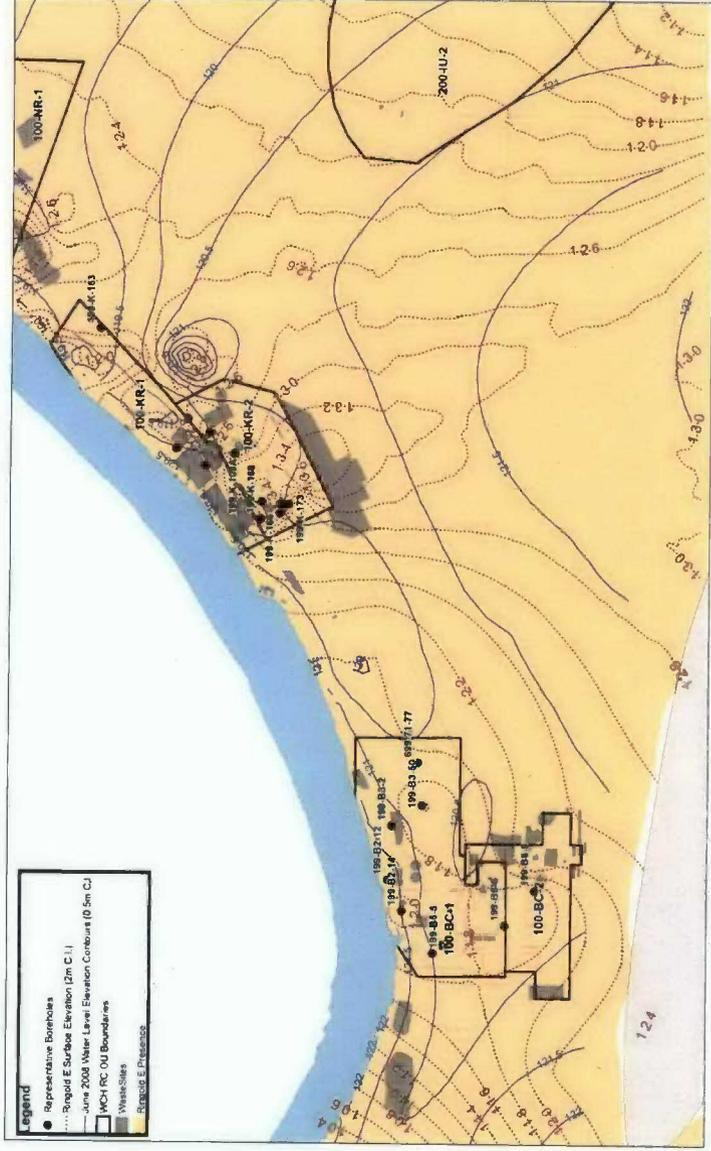


Figure 3-4. Borehole Locations for 100-B and 100-K Areas

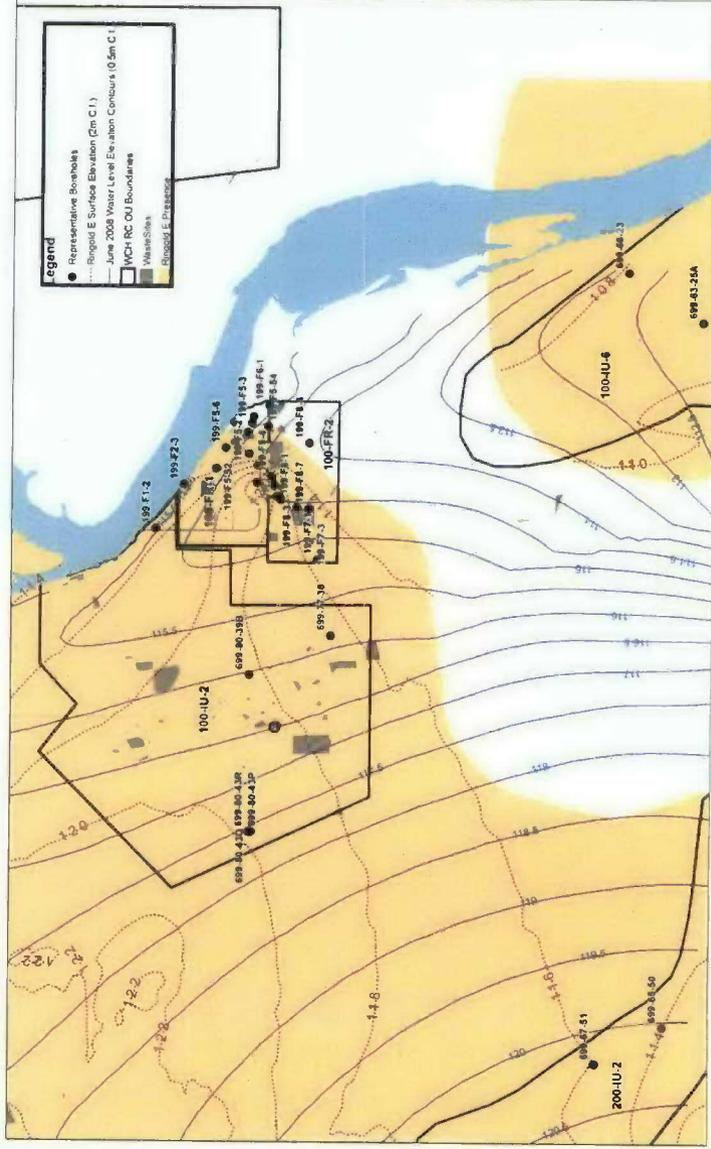


Figure 3-5. Borehole Locations for 100-F and 100-IJ Areas

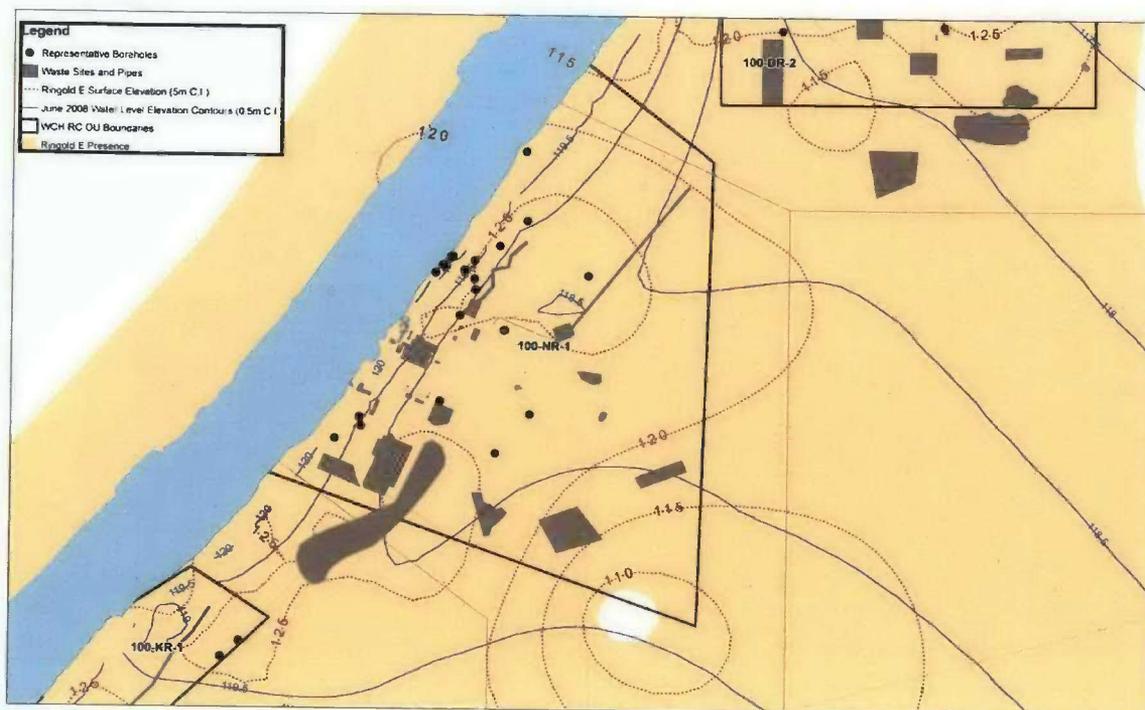


Figure 3-6. Borehole Locations for 100-N Area

Representative columns were identified by collecting and reviewing geologic data from 86 boreholes nearest to the waste sites in each geographic area. All borehole data were taken from the Hanford Environmental Information System (HEIS) borehole database. The columns include the VZ and the unconfined aquifer. The water table elevations of June 2008 were selected to provide representative (not extreme) high water table conditions; the month of June is typically when the highest river stages occur in this reach of the Columbia River. Use of water table elevations from the high water stage period (represented by the June 2008 data) result in a conservative (smaller) thickness of the VZ for each well and borehole to develop the representative stratigraphic profiles. Imposing conservative bias towards a smaller thickness was made to reduce the travel distance for contaminants in the vadose zone, and thereby bias the resulting peak groundwater concentration calculated to arrive sooner and greater magnitude—resulting in lower SSL and PRG values than otherwise. These borehole data also provided estimates of the thicknesses of each lithologic unit within the VZ and within the aquifer. The boreholes in each geographic area were divided into groups based on the proportion of each lithologic unit and total VZ thickness. A representative stratigraphic column was selected for each borehole group within each geographic area; this yielded from two to seven stratigraphic columns for each geographic area (see Section **Error! Reference source not found.** below).

The total column thickness, VZ thickness, and aquifer thickness of the representative columns vary with the borehole geology for each geographic area. Only the thickness of the clean backfill was held constant at 4.6 m (15 ft.) for all representative columns based on the Interim Action Record of Decision (ROD) for the 100 Area sites (EPA/ROD/R10-99/039, *EPA Superfund Record of Decision: Hanford 200-Area (USDOE) and Hanford 100-Area (USDOE)*). Thickness of the VZ, thickness of the SZ, and percentages of the different lithologic units in each zone were determined using the selected borehole logs. Table 3-1

presents the number of boreholes evaluated in each geographic area along with the range in vadose zone and saturated zone thickness. For a given borehole, a conservative (thinner) estimate of VZ thickness was calculated by taking the difference between ground surface elevation and the June 2008 water table elevation, which is representative of the seasonal high water table elevation. Boreholes belonging to the 100-IU-2 and 100-IU-6 geographic areas were combined to produce shared representative columns. This was done due to lack of borehole data across both geographic areas.

Table 3-1. Vadose and Saturated-Zone Thicknesses in the 100 Area Geographic Areas

Geographic area	Number of Boreholes	Vadose Zone Thickness (m)			Saturated Zone Thickness (m)		
		Minimum	Average	Maximum	Minimum	Average	Maximum
100-D	18	16.7	23.6	26.6	1.2	5.7	8.1
100-H	17	8.4	11.8	13.4	2.3	5.2	8.2
100-K	8	15.8	21.8	25.1	14.9	25.3	28.7
100-BC	8	12.2	19.2	30	30.9	34.5	48.2
100-F	17	7.5	10.9	13.4	1.2	6.4	11.8
100-N	10	19.2	21.0	25.4	8.8	11.6	16.2
100-IU-2 & 100-IU-6	8	7.4	14.5	40.0	4.6	8.9	24.0

Representative stratigraphic columns for each geographic area were derived from groupings of the borehole data by VZ thickness and lithologic composition (Table 3-2 through Table 3-8). The objective was to create a limited number of representative stratigraphic columns for each geographic area so that the number of STOMP simulations would be feasible given resource constraints, while capturing the range of variability within each area. This was accomplished by dividing the boreholes for each geographic area into groups based on a range of VZ-thickness intervals and then identifying one, or more, representative lithologic compositions (see Appendix A for more details). For example, the set of 100-D boreholes was divided into three groups according to VZ thickness: 25, 20, and 15 m, whereas the 100-H boreholes were divided into two groups with 12 and 8 m thicknesses, respectively (Table 3-2 and Table 3-3). Examination of all wells within the 100-D 25-m-thickness group revealed a range of compositions for the VZ, but the 12 boreholes in this group were divided into three sub-groups based on relative fraction of lithologies:

- 100% Hanford formation
- 80% Hanford formation – 20% Ringold E unit
- 60% Hanford formation – 40% Ringold E unit (Table 3-2)

A 5-m thickness of the SZ was used in STOMP simulations in accordance with WAC 173-340-747(5)(f)(i) and equation 747-4 for A, aquifer mixing zone. If the thickness of the SZ was less than 5 m, then the thickness of the SZ was assumed as 5 m. Table 3-2 through Table 3-8 compares the actual to the representative compositions for each geographic area. The procedure for determining representative boreholes and thickness of VZ and SZ is presented in Appendix A of this report.

Table 3-2. Determination of Vadose Zone Thickness and Geology for Geographic Area 100-D

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ ¹ Composition
1	25	100% Hanford	25	0	199-D4-83	100% Hanford	24.32	5.25	6.48	100% Hanford
					199-D5-17		25.4	6.15		
					199-D5-97		25.81	7.41		
					199-D5-99		26.09	7.29		
					199-D8-4		25.21	6.31		
2	20	100% Hanford	20	0	199-D2-5	100% Hanford	22.64	4.80	5.13	100% Hanford
					199-D8-97		23.14	5.06		
					199-D8-98		20.37	5.53		
3	25	75% Hanford 25% Ringold E	20	5	199-D4-101	76% Hanford 24% Ringold E	25.35	6.66	7.35	100% Ringold E
					199-D5-103	83% Hanford 17% Ringold E	25.69	8.05		
4	20	80% Hanford 20% Ringold E	16	4	199-D8-89	80% Hanford 20% Ringold E	19.76	4.01	4.01	100% Ringold E
5	25	60% Hanford 40% Ringold E	15	10	199-D4-25	63% Hanford 37% Ringold E	24.79	6.15	4.91	100% Ringold E
					199-D5-12	59% Hanford 41% Ringold E	25.96	1.17		
					199-D5-120	63% Hanford 37% Ringold E	25.76	7.16		
					199-D5-19	63% Hanford 37% Ringold E	24.14	4.66		
					199-D5-34	62% Hanford 38% Ringold E	26.6	5.40		
6	15	60% Hanford 40% Ringold E	9	6	199-D8-54B	63% Hanford 37% Ringold E	16.82	6.35	5.34	100% Ringold E
					199-D8-55	55% Hanford 45% Ringold E	16.7	4.33		

Note, VZ: vadose zone; SZ: saturated zone.

Table 3-3. Determination of Vadose Zone Thickness and Geology for Geographic Area 100-H

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ Composition
1	12	100% Hanford	12	0	199-H3-1	100% Hanford	12.90	4.17	5.25	100% Hanford
					199-H3-25		11.31	5.75		
					199-H3-2A		11.39	5.37		
					199-H3-2B		11.26	6.11		
					199-H3-2C		11.36	5.40		
					199-H4-1		11.62	6.14		
					199-H4-11		10.82	7.16		
					199-H4-14		11.42	6.56		
					199-H4-2		11.66	8.15		
					199-H4-46		13.07	5.53		
					199-H4-49		13.36	3.40		
					199-H4-69		12.53	5.75		
					199-H4-70		12.97	4.10		
					199-H4-72		11.90	5.17		
199-H4-9	11.34	2.83								
					199-H6-2		12.92	2.32		
2	8	100% Hanford	8	0	699-99-41	100% Hanford	8.35	3.84	3.84	100% Hanford

Note; VZ: vadose zone; SZ: saturated zone

Table 3-4. Determination of Vadose Zone Thickness and Geology for Geographic Area 100-K

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ Composition
1	25	100% Hanford	25	0	199-K-173	100% Hanford	25.12	28.07	28.07	8% Hanford 92% Ringold E (100% Ringold E selected in the model)
2	15	70% Hanford 30% Ringold E	10.5	4.5	199-K-32B	70% Hanford 30% Ringold E	15.77	25.68	20.305	100% Ringold E
					199-K-163	66% Hanford 34% Ringold E	18.6	14.93		
3	20	50% Hanford 50% Ringold E	10	10	199-K-109A	52% Hanford 48% Ringold E	22.71	24.54	24.51	100% Ringold E
4	20	40% Hanford 60% Ringold E	8	12	199-K-111A	38% Hanford 62% Ringold E	21.01	26.33	26.33	100% Ringold E
5	20	30% Hanford 70% Ringold E	6	14	199-K-165	35% Hanford 65% Ringold E	24.96	28.69	27.67	100% Ringold E
					199-K-166	34% Hanford 66% Ringold E	24.02	27.26		
					199-K-106A	28% Hanford 72% Ringold E	22.48	27.05		

Note; VZ: vadose zone; SZ: saturated zone

Table 3-5. Determination of Vadose Zone Thickness and Geology for Geographic Area 100-F

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ Composition
1	12	100% Hanford	12	0	199-F5-46	100% Hanford	12.40	4.82	6.14	100% Hanford
					199-F5-45		11.81	3.89		
					199-F5-52		12.22	7.90		
					199-F5-2		11.38	11.79		
					199-F5-54		11.53	9.74		
					199-F5-47		13.42	5.63		
					199-F5-4		12.10	3.14		
					199-F8-4		11.31	2.86		
					199-F8-2		11.00	5.46		
2	10	100% Hanford	10	0	199-F5-5	100% Hanford	10.77	11.18	10.39	100% Hanford
					199-F5-6		10.95	10.08		
					199-F5-3		9.90	9.91		
3	8	100% Hanford	8	0	199-F5-1	100% Hanford	9.00	9.90	4.94	100% Hanford
					199-F8-3		7.45	1.70		
					199-F6-1		8.28	6.96		
					199-F8-7		8.53	1.22		
4	12	40% Hanford 60% Ringold E	4.8	7.2	199-F5-48	43% Hanford 57% Ringold E	12.76	3.09	3.09	100% Ringold E

Note; VZ: vadose zone; SZ: saturated zone

Table 3-6. Determination of Vadose Zone Thickness and Geology for Geographic area 100-BC

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ Composition
1	14		14	0	199-B3-2		14.24	32.4	32.4	100% Hanford
2	23		23	0	699-71-77		23.61	31.26	31.26	2% Hanford 98% Ringold E (100% Ringold E selected in the model)
3	14		14	0	199-B5-5		14.34	48.15	48.15	4% Hanford 96% Ringold E (100% Ringold E selected in the model)
4	30	100% Hanford	30	0	199-B8-9	100% Hanford	29.98	34.49	34.49	15% Hanford 85% Ringold E
					199-B3-50		22.18	31.77		17% Hanford 83% Ringold E (15% Hanford 85% Ringold E selected in the model)
5	22		22	0	199-B5-6		24.18	34.03	32.9	12% Hanford 88% Ringold E (15% Hanford 85% Ringold E selected in the model)
6	12	30% Hanford 70% Ringold E	3.6	8.4	199-B2-12	32% Hanford 68% Ringold E	12.16	33.41	33.41	100% Ringold E
7	13	80% Hanford 20% Ringold E	10.4	2.6	199-B2-14	78% Hanford 22% Ringold E	12.65	30.85	30.85	100% Ringold E

Note; VZ: vadose zone; SZ: saturated zone

Table 3-7. Determination of Vadose Zone Thickness and Geology for Geographic areas 100-IU-2 and 100-IU-6

Representative Column Index	Representative VZ Thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Wells	Actual VZ Composition	Actual VZ Thickness (m)	Actual Aquifer Thickness (m)	Average Aquifer Thickness (m)	SZ Composition
1	40	100% Hanford	40	0	699-67-51	100% Hanford	40.02	23.99	23.99	17% Hanford; 83% Ringold E
2	22	100% Hanford	22	0	699-65-50	100% Hanford	22.54	12.51	12.51	100% Hanford
3	10	100% Hanford	10	0	699-76-36	100% Hanford	10.19	5.05	6.49	100% Hanford
					699-80-43P		9.11	4.61		
					699-63-25A		9.10	9.80		
4	8	100% Hanford	8	0	699-80-39B	100% Hanford	7.42	5.69	5.11	100% Hanford
					699-80-43Q		8.84	4.88		
					699-80-43R		8.94	4.78		

Note; VZ: vadose zone; SZ: saturated zone

Table 3-8. Determination of Vadose Zone Thickness and Geology for Geographic Area 100-N

Representative Column Index	Representative VZ thickness (m)	Representative VZ Composition	Thickness of Hanford in VZ (m)	Thickness of Ringold E in VZ (m)	Corresponding Wells	Actual VZ Composition	Actual VZ thickness (m)	Actual Aquifer thickness (m)	Average Aquifer thickness (m)	SZ Composition
1	20	85% Hanford, 15% Ringold E	17	3	199-K-150	85% Hanford, 15% Ringold E	19.46	14.68	13.44	100% Ringold E
					199-K-160		19.78	16.18		
					699-86-60		19.82	9.44		
2	21	60% Hanford, 40% Ringold E	12.5	8.5	199-N-105A	64% Hanford, 36% Ringold E	20.49	8.77	9.75	100% Ringold E
					199-N-69	59% Hanford, 41% Ringold E	21.62	9.16		
					199-N-70	56% Hanford, 44% Ringold E	20.37	11.33		
3	23	72% Hanford, 28% Ringold E	17	6	199-N-106A	70% Hanford, 30% Ringold E	25.36	10.91	10.80	100% Ringold E
					199-N-71	75% Hanford, 25% Ringold E	22.43	10.90		
					699-84-59	72% Hanford, 28% Ringold E	21.81	10.60		
4	19.5	95% Hanford, 5% Ringold E	18.5	1.0	199-K-159	95% Hanford, 5% Ringold E	19.21	14.31	14.31	100% Ringold E

Note: VZ = vadose zone, SZ = saturated zone

3.2 Modeling Features, Events, Processes, and Assumptions

This section provides a summary of key FEPs that are considered in the development of the VZ flow and transport models for the River Corridor. These FEPs are important in developing the conceptual models as they affect the transport of contaminants through the VZ. Section 3.2.4.6 lists key modeling assumptions.

3.2.1 Climate and Vegetation

The DOE's Hanford Site lies within the semiarid shrub-steppe Pasco Basin of the Columbia Plateau in south-central Washington State. The region's climate is greatly influenced by the Pacific Ocean and the Cascade Mountain Range to the west, and other mountain ranges to the north and east. The Pacific Ocean moderates temperatures throughout the Pacific Northwest, and the Cascade Range generates a rain shadow effect that limits rain and snowfall in the eastern half of Washington State. The Cascade Range also serves as a source of cold air drainage, which has a considerable effect on the wind regime on the Hanford Site. Mountain ranges to the north and east of the region shield the area from the severe winter storms and frigid air masses that move southward across Canada. The following climate information summary is extracted from information reported in PNNL-6415, *Hanford Site National Environmental Policy Act (NEPA) Characterization*.

Climatological data for the Hanford Site are compiled at the Hanford Meteorology Station (HMS), which is located on the Hanford Site's Central Plateau, just outside the northeast corner of the 200 West Area and about 4 kilometers (km) (3 miles [mi]) west of the 200 East Area. Meteorological measurements have been made at the HMS since late 1944. Before the HMS was established, local meteorological observations were made at the old Hanford town site (1912 through late 1943) and in Richland (1943 to 1944). A climatological summary for Hanford is provided in a report by PNNL-15160, *Hanford Site Climatological Summary 2004 with Historical Data*. Data from the HMS capture the general climatic conditions for the region and describe the specific climate of the Hanford Site's Central Plateau. The size of the Hanford Site and its topography give rise to substantial spatial variations in wind, precipitation, temperature, and other meteorological characteristics. To characterize meteorological differences accurately across the Hanford Site, the HMS operates a network of monitoring stations. These stations, which currently number 30, are situated throughout the Hanford Site and in neighboring areas.

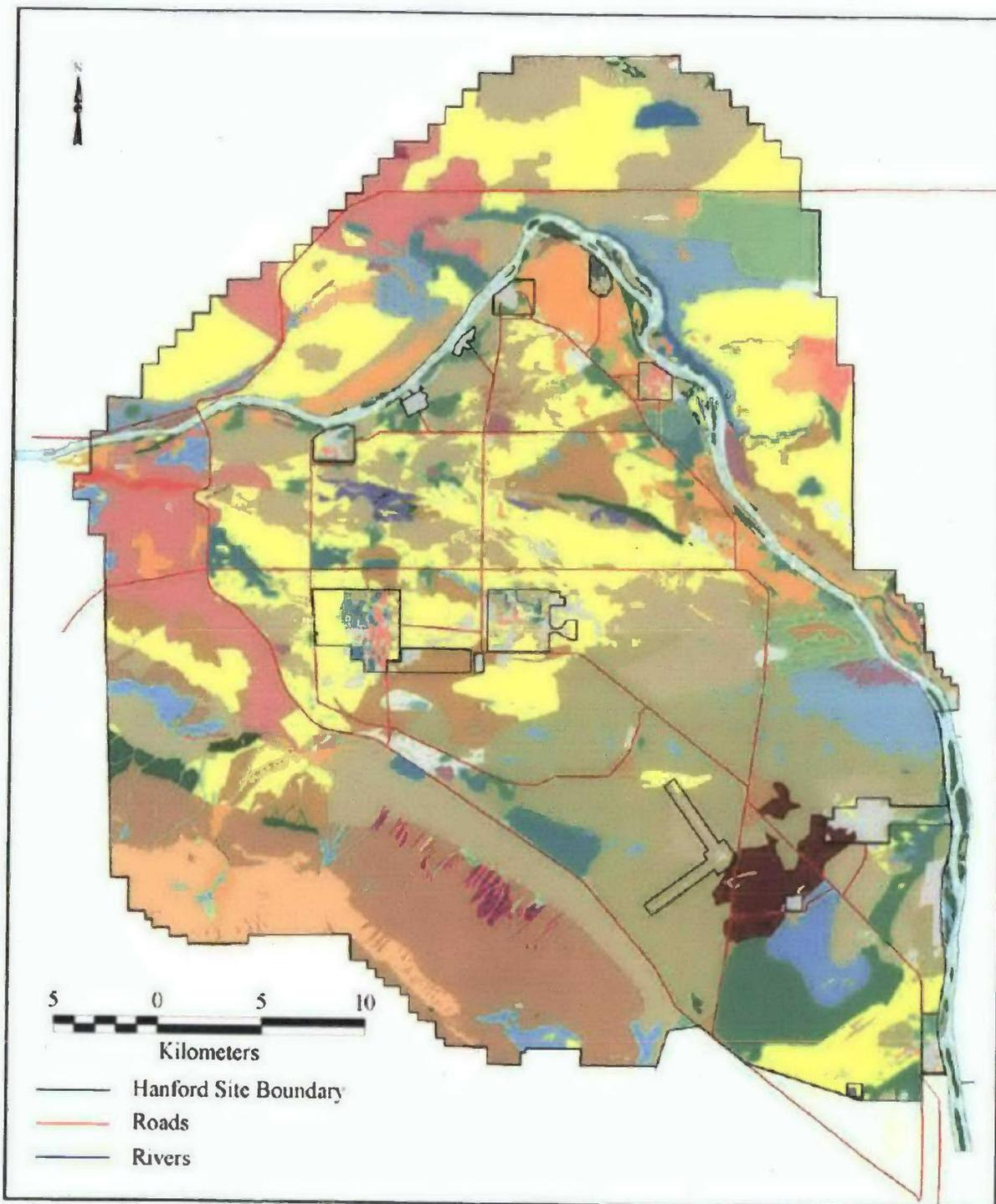
The prevailing surface winds on Hanford's Central Plateau are from the northwest and occur most frequently during the winter and summer. During the spring and fall, there is an increase in the frequency of winds from the southwest and a corresponding decrease in winds from the northwest. Monthly and annual joint-frequency distributions of wind direction versus wind speed for the HMS are reported in PNNL-15160. Monthly average wind speeds 15.2 m (50 ft.) above the ground are lower during the winter months, averaging 2.7 to 3.1 m/s (6 to 7 miles per hour [mph]) and faster during the spring and summer, averaging 3.6 to 4.0 m/s (8 to 9 mph). The fastest wind speeds at the Hanford Site are usually associated with flow from the southwest. However, the summertime drainage winds from the northwest frequently exceed speeds of 13 m/s (30 mph). The maximum speed of the drainage winds (and their frequency of occurrence) tends to decrease at locations toward the southeast. The HMS averages 156 days per year with peak wind gusts greater than or equal to 11 m/s (25 mph) (ranging from a low of about 7 days in December to a high of nearly 20 days in June and July). Of these, an average of 57 days occur with peak gusts greater than or equal to 16 m/s (35 mph) (from a low of about 3 days in September and October to a high of about 6 days during the months of April through July).

Monthly averages and extremes of temperature, dew point, and humidity are presented in PNNL-15160. Based on data collected from 1946 through 2004, the average monthly temperatures at the HMS range from a low of -0.7°C (31°F) in January to a high of 24.7°C (76°F) in July. The highest winter monthly average temperature was 6.9°C (44°F) in February 1958 and February 1991, and the lowest average monthly temperature was -11.1°C (12°F) in January 1950. The highest monthly average temperature was 27.9°C (82°F) in July 1985, and the lowest summer monthly average temperature was 17.2°C (63°F) in June 1953. Daily maximum temperatures at the HMS vary from an average of 2°C (35°F) in late December and early January to 36°C (96°F) in late July. There are, on average, 52 days during the summer months with maximum temperatures greater than or equal to 32°C (90°F) and 12 days with maxima greater than or equal to 38°C (100°F). From mid-November through early March, the average daily minimum temperature is below freezing; the daily minimum in late December and early January is -6°C (21°F). On average, the daily minimum temperature of less than or equal to -18°C (approximately 0°F) occurs only 3 days per year; however, only about one winter in two experiences such low temperatures. The annual average relative humidity at the HMS is 55%. It is highest during the winter months, averaging about 76%, and lowest during the summer, averaging about 36%. The annual average dew point temperature at the HMS is 1°C (34°F). In the winter, the dew point temperature averages about -3°C (27°F), and in the summer, it averages about 6°C (43°F).

Average annual precipitation at the HMS is 17 centimeters (cm) (6.8 inches [in.]). During 1995, the wettest year on record, 31.3 cm (12.3 in.) of precipitation was measured; during 1976, the driest year, only 7.6 cm (3 in.) was measured. For the year chosen to represent the annually occurring highest water table (2008) in this model, the measured precipitation was 14.0 cm (5.49 in.). The wettest season on record was the winter of 1996-1997, with 14.1 cm (5.4 in.) of precipitation; the driest season was the summer of 1973, when only 0.1 cm (0.03 in.) of precipitation was measured. Most precipitation occurs during the late autumn and winter, with more than half of the annual amount occurring from November through February. Days with greater than 1.3 cm (0.50 in.) precipitation occur on average less than one time each year. Average snowfall ranges from 0.25 cm (0.1 in.) during October to a maximum of 13.2 cm (5.2 in.) during December, and decreases to 1.3 cm (0.5 in.) during March. The record monthly snowfall of 59.4 cm (23.4 in.) occurred during January 1950. The seasonal record snowfall of 142.5 cm (56.1 in.) occurred during the winter of 1992-1993. Snowfall accounts for about 38% of all precipitation from December through February. Note that recharge measurements include all precipitation, including snowfall.

Vegetation communities in this region are subject to change depending on soil type, climate conditions, physical disturbance, and plant succession. Figure 3-7 illustrates the distribution of vegetation types and areas on the Hanford Site before the major fire that occurred in 2000 (Legend for Figure 3-7 is provided in Figure 3-8). The extent of the year 2000 fire is shown in Figure 3-9.

Shrublands occupy the largest area in terms of acreage and comprise seven of the nine major plant communities on the Hanford Site (PNNL-13688, *Vascular Plants of the Hanford Site*). Of the shrubland types, sagebrush-dominated communities are predominant, with other shrub communities varying with changes in soil and elevation. About 287 square kilometers (km^2) (111 square miles [mi^2]) of shrub habitat dominated by big sagebrush was destroyed in the 2000 fire; this area is in various stages of recovery. Of the vegetation types found on the Hanford Site, those with a shrub component (i.e., big sagebrush, threetip sagebrush [*Artemisia tripartita*], bitterbrush [*Purshia tridentata*], gray rabbitbrush [*Ericameria nauseous*, previously *Chrysothamnus nauseosus*], green rabbitbrush [*Chrysothamnus viscidiflorus*], black greasewood [*Sarcobatus vermiculatus*], winterfat [*Krascheninnikovia (Ceratooides) lanata*], snow buckwheat [*Eriogonum niveum*], and spiny hopsage [*Grayia (Atriplex) spinosa*]) are



Source: PNNL-6415

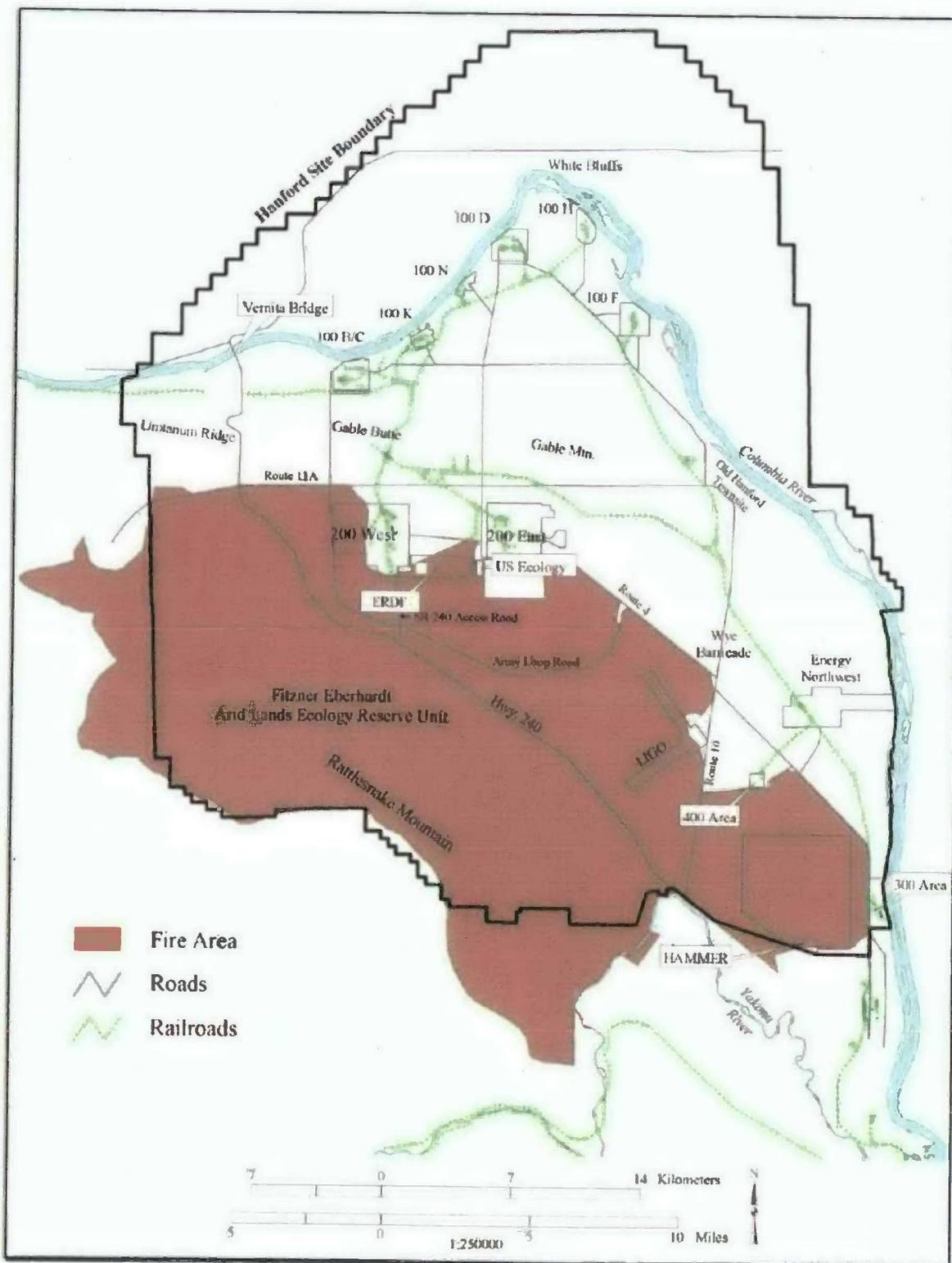
Figure 3-7. Distribution of Vegetation Types and Areas on the Hanford Site, Washington, before the Year 2000 Fire

LEGEND

	Abandoned Old Agricultural Fields
	Alkali Saltgrass - Cheatgrass
	Big Sagebrush - Bitterbrush / Bunchgrass
	Big Sagebrush - Bitterbrush / Needle-and-Thread Grass
	Big Sagebrush - Bitterbrush / Sandberg's Bluegrass
	Big Sagebrush - Rigid Sagebrush / Bunchgrass
	Big Sagebrush - Rock Buckwheat / Bunchgrass
	Big Sagebrush - Spiny Hopsage / Bunchgrass
	Big Sagebrush - Spiny Hopsage / Sandberg's Bluegrass - Cheatgrass
	Big Sagebrush / Bluebunch Wheatgrass
	Big Sagebrush / Bunchgrass
	Big Sagebrush / Needle-and-Thread Grass
	Big Sagebrush / Sand Dropseed
	Big Sagebrush / Sandberg's Bluegrass - Cheatgrass
	Bitterbrush / Bunchgrass
	Bitterbrush / Indian Ricegrass
	Bitterbrush / Needle-and-Thread Grass
	Black Greasewood / Alkali Saltgrass
	Bluebunch Wheatgrass - Needle-and-Thread Grass
	Bluebunch Wheatgrass - Sandberg's Bluegrass
	Bunchgrass - Cheatgrass
	Crested Wheatgrass
	Disturbed
	Gray Rabbitbrush - Snow Buckwheat / Bunchgrass
	Gray Rabbitbrush / Bunchgrass
	Gray Rabbitbrush / Cheatgrass
	Gray Rabbitbrush / Needle-and-Thread Grass
	Gray Rabbitbrush / Sand Dropseed
	Gray Rabbitbrush / Sandberg's Bluegrass - Cheatgrass
	Needle-and-Thread Grass - Indian Ricegrass
	Needle-and-Thread Grass - Sandberg's Bluegrass
	Non-Riverine Wetlands and Associated Deepwater Habitats
	Rabbitbrush / Bunchgrass
	Rigid Sagebrush / Sandberg's Bluegrass
	Riparian
	Riverine Wetlands and Associated Deepwater Habitats
	Sand Dropseed - Sandberg's Bluegrass - Cheatgrass
	Sandberg's Bluegrass - Cheatgrass
	Snow Buckwheat - Bitterbrush / Bunchgrass
	Snow Buckwheat / Bunchgrass
	Snow Buckwheat / Sandberg's Bluegrass - Cheatgrass
	Spiny Hopsage / Sandberg's Bluegrass - Cheatgrass
	Talus
	Threelobe Sagebrush / Bunchgrass
	Thymelaf Buckwheat / Sandberg's Bluegrass
	Vernal Pool
	White Bluffs
	Winterfat / Bunchgrass

Source: PNNL-6415

Figure 3-8. Legend for Figure 3-7



Source: PNNL-6415

Figure 3-9. Extent of Hanford Site, Washington, Burned as a Result of the June 27 to July 2, 2000 Wildfire

considered shrub-steppe. These stands typically have an understory dominated by bunchgrasses such as bluebunch wheatgrass (*Pseudoroegneria spicata*, previously *Agropyron spicatum*), Sandberg's bluegrass

(*Poa sandbergii [secunda]*), needle-and-thread grass (*Hesperostipa comate*, previously *Stipa comata*), Indian ricegrass (*Achnatherum hymenoides*, previously *Oryzopsis hymenoides*), bottlebrush squirreltail (*Elymus elymoides*, previously *Sitanion hystrix*), and prairie junegrass (*Koeleria cristata*), as well as a number of broad-leaf forbs. Heavily grazed or disturbed areas often have an understory dominated by cheatgrass. Heterogeneity of species composition varies with soil, slope, and elevation. Vegetation types with a significant cheatgrass component are generally of lower habitat quality than those with bunchgrass understories.

Most grasses occur as understory in shrub-dominated plant communities. Because shrubs have been removed by fire in many areas, there are large areas of grass-dominated communities on the Hanford Site. Cheatgrass has replaced many native perennial grass species and is well established in many low-elevation (less than 244 m [800 ft.]) and/or disturbed areas. Of the native grasses that occur on the Hanford Site, bluebunch wheatgrass occurs at higher elevations. Sandberg's bluegrass is widely distributed throughout the Columbia Basin and the intermountain west. Needle-and-thread grass, Indian ricegrass, and thickspike wheatgrass (*Elymus macrourus*, previously *Agropyron dasytachyum*) occur in sandy soils and dune habitats.

Within the past few hundred years, the Hanford Site upland landscape had few trees and the Columbia River shoreline supported a few scattered cottonwood (*Populus spp.*) or willows (*Salix spp.*). Homesteaders and Manhattan Project construction workers planted trees in association with agricultural areas and housing camps. Shade and ornamental trees were planted in the 1950s around former military installations and industrial areas on the Hanford Site. Currently, approximately 23 species of trees occur on the Site. The most commonly occurring species are black locust (*Robinia pseudo-acacia*), Russian olive (*Eleagnus angustifolia*), cottonwood (*Populus trichocarpa*), mulberry (*Morus alba*), sycamore (*Platanus occidentalis*), and poplar (*Populus spp.*). These trees are not commonly found in waste disposal locations.

3.2.2 Recharge and Evapotranspiration

Recharge is the flux of water transmitted across the water table from the VZ to the SZ. Direct measurement of recharge at the water table is typically impractical due to the inaccessibility, especially at Hanford where the water table is commonly located at depths below ground surface (bgs) of 80 m or more. Natural recharge is that recharge that originates as meteoric water. Other aquifer-influencing operations, such as artificial discharges (from anthropogenic discharges such as those associated with past waste management operations at the Hanford Site) or perturbations to the aquifer system from remedial action pump and treat systems, where present, would complicate efforts at making a direct measurement of natural recharge for a deep water table. Instead, measurements and analyses in the unsaturated zone at shallow depths are used to characterize deep drainage. Deep drainage is defined here as the water flux leaving the depth below which the processes of evapotranspiration can return water from the unsaturated soil to the atmosphere (PNNL-17841, *Compendium of Data for the Hanford Site (Fiscal Years 2004 to 2008) Applicable to Estimation of Recharge Rates*). This deep drainage, with sufficient time, will be manifest as the natural recharge flux. The time required for this to happen will depend on the thickness and hydraulic properties of the VZ and the deep drainage rate itself. Changes in the deep drainage rate, such as would result from changes in surface vegetative conditions that increase or decrease the evapotranspiration rate, can take many years to be reflected in the recharge rate for a thick VZ in arid conditions such as at the Hanford Site and can be an important consideration in characterizing recharge as well (PNNL-17841).

Important physical properties and processes that influence recharge include climate, soil hydraulic properties and stratigraphy, vegetative cover, land use, and topography (PNNL-17841). Climate determines the driving forces for recharge, namely the quantity of precipitation available for the land-surface water balance, and the energy fluxes that are determinant in the partitioning of precipitation into evaporation, transpiration, and recharge. Soil hydraulic properties and stratigraphy determine the rate at which water is transmitted through the VZ, and hence the effective time for processes of evaporation and transpiration to influence the net downward flux. Vegetative cover determines the strength of the transpiration portion of the land-surface water balance. Land use will change the influencing factors including the vegetative cover and surface soils, and hence the hydraulic properties and soil stratigraphy of a site, and hence transpiration rates. Topography is the primary determinant for the portion of precipitation that is subject to overland flow, either "run-on" or "run-off," for a given site. Knowledge of all of the influences is important to the estimation of recharge at a given location.

There has been considerable study devoted to estimation of recharge rates at the Hanford Site to support flow and transport modeling needs. PNL-10285, *Estimated Recharge Rates at the Hanford Site*, produced a defensible map of estimated recharge rates across the Hanford Site for current climate and 1991 vegetation/and use patterns. Various recharge data packages have been prepared to support performance assessments (e.g., PNNL-13033, *Recharge Data Package for the Immobilized Low-Activity Waste 2001 Performance Assessment*, PNNL-14744, *Recharge Data Package for the 2005 Integrated Disposal Facility Performance Assessment*; PNNL-16688, *Recharge Data Package for Hanford Single-Shell Tank Waste Management Areas*) and site-wide assessments (e.g., PNNL-14702). These studies, in turn, have been supported by a significant field research program (e.g., PNL-6403, *Recharge at the Hanford Site: Status Report*; PNL-6810, *The Field Lysimeter Test Facility (FLTF) at the Hanford Site: Installation and Initial Tests*; PNL-7209, *Field Lysimeter Test Facility: Second Year (FY 1989) Test Results*; Gee et al. [2005], "Measurement and Prediction of Deep Drainage from Bare Sediments at a Semiarid Site"; Gee et al. [2007], "Hanford Site Vadose Zone Studies: An Overview"; PNNL-17841).

For numerical simulation, two general approaches are available with regard to addressing recharge. In the first, the surface energy and fluid balance can be explicitly simulated as part of the larger VZ model numerical implementation. In this approach, meteorological data (precipitation, wind speed, humidity, solar radiation, air temperature), surface soil parameters, and vegetation parameters (root density and depth with time, leaf area index with time, growth cycle dates, etc.) would be used to directly simulate the surface water balance and thereby estimate net deep recharge. Under this approach, the processes simulated for the upper boundary would dominate time step control of the simulation, particularly as this approach would require high-temporal-resolution meteorological data (e.g., hourly) to support a reasonably accurate simulation of the processes in question. A second approach is to segregate the simulation of the surface balance processes to arrive at a net recharge rate used for deeper VZ simulations. In this approach the full process-based simulation described for the surface soil is still performed, but only for the near surface. This has been done, and the effective net recharge rates are available in references such as PNNL-14702 for application to deeper VZ simulations. The second approach is clearly more efficient and is preferred. It is noted that the recharge rates from the second approach are strongly a function of vegetation cover and surface soil type, and that due to land-surface condition changes in time, these rates will change over time. A typical progression might be from a pre-operational natural vegetation cover (low recharge due to vegetation efficiently returning a high proportion of meteoric water to the atmosphere through transpiration) to an operational cover (such as gravel maintained vegetation-free with high recharge) to a transitional period following remediation with declining recharge rates, and finally a return to a mature native plant community with low recharge once

again. Thus, the historic and projected land cover condition is the determining factor for selecting recharge rates to apply with time.

3.2.3 Columbia River – Aquifer Interactions

The groundwater flow in the aquifer and exchange with the Columbia River impacts contaminant transport within the geographic areas in the River Corridor. Flow paths in the groundwater/river zone of interaction vary with daily and seasonal fluctuations in river stage. River water infiltrates the banks during high river stages, moves inland, then reverses flow as the river stage subsides, and moves back through the hyporheic zone and discharges to the riverbed. Monitoring and modeling studies suggest that this back-and-forth motion of groundwater and river is very cyclical in response to the diurnal river stage cycle, which typically includes two high stages and two low stages in response to power peaking demands on the Priest Rapids hydroelectric dam located upstream of the Hanford Site. Review of past modeling studies in addition to new studies conducted for the Remedial Process Optimization (RPO) and 100-Area RI/FS suggests that there is a significant back-and-forth or sloshing action due to flow reversals within the aquifer resulting from river stage changes. For example, an individual Cr(VI) atom may experience a discontinuous path on its way to the river. It will experience numerous reversals in flow direction before it eventually reaches the water column in the river.

The flow reversal is very significant process with respect to the fate and transport of Cr(VI) (the most prevalent contaminant in the 100 Area). This is because it allows for the partial replenishment or resetting of the geochemical factors that promote reduction, adsorption, and precipitation of Cr(VI) that are close to being maxed out (nutrient limited, adsorption site limited) towards the distal end of the groundwater flow path. Modeling studies (e.g., PNNL-13674, *Zone of Interaction Between Hanford Site Groundwater and Adjacent Columbia River*) indicate that the movement of groundwater in response to river stage is predominantly piston-type flow. This action likely replenishes the geochemical environment and allows for continued reduction, adsorption, and precipitation in the hyporheic zone and adjacent groundwater.

Work by the Pacific Northwest National Laboratory (PNNL) at the Integrated Field Research Challenge site at the Hanford 300 Area illustrates the water action in terms of river stage versus contaminant concentration in the hyporheic zone. In this case, the contaminant of concern is uranium. The figure below (Figure 3-10) shows uranium concentration in hyporheic zone in black versus the river stage (gray line). There is a pronounced inverse relationship in which as the river elevation rises, uranium concentrations decline; this may be due to reversal of flow direction and/or dilution. Similar observations have been made for years in the 100-Area of Cr(VI) concentrations in response to the spring runoff.

Studies of Cr(VI) reduction in river water (Świetlik, 2002, “Kinetic Study of Redox Processes of Chromium in Natural River Water”) indicate Cr(VI) reduction rates with a half-life ($t_{1/2}$) on the order of 2–19 hours, indicating that Cr(VI) will be fully reduced in a river within a day to a week’s time. Because of the river-stage changes, river water of differing chemistry is brought into contact with the near-field groundwater system adjacent to the river. This “rinsing” action allows the geochemical properties of the aquifer matrix to be refreshed, and allows for continued geochemical reduction, adsorption, and precipitation of contaminated groundwater upon contact with the sediment when the river stage drops and groundwater flows towards the river.

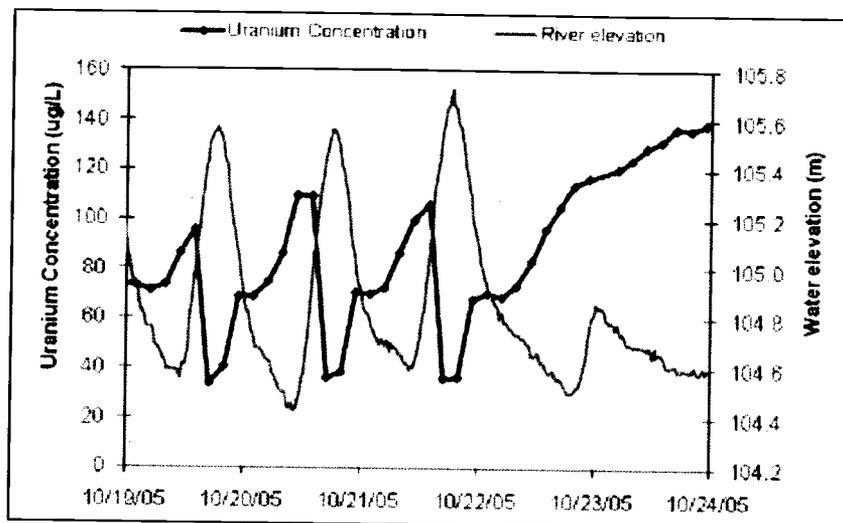


Figure 3-10. Relationship of Uranium Concentration to River Stage in the 300 Area Hyporheic Zone

An important addition to our understanding of the fate and transport of Cr(VI) is that in addition to chemical reduction of Cr(VI) to Cr(III) the reduction also may occur biologically, mediated by bacteria. Chandler et al. (1997), "Phylogenetic Diversity of Archaea and Bacteria in a Deep Subsurface Paleosol," described the wide variety of microbes present in the Hanford subsurface. Their studies focused on the VZ. A number of studies have been conducted on deeper Hanford bacteria in the groundwater. Recent studies of 100-H Area groundwater microbial ecology (Han et al., 2010, *Physiological and Transcriptional Studies of Cr(VI) Reduction Under Aerobic and Denitrifying Conditions by an Aquifer-Derived Pseudomonad*) suggest that bacteria can use multiple electron donors to reduce Cr(VI), depending on whether conditions are aerobic or anaerobic. PNNL-18784, *Hanford 100-D Area Biostimulation Treatability Test Results*, described results from biostimulation treatability tests at 100-D. They observed that following the injection of a carbon substrate, "...microbial activity and ability to reduce the targeted species were observed throughout the monitored zone." These general mechanisms are described in the *Chromium(VI) Handbook* (CRC Press, 2005).

A field study conducted by Washington Closure Hanford (WCH-380, *Field Summary Report for Remedial Investigation of Hanford Site Releases to the Columbia River, Hanford Site, Washington*) in 2010 involved the collection of pore water samples under extremely low-stage river-stage conditions. The study included preliminary mapping and measurement of site contaminants in sediment, pore water, and surface water in areas where groundwater upwelling occurred. Trident probe and associated river-stage-specific sampling was used to collect samples of pore water at 20 to 31 cm (8 to 12 in.) below the riverbed surface. Sediment coring and grab sampling techniques were then used concurrently with the Trident probe to assess the likelihood of potential ecological risk where contaminated groundwater was found entering the river. In total, 972 sample locations were measured. Groundwater upwelling locations were mapped using conductivity and temperature at 685 sample locations. Study results showed groundwater upwelling was not uniformly distributed, and varied by water depth, season, and proximity to the shoreline. Evaluation of laboratory quality assurance/quality control (QA/QC) results indicates that a number of initially high values were unsubstantiated due to laboratory analysis issues coupled with poor comparison to low total Cr values. Pore-water samples collected from the hyporheic zone in the river-bed sediments indicate that total Cr is occasionally present in the river substrate at selected locations and is detected above aqueous WQS both near shore and offshore. However, the Trident probe measurement

methodology collects a sample within tens of minutes and does not meet the 4-day criteria to estimate the Criterion Continuous Concentration (CCC). [The CCC is an estimate of the highest concentration of a material in surface water to which an aquatic community can be exposed indefinitely without resulting in an unacceptable effect.]

Review of the geochemistry of the aquifer matrix and groundwater at the 100-HR-3 and 100-KR-4 OUs indicates the presence of conditions that favor moderate amounts of reduction, adsorption, and precipitation of Cr(VI). PNNL-14202, *Mineralogical and Bulk-Rock Geochemical Signatures of Ringold and Hanford Formation Sediments*, conducted mineralogical studies of the Ringold formation and the Hanford formation. The results of these studies suggest that both formations contain sufficient iron, mica, and other critical components to be able to foster Cr(VI) reduction as well as adsorption of the anionic Cr(VI) species to positively charged surfaces such as along the edges of mica sheets and related clay weathering products. While these mechanisms act continuously in the aquifer, they are not likely to have a statistically significant measurable impact on highly contaminated Cr(VI) plumes; however, as active remediation such as pump-and-treat systems operate and Cr(VI) concentrations in the aquifer decline, these mechanisms become significant at lower concentrations.

Very high concentrations of Cr(VI) at the main hotspot in the 100-D South plume and relatively high concentrations in the adjacent 100-D North plume continue to be problematic. The DR-5 pump-and-treat system has removed relatively large amounts of Cr(VI) from just four extraction wells in this area; however, impact on the overall footprint of the plumes from DR-5 operation is minimal. The In Situ Redox Manipulation (ISRM) Barrier, which enhances the natural reductive capacity of the aquifer through the addition of sodium dithionite, was installed downgradient of the south plume in Year 2000. The barrier has exhibited uneven performance, although it appears to work well at the upstream end where the aquifer is thicker, and the concentrations in the aquifer are lower along the east margin of the plume. Immediately downgradient of the hotspot, there is breakthrough of the plume. Most likely, the barrier is reducing Cr(VI) at a fairly steady rate across the length of the barrier, or at least per unit thickness of aquifer. At the location where the aquifer is thinner and the concentrations are higher, the reduction capacity is likely being exceeded, resulting in the observed break through.

An important outcome of the Expert Panel study (SGW-39305, 2008) was the recommendation to assess the 1:1 factor within the context of the U.S. Environmental Protection Agency (EPA) guidance on attenuation¹. As the EPA guidance notes, the primary mechanism for attenuation of Cr(VI) is the natural reduction in the environment in the presence of iron and enhanced by bacteria. Additional attenuation can occur via chemical precipitation and adsorption to mineral grains. Biostimulation of bacterial growth via addition of carbon substrates is a common method of accelerating this reduction. However, the ambient bacterial population will still generate Cr(VI) reduction at some rate.

The Expert Panel on groundwater-surface water interaction correctly noted that much of the flow within the aquifer adjacent to the hyporheic zone is likely to be laminar flow. Some mixing will occur under these conditions; however, this is likely to be relatively minimal owing to local variations in hydraulic conductivity. The main mechanism will be the transgression and regression of river water through the hyporheic zone and into the adjacent aquifer. This movement must obey the usual rules of flow within a potential field such as that found in groundwater; consequently, the resulting movement will be much like piston flow with river water invading and receding from the formation. The significance of this action is

¹ The interim groundwater cleanup target for Cr(VI) in the pump and treat system (22 µg/L) have been set with the expectation that the groundwater discharging to the river will be subject to at least a 1:1 dilution, which will result in concentrations below the ambient freshwater aquatic life chronic toxicity target value of 11 µg/L.

that the geochemical reduction capacity of the aquifer matrix is refreshed with each successive wave of fresh water that pulses through the aquifer. Some adsorption likely occurs, although it is probably limited given the $\text{Cr}_2\text{O}_4^{2-}$ forms the majority of the Cr. Adsorption sites in the more concentrated portions of the plumes are likely saturated until remediation has advanced to a point where enough Cr(VI) has been removed from the system to free up binding sites. This may allow Cr precipitates such as $\text{Cr}(\text{OH})_3$ to be removed as particles.

The EPA guidance recommends evaluating concentrations along a flow path and estimating the attenuation that is occurring. A good example is looking at the margins of the diffuse plume in the Horn area between 100-D and 100-H. Figure 3-11 shows the evolution of Cr(VI) and specific conductance along an approximate streamline through wells 699-97-45 and 699-99-44 and aquifer tube C6288. In the wells in the aquifer, specific conductance is constant at about 420 microsiemens per centimeter ($\mu\text{S}/\text{cm}$) while Cr(VI) drops from 55 to 45 micrograms per liter ($\mu\text{g}/\text{L}$). Further downgradient at the aquifer tube, specific conductance has dropped to about 220 $\mu\text{S}/\text{cm}$ and Cr(VI) to 12 $\mu\text{g}/\text{L}$. Typical specific conductance in the river is 100–125 $\mu\text{S}/\text{cm}$; a river effect is apparent. The specific conductivity has dropped in half. If the same mechanism was operating on the Cr(VI), the expected value might be closer to 22 than 12 $\mu\text{g}/\text{L}$, suggesting that other mechanisms are impacting Cr(VI) concentrations.

The main factors of Cr(VI) attenuation are chemical and biological factors of reduction, precipitation, and adsorption. Reduction occurs within the aquifer and appears to be enhanced where river water refreshes the geochemical sites on the aquifer matrix in and adjacent to the hyporheic zone. Pore-water samples collected from the hyporheic zone in river-bed sediments indicate that Cr(VI) is occasionally present in the river substrate at selected locations at concentrations that exceed the ambient water quality criterion.

3.2.4 Historical Discharges and Unintended Releases

Irradiated uranium fuel production at the 100 Area sites containing the original eight reactors generated large volumes of effluent wastewater over a span of 22 years. Reactor processes were similar at all eight reactors leading to similar waste products at all sites. The primary generating process for these wastes was the production, use and disposal of reactor cooling water. Maximum quantities of cooling water were used because cooling water passed through each system once and was then discharged, hence the description of these reactors as single pass reactors.

To generate cooling water, several processes were needed. First, river water was collected and treated to remove impurities. Then other chemicals were added to enhance cooling water performance. After passage through the reactor, cooling water was discharged directly into the Columbia River or diverted to a series of retention basins and trenches to allow for short-term radioactive decay and cooling before discharge into the Columbia River. Fluid losses from the various facilities used to generate and transfer coolant after use were common occurrences. The fraction of total coolant and other waste volumes that discharged directly into the Columbia River versus into the subsurface through leaking facilities is not well known. However, leaking fluid volumes from retention basins, storage tanks, trenches, cribs and pipelines were sufficient to create and sustain groundwater mounds underneath them throughout operations. The fluids contained additive chemicals and radionuclides from ruptured fuel elements. These constituents have been and continue to be the primary sources of groundwater contamination. The most widespread subsurface contaminant is Cr, which was added to minimize corrosion of aluminum cooling pipes in the reactor cores. Cumulative estimates of coolant volumes and Cr inventory at each of the reactors are shown in Table 3-9.

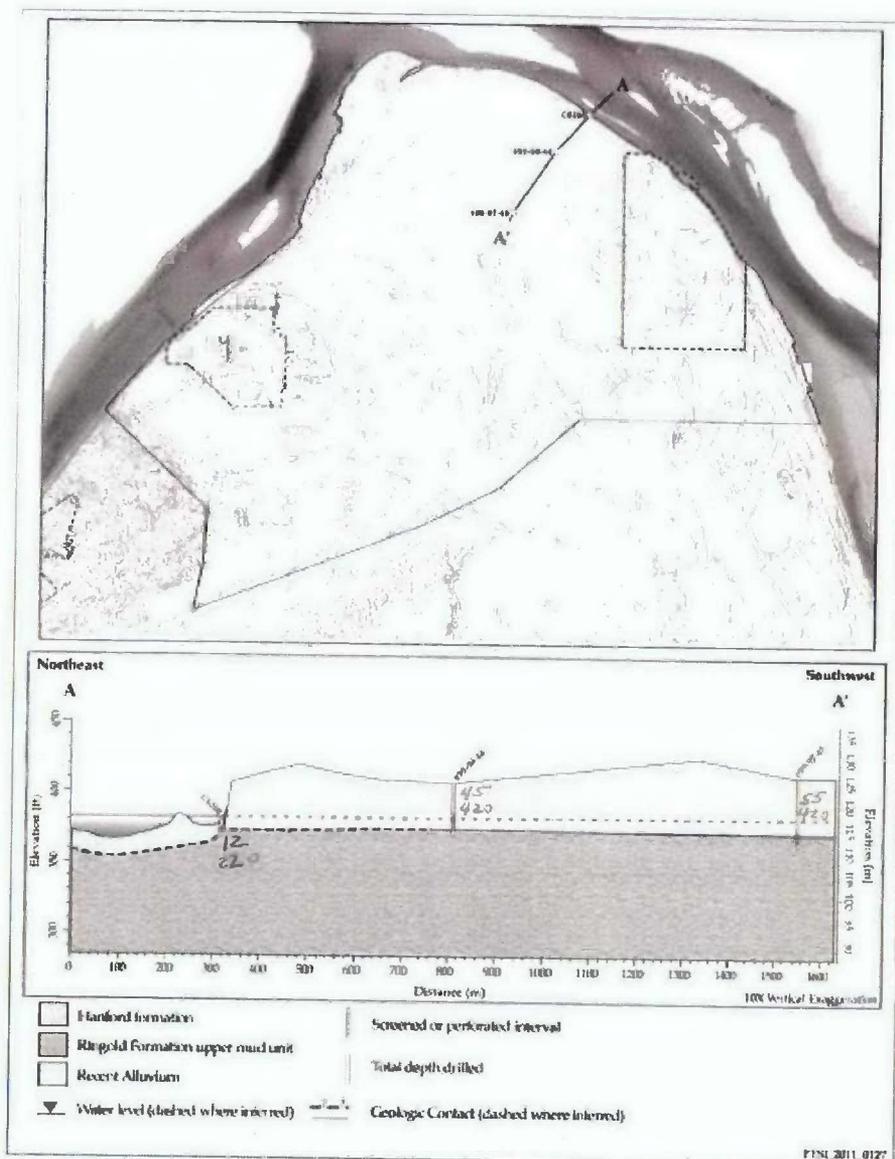


Figure 3-11. Cross Section Along a Streamline in the Horn Area Showing Cr(VI) Concentration (upper number) and Specific Conductance (lower number) as Groundwater Discharges to the Columbia River

Table 3-9. Cumulative Reactor Coolant Volumes and Cr Quantities Used in Single Pass Reactor Operations

Reactor	Operations Period	Coolant Volume (L)	Cr(VI) Inventory (kg)
B and C	1944-1969	5.3E+12	2.8E+6
KE and KW	1955-1971	1.2E+13	6.3E+6
D and DR	1944-1967	4.5E+12	2.6E+6
H	1949-1965	2.1E+12	1.4E+6
F	1945-1965	2.3E+12	1.6E+6

In addition to reactor coolant, decontamination fluids and gas purification condensates were discharged. The decontamination fluids were generated by cleanup of reactor parts and typically contaminated with nitric and chromic acid and radionuclides. Finally, raw water basins leaked extensively into the subsurface and influenced the local groundwater flow patterns significantly.

In the following sections, the large discharge storage and disposal facilities are described. Where available for historical record, waste fluid types, fluid volumes, and estimates of Cr and total radionuclide inventories are summarized.

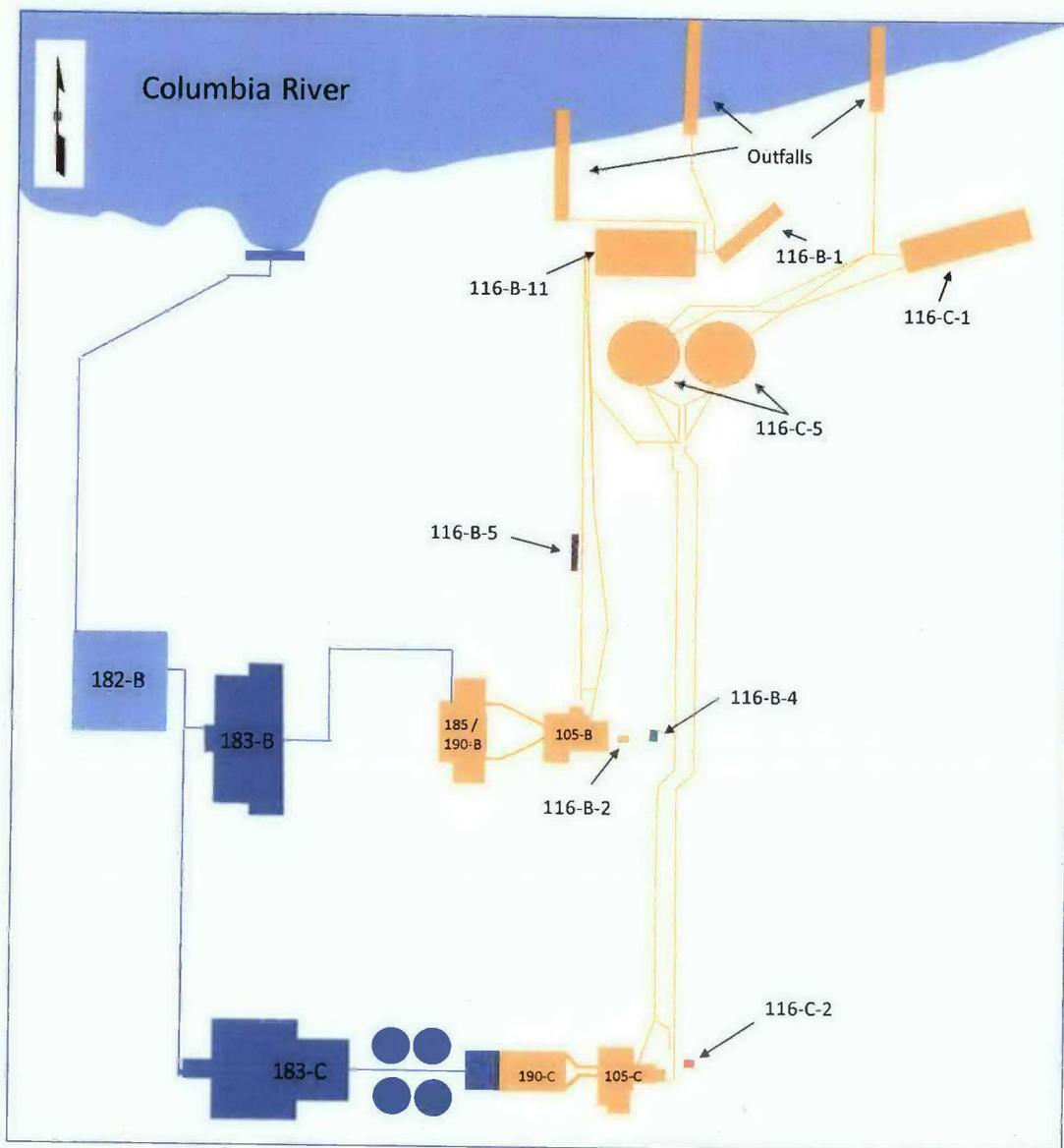
3.2.4.1 100-BC Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD3 Rev 0, *Integrated 100 Area Remedial Investigation/Feasibility Study Work Plan Addendum 3: 100-BC-1, 100-BC-2, and 100-BC-5 Operable Units*. The major structures used to create, use, and dispose of reactor coolant at the 100 B/C Area are shown in Figure 3-12. River water was pumped and stored in the 182-B reservoir prior to transfer to 183-B and 183-C. At 183-B and 183-C, Columbia River water was purified and transferred to 190-B and 190-C, respectively, where sodium dichromate was added. Concentrated sodium dichromate starting materials, first as solids (until the mid-1950s at 105-C and around 1960 at 105-B) and then solutions, were stored at 190-B and 190-C and added to the purified Columbia River water to make reactor coolant. Some loss of the highly concentrated sodium dichromate solution occurred around the storage tank at 183-C.

The reactor coolant was then routed through the reactors (105-B and 105-C) and piped to either the 116-B-11 or 116-C-5 retention basins. From these facilities, most of the coolant was then discharged to the river through three outfalls. Because of intermittent overflow of the retention basins or decisions to sequester specific coolant volumes contaminated by exposure to ruptured fuel elements, reactor coolant was also routed to the 116-B-1 and 116-C-1 trenches. An additional discharge event occurred during early operations (1946) in which highly contaminated fuel storage basin water was discharged to the 116-B-2 trench. Leaks were ubiquitous in pipelines and the retention basin. However, the fraction of discharged volume that entered the Columbia River versus leakage into the VZ through infrastructure leaks is not known.

Decontamination solutions were typically discharged into cribs such as 116-B-4 (shown in Figure 3-12) 116-B-3, 116-B-6A and 116-B-6B. Reported cumulative discharge volumes at these sites are less than a million L except for 116-B-4 (10 million L). A unique set of waste streams were sent to the 116-B-5 trench, including wastewater from tritium production in the early 1950s and then laboratory waste associated with ruptured fuels examination.

Characteristics of the discharged liquids are summarized in Table 3-10. Small volume Cr discharges have also been reported, including an accidental discharge of concentrated sodium dichromate solution (53,980 L) into the sewer at 183-C in 1966 (4,000 kg in 4,000 L), and small quantities of chromic acid to the 116-B-6A/6B crib (a total of 38 kg of Cr [PNL-6456, *Hazard Ranking System Evaluation of CERCLA Inactive Waste Sites at Hanford*]). A mixture of radionuclides has been measured frequently in characterized soils including cesium-137, strontium-90, cobalt-60, europium isotopes, and uranium isotopes.



Color Key: facilities for management of reactor coolant: supply, use, and disposal; discharge cribs.

Figure 3-12. Map of Major 100 B/C Area Liquid Storage and Discharge Locations

Table 3-10. Liquid Discharge Characteristics at the Major 100 B/C Area Sites

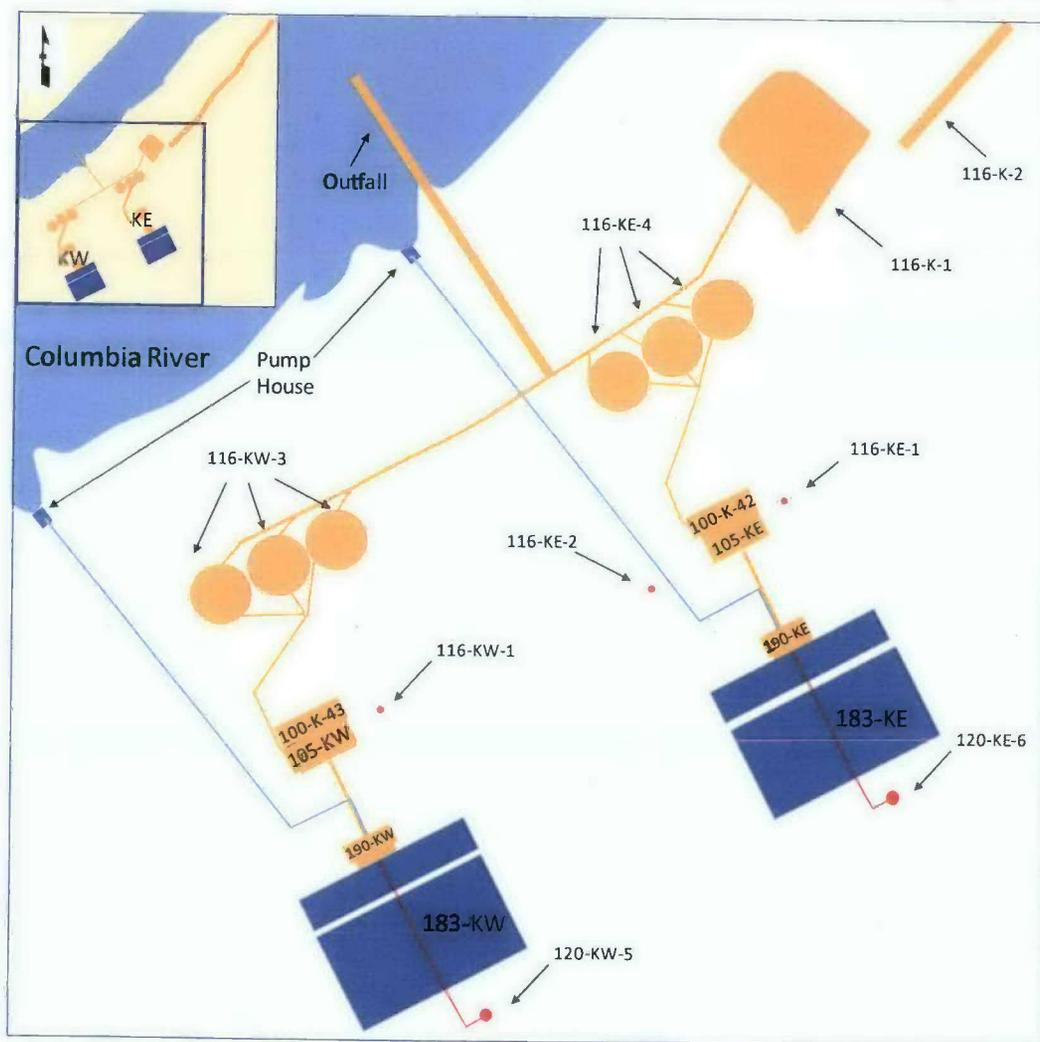
Facility	Waste Characteristics	Contaminant Inventory
116-B-1 Trench	<u>Operation Period:</u> 1946-1955 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 6E+7 L	<u>Chromium:</u> 23 kg <u>Radionuclides:</u> 3.1 Ci
116-B-2 Trench (Fuel Storage Basin Trench)	<u>Operation Period:</u> 1946 <u>Waste Type:</u> Fuel Storage Basin Coolant <u>Discharge Volume:</u> 4E+6 L	<u>Chromium:</u> No estimate <u>Radionuclides:</u> 15 Ci
116-B-4 Trench	<u>Operation Period:</u> 1957-1968 <u>Waste Type:</u> Decontamination Fluids <u>Discharge Volume:</u> 3E+5 L	<u>Chromium:</u> 380 kg <u>Radionuclides:</u> 2 Ci
116-B-5 Crib	<u>Operation Period:</u> 1950-1968 <u>Waste Type:</u> Tritium Production Waste, Laboratory Waste <u>Discharge Volume:</u> 1E+7 L	<u>Chromium:</u> None <u>Radionuclides:</u> 190 Ci of tritium as of 1988
116-B-11 Retention Basin	<u>Operation Period:</u> 1944-1968 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate
116-C-1 Trench	<u>Operation Period:</u> 1952-1968 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 1E+8 to 7E+8 L plus 1968 Infiltration Test Water Volume of 1E+10 L	<u>Chromium:</u> 38 kg <u>Radionuclides:</u> 150 Ci
116-C-2 Crib	<u>Operation Period:</u> 1952-1968 <u>Waste Type:</u> Reactor Coolant, Decontamination Fluids <u>Discharge Volume:</u> 7.5E+6 L	<u>Chromium:</u> 376 kg <u>Radionuclides:</u> < 1 Ci
116-C-5 Retention Basins	<u>Operation Period:</u> 1952-1969 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate

3.2.4.2 100-K Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD2, *Integrated 100 Area Remedial Investigation/Feasibility Study Work Plan Addendum 2: 100-KR-1, 100-KR-2, and 100-KR-4 Operable Units*. The major structures used to create, use, and dispose of reactor coolant at the 100 K Area are shown in Figure 3-13. Two reactors (105-KW and 105-KE) were constructed and operated with separated systems for creating reactor coolant. Columbia River water was pumped at two pump houses, one for each reactor, and transferred to 183-KW and 183-KE. At 183-KW and 183-KE, This water was purified and transferred to 190-KW and 190-KW, respectively, where sodium dichromate was added. Concentrated sodium dichromate liquid starting materials were stored in tanks (120-KW-5 and 120-KE-6)

next to the 183-KW and 183-KE sedimentation basins. Some losses of the highly concentrated sodium dichromate solution occurred around the storage tanks (120-KW-5 and 120-KE-6) during transfer from railroad cars. These losses are presumed to be the primary sources of the maximum groundwater concentration zones underlying the reactors. The high concentration solutions were then piped underneath these basins to a mixing tank at 190-KW and 190-KE. Two dilution steps were completed to make up reactor coolant concentrations.

The reactor coolant was then routed through the reactors (105-KW and 105-KE) and piped to the 116-KW-3 or 116-KE-4 retention basins, respectively. From these facilities, coolant was then discharged to either the 116-K-1/116-K-2 system or the river through the 1908 outfall. Leaks were ubiquitous in pipelines and retention basins. Estimates at 116-KE-4 were on the order of 57,000 to 114,000 L/min. The 116-K-2 trench also overflowed frequently. Other much smaller liquid waste discharges to cribs were condensate from reactor gas purification systems (116-KE-1 and 116-KW-1) and cleanup column waste from the 1706-KER facility that was used to test the performance of various reactor components.



Color Key: facilities for management of reactor coolant supply, use, and disposal; concentrated sodium dichromate liquid storage tanks.

Figure 3-13. Map of Major 100 K Area Liquid Storage and Discharge Locations

Characteristics of the discharged liquids are summarized in Table 3-11. The great majority of fluids discharged to the Columbia River or the retention basin/trench system were reactor coolants. Because of extensive leakage of these systems and variable Cr content over time, the fraction of Cr that discharged directly into the Columbia River versus the subsurface is uncertain. The estimate for the 116-K-2 facility (300,000 kg) is an approximation for the VZ discharge, and constitutes about 5% of the total amount used during operations of 105-KW and 105-KE. The estimated radionuclide releases from reactor coolant, fuel storage basin coolant, and decontamination fluids are also dominated by the 116-K-2 trench estimate of about 2,100 Ci. Primary radionuclides in this estimate include europium isotopes, nickel-63, and cesium-137. The gas purification system condensate contained mostly carbon-14 and tritium, and the cleanup column waste contained a mixture of fission products including cobalt-60, strontium-90, and europium isotopes.

Table 3-11. Liquid Discharge Characteristics at the Major 100 K Area Sites

Facility	Waste Characteristics	Contaminant Inventory
116-K-1 Crib	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 4E+7 L	<u>Chromium:</u> 15 kg <u>Radionuclides:</u> 46 Ci
116-K-2 Trench	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Reactor Coolant, Fuel Storage Basin Coolant <u>Discharge Volume:</u> 3E+11 L	<u>Chromium:</u> 114,000 kg <u>Radionuclides:</u> 2,100 Ci
116-KE-1 Crib	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Gas Purification System Condensate <u>Discharge Volume:</u> 8E+5 L	<u>Chromium:</u> 0 kg <u>Radionuclides:</u> < 240 Ci (C-14, H-3)
116-KW-1 Crib	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Gas Purification System Condensate <u>Discharge Volume:</u> 8E+5 L	<u>Chromium:</u> 0 kg <u>Radionuclides:</u> < 240 Ci (C-14, H-3)
116-KE-2 Crib	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Cleanup Column Waste from Reactor Component Tests <u>Discharge Volume:</u> 3E+6 L	<u>Chromium:</u> 0 kg <u>Radionuclides:</u> 38 Ci
116-KW-3 and 116-KE-4 Retention Basins	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate (extensive leakage)	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate
120-KE-6 and 120-KW-5 Sodium Dichromate Storage Tanks	<u>Operation Period:</u> 1955-1971 <u>Waste Type:</u> Reactor Coolant, Decontamination Fluids <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> 0 Ci

3.2.4.3 100-D Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD1, *Integrated 100 Area Remedial Investigation/Feasibility Study Work Plan Addendum 1: 100-DR-1, 100-DR-2, 100-HR-1, 100-HR-2, and 100-HR-3 Operable Units*. The major structures used to create, use, and dispose of reactor coolant at the 100 D Area are shown in Figure 3-14. Coolant production went through a number of modifications over time. In all cases, the process began with pumping Columbia River water and storing it in the 182-D reservoir prior to transfer to 108-D until about 1950, and thereafter to 183-D and 183-DR. At these facilities, the river water was treated to reduce total dissolved solids in preparation for the addition of Cr and other chemicals to make reactor coolant.

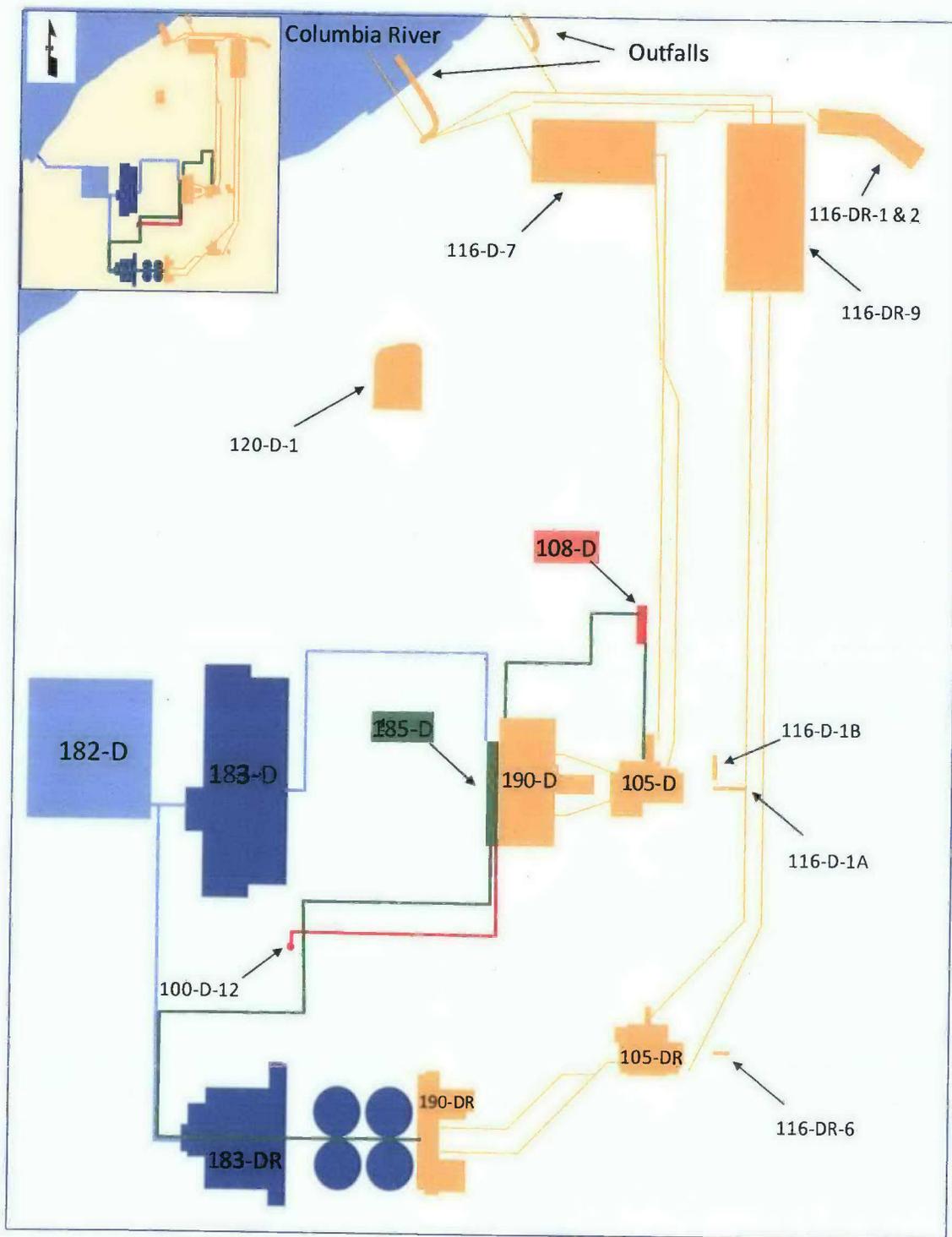
The initial sodium dichromate preparation process was done at 108-D between 1944 and 1950. Crystalline sodium dichromate was dissolved in water to make up the so-called 10% to 15% solution containing about 43 to 64 g/L of Cr, and then piped either to 105-D directly or to 185-D and 190-D where mixing with the treated Columbia River water caused additional dilution of Cr to about 700 µg/L. This diluted solution was then pumped through reactor 105-D.

After 1950, 108-D was eliminated from the coolant production process, and at some point, starting materials were switched from solids to liquids with Cr concentrations of about 466 g/L, referred to as the 70% solution. Around 1959–1960, the 100-D-12 transfer station was built, which is where the 70% solution was supplied by rail car and tankers. This solution was then pumped to storage tanks at 185-D and diluted to the 10% to 15% solution. For coolant supply to 105-D, the 10% to 15% solution was again diluted to the 700 µg/L level as it passed through 190-D and into the 105-D reactor. For coolant supply to 105-DR, the 10% to 15% solution was piped to 183-DR and then 190-DR for mixing with Columbia River water to achieve the 700 µg/L reactor coolant levels.

Following passage through the reactors, coolant was pumped to a retention basin system and to associated smaller cribs. The facilities receiving the bulk of the reactor coolant volume are listed in Table 3-12 with Cr estimates where available. Most fluids went to the retention basins and then directly to the outfalls. Piping and basin structures leaked extensively, and some fraction of the total volume went directly into the subsurface in quantities sufficient to create and sustain groundwater mounds under these facilities. A notable exception to this practice was a deliberate coolant discharge event in 1967 when three months' worth of coolant production ($1.3E+10$ L) was deliberately discharged into 116-DR 1 & 2 in an attempt to provide a longer transport path to the Columbia River. This event propagated a large plume eastward across the Horn. Discharges at the 100-D-12 transfer station are also listed in Table 3-12 because the 70% solution was regularly discharged into a French drain at the end of a transfer process when rail cars were sluiced after the bulk of the fluids had been transferred into the transfer station. The volume of clean out fluids discharged in this manner is not quantifiable, but hundreds to thousands of kilograms of Cr could have gone down the French drain because of maximum concentrations in the 70% solution. Several hundred thousand kilograms of Cr were transferred through 100-D-12.

Other large volumes of uncontaminated water were released at the 120-D-1 Pond and from a leaking 182-D Reservoir which is still operating. Discharge and leakage has been sufficient to create and sustain groundwater mounds underneath these facilities.

Characteristics of the discharged liquids are summarized in Table 3-12. The major contaminant in these facilities is Cr with variable amounts of radionuclides. A mixture of radionuclides has been measured frequently in characterized soils including cesium-137, strontium-90, cobalt-60, europium isotopes, and uranium isotopes.



Color Key: facilities for management of reactor coolant supply, use, and disposal; concentrated sodium dichromate liquid storage tanks; sodium dichromate dilution.

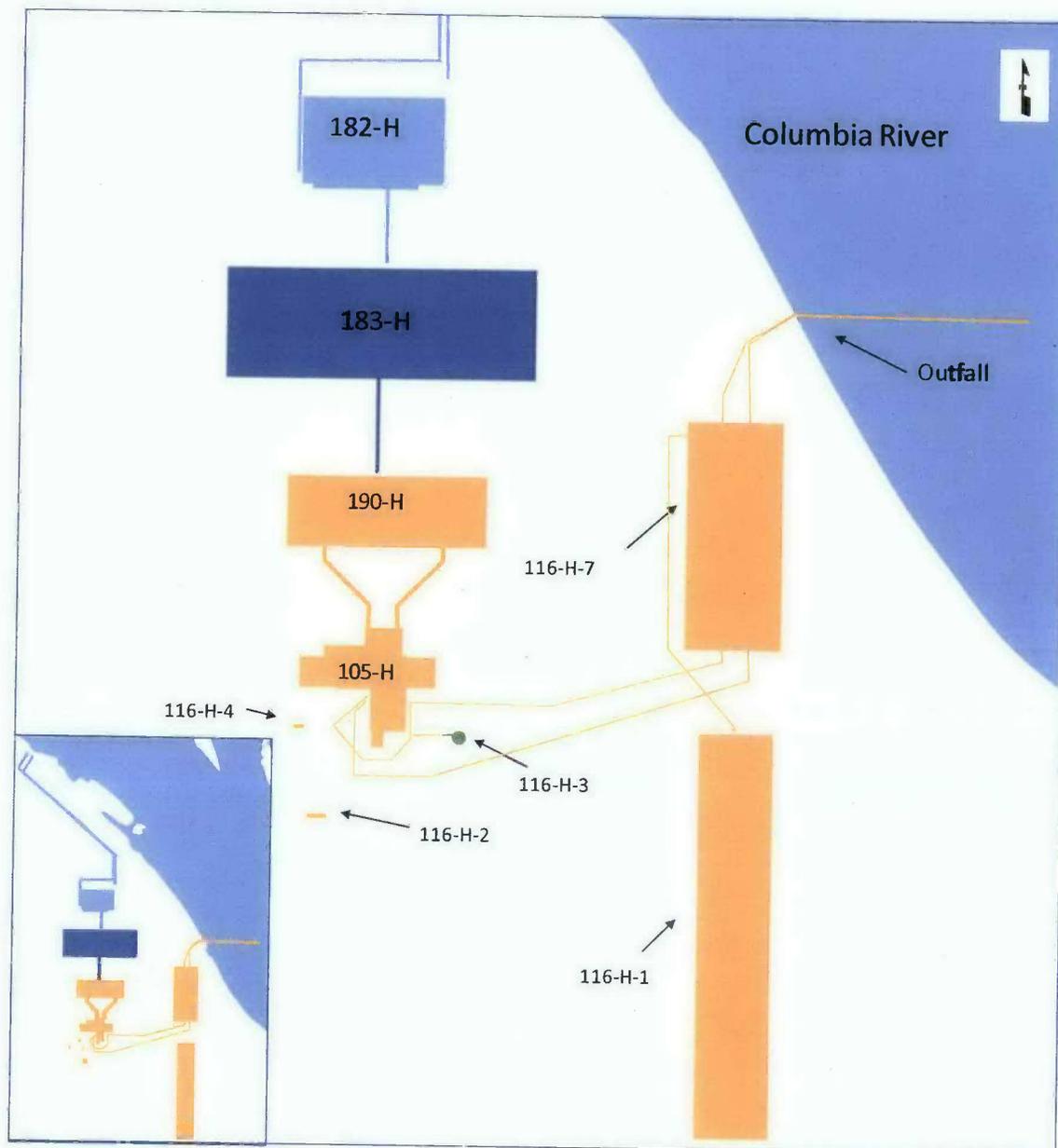
Figure 3-14. Map of Major 100 D Area Liquid Storage and Discharge Locations

Table 3-12. Characteristics of Significant Liquid Discharges at the 100 D Area Sites

Facility	Waste Characteristics	Contaminant Inventory
116-D-1A Trench	<u>Operation Period:</u> 1947-1952 <u>Waste Type:</u> Fuel Storage Basin Coolant <u>Discharge Volume:</u> 2E+5 L	<u>Chromium:</u> 380 kg <u>Radionuclides:</u> 4.7 Ci
116-D-1B Trench	<u>Operation Period:</u> 1953-1967 <u>Waste Type:</u> Fuel Storage Basin Coolant, Reactor Coolant <u>Discharge Volume:</u> 8E+6 L	<u>Chromium:</u> 266 kg <u>Radionuclides:</u> 2.6 Ci
116-D-7 Retention Basin	<u>Operation Period:</u> 1944-1967 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> 5-400 Ci
116-DR-9 Retention Basin	<u>Operation Period:</u> 1950-1967 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> 5-400 Ci
116-DR-1 & 2 Trench	<u>Operation Period:</u> 1950-1967 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 4E+7 L (does not include the volume [1.3E+10 L] discharged intentionally in 1967)	<u>Chromium:</u> 30 kg <u>Radionuclides:</u> 3.1 Ci
116-DR-6-Trench	<u>Operation Period:</u> 1953-1965 <u>Waste Type:</u> Reactor Coolant and Decontamination Fluid <u>Discharge Volume:</u> 7E+6 L	<u>Chromium:</u> 0.8 kg <u>Radionuclides:</u> No estimate
120-D-1 Pond	<u>Operation Period:</u> 1977-1994 <u>Waste Type:</u> Filtered Water from 183-D Sand Filter and 185/189 <u>Discharge Volume:</u> 2E+9 L	<u>Chromium:</u> None <u>Radionuclides:</u> None
100-D-12 Transfer Station	<u>Operation Period:</u> 1959-1965 <u>Waste Type:</u> Concentrated Sodium Dichromate <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> No estimate <u>Radionuclides:</u> None

3.2.4.4 100-H Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD1. The major structures used to create, use, and dispose of reactor coolant at the 100-H Area are shown in Figure 3-15. River water was pumped and stored in the 182-H reservoir prior to transfer to 183-H. Columbia River water was purified at 183-H and transferred to 190-H where sodium dichromate was added. Concentrated sodium dichromate starting materials, first as solids (until 1959) and then solutions, were stored at 190-H and added to the purified Columbia River water to make reactor coolant. Unlike processes at the 100-D and 100-K Areas, there is no indication of concentrated sodium dichromate leaks or discharges into the subsurface.



Color Key: facilities for management of reactor coolant supply, use, and disposal; French drain discharge.

Figure 3-15. Map of Major 100 H Area Liquid Storage and Discharge Locations

The reactor coolant was then routed through the reactor (105-H) and piped to the 116-H-7 retention basin. From this facility, most of the coolant was then discharged to the river, primarily through the 1904-H (116-H-5) outfall. Because of intermittent overflow of the 116-H-7 retention basin, reactor coolant was also routed to the 116-H-1 trench. An additional discharge route was also used early in the operations period in which reactor coolant used to cool fuel in the fuel storage basin at the reactor was routed to the 116-H-4 crib (1950–1952). Leaks were ubiquitous in pipelines and the retention basin. However, the fraction of discharged volume that entered the Columbia River is not known. Decontamination solutions were typically discharged into the 116-H-3 French drain and sometimes mixed with reactor coolant pumped through the 116-H-7 retention basin.

Characteristics of the discharged liquids are summarized in Table 3-13. The major contaminant in these facilities is Cr with variable amounts of radionuclides. The high inventory for the 116-H-3 French drain may indicate a chromic acid component in the decontamination fluids. Mixtures of radionuclides have been measured frequently in characterized soils, including cesium-137, strontium-90, cobalt-60, europium isotopes, and uranium isotopes.

Table 3-13. Characteristics of Significant Liquid Discharges at the 100 H Area Sites

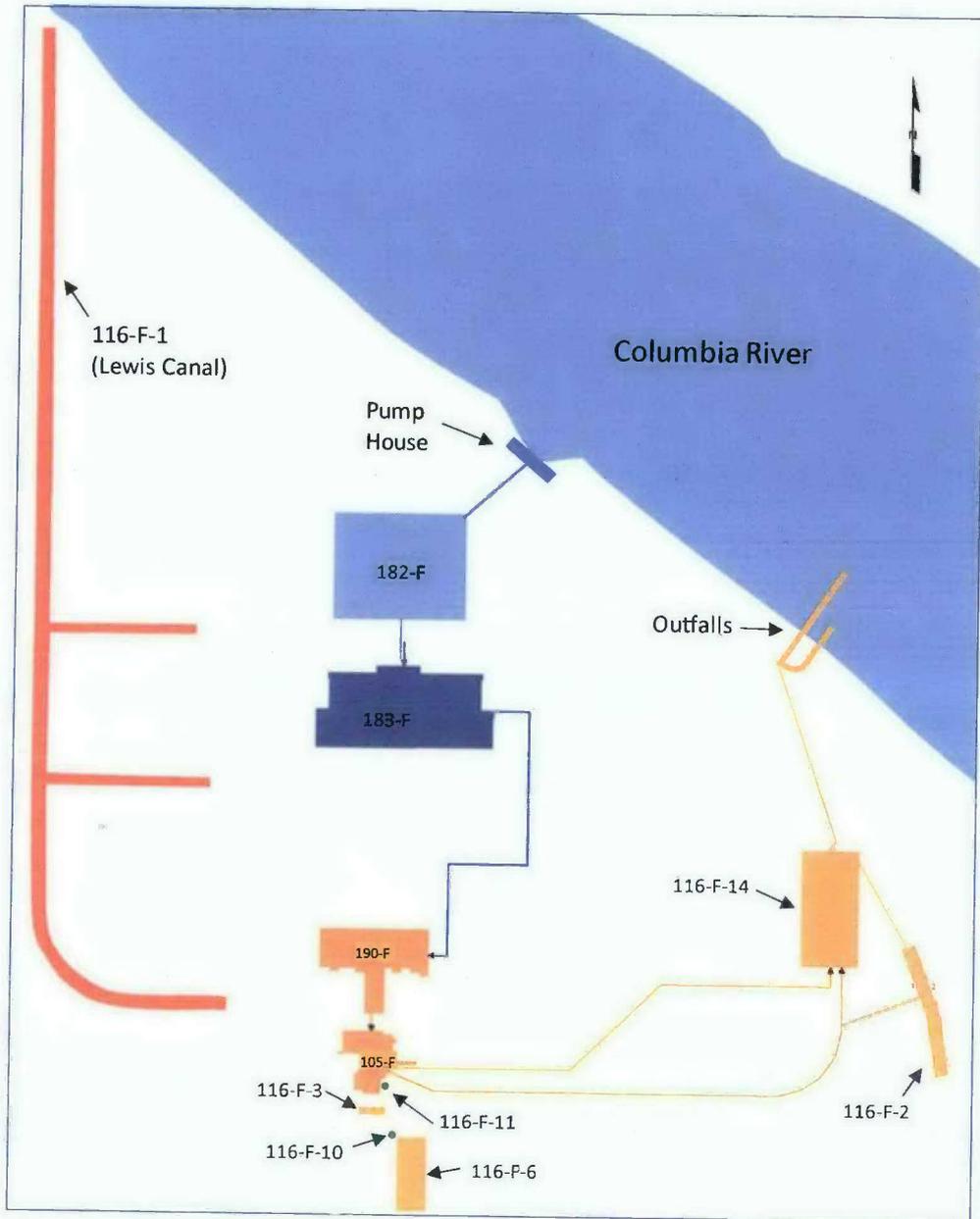
Facility	Waste Characteristics	Contaminant Inventory
116-H-1 Trench	<u>Operation Period:</u> 1952-1965 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 9E+7 L	<u>Chromium:</u> 60 kg <u>Radionuclides:</u> 33 Ci
116-H-2 Trench	<u>Operation Period:</u> 1953-1965 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 6E+8 L	<u>Chromium:</u> 400 kg <u>Radionuclides:</u> 1.4 Ci
116-H-3 French Drain	<u>Operation Period:</u> 1950-1965 <u>Waste Type:</u> Decontamination Fluids <u>Discharge Volume:</u> 4E+5 L	<u>Chromium:</u> 1330 kg <u>Radionuclides:</u> 0.07 Ci
116-H-4 Crib	<u>Operation Period:</u> 1950-1952 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> No estimate	<u>Chromium:</u> 466 kg <u>Radionuclides:</u> 270 Ci in 1953
116-H-7 Trench	<u>Operation Period:</u> 1949-1965 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 4E+7 L	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate

3.2.4.5 100-F Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD4, *Integrated 100 Area Remedial Investigation/Feasibility Study Work Plan Addendum 4: 100-FR-1, 100-FR-2, 100-FR-3, 100-IU-2, and 100-IU-6 Operable Units*. The major structures used to create, use, and dispose of reactor coolant at the 100-F Area are shown in Figure 3-16. River water was pumped and stored in the 182-F reservoir prior to transfer to 183-F. Columbia River water was purified at 183-F and transferred to 190-F, where sodium dichromate was added. Concentrated sodium dichromate starting materials, first as solids (until 1959) and then solutions, were stored at 190-F and added to the purified Columbia River water to make reactor coolant. Unlike processes at the 100-D and 100-K Areas, there is no indication of concentrated sodium dichromate leaks or discharges into the subsurface.

The reactor coolant was then routed through the reactor (105-F) into the 100-F-19 pipeline system to either the 116-F-4 retention basin, and to a much smaller extent, to the Lewis Canal (116-F-1). From these facilities, most of the coolant was then discharged to the river, primarily through the 1904-F (116-F-8) outfall. Because of intermittent overflow of the 116-F-4 retention basin, reactor coolant was also routed to the 116-F-2 trench. An additional discharge route was also used early in the operations period in which reactor coolant used to cool fuel in the fuel storage basin at the reactor was routed to the 116-F-3 crib (1947-1951). Leaks were ubiquitous in pipelines and the retention basin. However, the fraction of

discharged volume that entered the Columbia River is not known. Decontamination solutions were typically discharged into the Lewis Canal and the 116-F-10 and 116-F-11 French drains.



Color Key: facilities for management of reactor coolant supply, use, and disposal; French drain discharge; Lewis Canal.

Figure 3-16. Map of Major 100 F Area Liquid Storage and Discharge Locations

Characteristics of the discharged liquids are summarized in Table 3-14. Cr estimates for 116-F-2 appears to be conservatively high. Cr concentrations in reactor coolant were highest early in the operations period and were typically about 0.7 mg/L. Assuming this value and the reported discharge volumes, the Cr mass estimate from 116-F-2 would be 42 kg. The high inventory for the 116-3 trench may indicate a chromic acid component in the decontamination fluids. A mixture of radionuclides has been measured frequently

in characterized soils, including cesium-137, strontium-90, cobalt-60, europium isotopes, and uranium isotopes.

Table 3-14. Liquid Discharge Characteristics at the Major 100 F Area Sites

Facility	Waste Characteristics	Contaminant Inventory
116-F-1 Trench (Lewis Canal)	<u>Operation Period:</u> 1953-1965 <u>Waste Type:</u> Reactor Coolant, Decontamination Fluid <u>Discharge Volume:</u> 1E+8 L	<u>Chromium:</u> 40 kg <u>Radionuclides:</u> 3.4 Ci
116-F-2 Trench	<u>Operation Period:</u> 1950-1965 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 6E+7 L	<u>Chromium:</u> 228 kg <u>Radionuclides:</u> 15 Ci
116-F-3 Trench	<u>Operation Period:</u> 1947-1951 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 7E+6 L	<u>Chromium:</u> 1.5 kg <u>Radionuclides:</u> 0.0021 Ci
116-F-6 Trench	<u>Operation Period:</u> 1952-1965 <u>Waste Type:</u> Reactor Coolant <u>Discharge Volume:</u> 1E+5 L	<u>Chromium:</u> No estimate <u>Radionuclides:</u> 6.5 Ci
116-F-10 French Drain	<u>Operation Period:</u> 1948-1965 <u>Waste Type:</u> Decontamination and Radioactive Liquid Water Rinses <u>Discharge Volume:</u> 4E+5 L	<u>Chromium:</u> 760 kg <u>Radionuclides:</u> 6.5 Ci
116-F-11 French Drain	<u>Operation Period:</u> 1953-1965 <u>Waste Type:</u> Decontamination Fluids <u>Discharge Volume:</u> 2E+5 L	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate
116-F-14 Retention Basin	<u>Operation Period:</u> 1945-1965 <u>Waste Type:</u> Reactor Coolant, Fuel Storage Basin Coolant <u>Discharge Volume:</u> 8.2E+10 to 1.6E+11 L	<u>Chromium:</u> No estimate <u>Radionuclides:</u> No estimate

3.2.4.6 100-N Area Liquid Discharges

The information summarized here is taken from DOE/RL-2008-46-ADD5, *Integrated 100 Area Remedial Investigation Feasibility Study Work Plan Addendum 5 100-NR-1 and 100-NR-2 Operable Units*.

The majority of contaminant mass released to the environment was dissolved or suspended as particulates in various fluids discharged to LWDFs near the reactor, primarily 116-N-1 (1301-N) LWDF and 116-N-3 (1325-N) LWDF. Throughout the reactor operations period and for some time afterward, these facilities received liquid waste. The majority of the discharge volume went to 116-N-1 (1301-N) LWDF from 1964 to late 1985 and the remainder went to 116-N-3 (1301-N) LWDF from 1983 into 1993. The major type of fluids included the following:

- Reactor coolant and periphery cooling systems bleed off
- Reactor primary coolant loop decontamination rinse solution

- Spent fuel storage basin cooling water overflow
- Building drains where radioactive solutions were generated and disposed

With the exception of the primary coolant loop decontamination rinse solution, which was generated every 2 to 4 years (Groundwater Impact Assessment Report for the 1325-N Liquid Waste Disposal Facility [WHC-EP-0675]), all solutions were generated and discharged continuously. The coolant fluids and basin fluids were the primary sources of LWDF discharge (see Figure 4- 1, adapted from WCH-0675).

These fluids became contaminated by contact with ruptured fuel elements and subsequent dissolution of readily dissolvable isotopes. The fluids were piped from the N Reactor or the fuel storage basin to the 1322-N Facility, then to the 13 10-N Storage Facility or the cribs, depending on the contamination levels. Fluids with unacceptably high contamination levels went to 13 10-N and were transported by rail to the 200 Area for disposal.

3.2.5 Modeling Assumptions

Various modeling assumptions are made to perform the PRG and SSL calculations. Some of the key assumptions are:

- The vadose zone is considered homogeneous in nature, within the stratigraphic cross sections developed for the simulations, without consideration to the presence of thin finer-grained material, which can retard the downward migration of contaminants.
- Groundwater is assumed to have negligible mixing with the Columbia River. In calculating the values for surface water protection, the point of compliance is assumed at the groundwater below the waste site. No attenuation or decay of contaminants is assumed between the source area and the groundwater or the river.
- The vadose zone is assumed to be fully or partially contaminated depending on the distribution coefficient of the contaminant. For fully contaminated vadose zone scenario, two nodes above the water table were kept clean to avoid numerical issues due to boundary effects. This scenario is referred as effective fully contaminated in this document. The SSL calculations use an irrigation recharge scenario but the PRG calculations use native vegetation recharge scenario based on reestablishment of natural infiltration.
- A linear equilibrium sorption isotherm is assumed to describe the sorption behavior of the contaminants of interest. The linear adsorption model, or K_d approach, is a useful and practical approach for modeling contaminant adsorption in transport performance assessments (PNNL-14576, *Applicability of the Linear Sorption Isotherm Model to Represent Contaminant Transport Processes in Site-Wide Performance Assessments*). Conditions exist for which this empirical approach is invalid, e.g., situations involving reactive transport (e.g., uranium transport the 300 Area), or where the concentrations of chemical parameters change rapidly within a small spatial zone (e.g., under a leaking high-level waste tank). However, evaluation of the contaminants of interest for the 100 Area and waste site conceptual site models does not reveal such situations, and the K_d approach is assumed a valid approximation of sorption behavior for this model.
- The calculations apply a derived K_d for Cr(VI) of 0.8 mL/g, which is taken from the lower end of the empirical cumulative distribution function based on the results of the batch leach testing at the 100 Area (ECF-Hanford-11-0165, *Evaluation of Hexavalent Chromium Leach Test Data Conducted on Vadose Zone Sediment Samples from the 100 Area*) and summarized below in Section 3.3.4. This is

therefore a bounding value that is applied to represent the residual fraction of Cr(VI) only that remains in the vadose zone after remediation; it does not apply to the more mobile fraction that has generally already migrated to groundwater prior to remediation. For all other contaminants of interest, K_d values will be defined by other environmental calculation files, with justification, for application in this model.

- The initial conditions for matric potential at the start of the flow and transport simulations represent a wetter vadose zone than is expected for such gravel-dominated sediments in an arid climate, thus allowing significantly higher water and solute flux values.
- The median hydraulic gradient value for each source area may be too small for waste sites near the Columbia River and may be several times too large for waste sites that are far inland from the river.
- In the modeling, revegetation of the area (from bare soil condition) is assumed to start after five years, with bare soil present for the first five years. This assumption results in more water infiltrating to the vadose zone than may actually occur.
- A minimum saturated aquifer thickness of 5 m is assumed.
- The longitudinal dispersivity in the transport calculations is set to zero to maximize the peak concentration in the groundwater.

Due to several of the above-mentioned conservative choices, the SSL and PRG concentrations are deemed to be bounding estimates (i.e., lead to the lowest reasonable threshold concentrations).

3.3 Nature and Extent of Contamination

This section presents an overview of the nature and extent of contamination by geographic area to be simulated with the model. This discussion is not comprehensive in the manner that will be presented in the RI reports to be prepared for these OUs, but does present sufficient information that is necessary to guide the development of this model. The term “contaminants of interest” is used to indicate those contaminants considered to aid in the development of this model because of prevalent groundwater contamination. This term is used cautiously because it is not the function of this model package report to identify COPCs or COCs: that will be the function of the RI reports for these OUs.

3.3.1 Geographic Area-specific Distribution of Contaminants in Vadose Zone

The 100 Area RI/FS process has identified and characterized residual contamination within the VZ. As a potential source of contamination to groundwater and the environment, understanding the distribution of contaminants in the subsurface is critical to developing numerical models to support risk assessment. The discussion is broken up into two parts. First, the general distribution of contaminants at each geographic area in the 100 Area is summarized. The summaries are based on information used to develop the work plans for each geographic area. Second, data collected as part of the RI/FS process are used to illustrate observed contaminant levels in the soil column in contrast to soil background levels, and where available the calculated SSL and final PRG values. The SSL and PRG values are calculated using Equation 2-1 and discussed in Section 5.2.

In discussing contaminants of interest specific to the areas below, note that lower mobility contaminants (that is, K_d values greater than about 1.0 mL/g) are the focus for model development because this model is constructed to address residual vadose zone contaminant still present. Higher mobility contaminants have

generally migrated to groundwater before the present, and consequently are not the focus for model development. This model will be used address to address the full range of K_d values for all contaminants to be evaluated. As discussed later, the Cr(IV) K_d bounding value selected (0.8 mL/g) is a value that pertains only to the residual fraction of Cr(VI) that remains in the soil after remediation. A K_d value at, or near, zero would be more appropriate to model past migration of the more mobile fraction of Cr(VI) that has already migrated to groundwater.

3.3.1.1 100-BC Vadose Zone Contaminant Distribution

Characterization of the 100-BC geographic area included field investigations of over 29 high-priority waste sites. Strontium-90, Cr(VI), and tritium were identified as contaminants of interest for groundwater within the 100-BC geographic area (DOE/RL-93-37, *Field Investigation Report for the 100-BC-5 Operable Unit*; DOE/RL-2008-46-ADD3). Characterization showed that waste sites that received enough liquid effluent to impact groundwater have contamination at varying levels throughout most of the VZ, especially for the more mobile contaminants. Contaminants with low contaminant distribution coefficients (near zero), such as Cr(VI), have migrated through the VZ and into the groundwater when the waste sites were operational. Where remediation has been completed, residual amounts of Cr(VI) exist in the VZ. However, limited data are available to quantify the quantities and distribution of mobile contaminants, including nitrate, tritium, and Cr(VI) in the VZ. Concentrations of less mobile contaminants generally decrease with depth below the disposal facility. Some waste sites only received small amounts of dilute liquids and are generally found to have soil contamination extending limited distances into the VZ beneath waste sites (i.e., burial grounds, reactor structures, and some unplanned releases).

In general, the following can be stated concerning the extent of contamination in the 100-BC geographic area based on contaminant soil-water partitioning coefficient (DOE/RL-2008-46-ADD4):

- **High soil partitioning contaminants:** The highest soil contaminant concentrations are expected within and near the point of release. Sufficiently high volumes of liquids discharged into a waste site can increase the vertical extent of contamination in the vadose zone. Where little or no liquid effluents were discharged to a waste site, soil contamination is expected to remain within and only slightly below the point of release.
- **Low soil partitioning contaminants:** The highest soil contaminant concentrations are expected to be away from the point of release but elevated levels may continue through the vadose zone to groundwater, depending on the discharge volume and infiltration rate. Soil contaminant levels generally decrease with depth, but contamination can be found at higher levels in lenses of fine materials. Limited data are available to evaluate vertical contaminant distribution behavior for several contaminants including nitrate, tritium, and Cr(VI).

3.3.1.2 100-K Vadose Zone Contaminant Distribution

The distribution of contaminants below high-volume remediated liquid waste disposal sites in the 100-K geographic area are highest at the bottom of the disposal facility and generally decrease with depth. Some of the contaminants are arsenic, total Cr, Cr(VI), mercury, lead, Cs-137, Co-60, Eu-152, Ni-63, Pu-239/240, U-238, and U-233/234. Soil samples collected and analyzed during interim remedial actions indicate residual contamination is located well above the water table and periodically re-wetted zone (the part of VZ that is saturated periodically due to river stage fluctuations). Waste sites that received small amounts of liquid are generally found to have soil contamination extending limited distances into the VZ

beneath the waste sites (i.e., burial ground, some unplanned releases, and liquid sites). Adverse impacts to groundwater are not expected from these sites (DOE/RL-2008-46-ADD2).

3.3.1.3 100-D, H Vadose Zone Contaminant Distribution

Cr(VI) is the principal environmental threat in 100-D/H geographic area. Other contaminants that are potential risks to human health and ecological receptors such as, arsenic, nitrate, tritium, U-233/234, U-235, and U-238, Tc-99, and Sr-90 are also present (DOE/RL-2008-46-ADD1). Field data indicate that contaminant distributions at high volume liquid waste sites like 116-DR-1&2 are highest near the bottom of the engineered structure, and generally decrease with depth but with occasional increases in contamination throughout the VZ. Soil samples collected at this site indicate that most of the contamination is high above the water table and does not exceed remedial action goals. However, soil data have not been collected throughout the VZ to make a complete assessment of contaminant distribution. Waste sites that received small amounts of dilute liquids are generally expected to have soil contamination extending limited distances into the VZ beneath waste sites (i.e., burial grounds, reactor structures, and some unplanned releases). There is little reason to believe that groundwater was impacted at waste sites that received minimal discharges. Field data from 116-DR-1&2 and 116-H-1 indicate that contaminant concentrations at high-volume liquid waste sites for contaminants (e.g., arsenic, total Cr, mercury, Cr(VI), lead, Cs-137, Co-60, Eu-152, Ni-63, Pu-239/240, U-238, and U-233/234) are highest at the bottom of the waste site and generally decrease with depth with observed sporadic increases throughout the VZ. Soil samples collected and analyzed during interim remedial actions (Borehole B8786 at 116-DR-1&2) indicate that residual contamination is located above the water table and the periodically re-wetted zone (DOE/RL-2008-46-ADD1).

3.3.1.4 100-F Vadose Zone Contaminant Distribution

Contaminants of interest for the 100-F geographic area include arsenic, Cr(VI), manganese, nitrate/nitrite, strontium-90, and tritium (DOE/RL-93-83, *Limited Field Investigation Report for the 100-FR-3 Operable Unit*). Contaminant profiles for sediments below the 116-F-4 crib and 116-F-14 retention basin indicate that contaminant concentrations generally decrease with depth, with the exception of total Cr. Higher concentrations are generally present between 1.5 to 3 m (10 ft.) bgs and are associated with the bottom of the engineered structure (DOE/RL-2008-46-ADD4).

3.3.1.5 100-N Vadose Zone Contaminant Distribution

The primary environmental threat in the 100-N geographic area is strontium-90 but six contaminants are identified in the sampling and analysis plan (DOE/RL-2009-42, *Sampling and Analysis Plan for the 100-NR-1 and 100-NR-2 Operable Units Remedial Investigation/Feasibility Study*). The highest concentrations of strontium-90 were found in surface sediments of the 116-N-1 and 116-N-3 cribs and the 116-N-1 trench. An estimated 2,454 Ci of strontium-90 was released to the 100-N cribs and trenches during reactor operations (DOE/RL-2008-46-ADD5, *Integrated 100 Area Remedial Investigation Feasibility Study Work Plan Addendum 5 100-NR-1 and 100-NR-2 Operable Units*). The acidic nature of the discharge (pH less than 2) at 100-N may have increased the mobility of the strontium-90 (HW-34499, *Adsorption and Retention of Strontium by Soils of the Hanford Project*; HW-56582, *Influence of Limestone Neutralization on the Soil Uptake of Sr-90 from a Radioactive Waste*). The effects can be observed in historic groundwater measurements with some wells recording pH levels around 2.0 (e.g., 199-N-14 in 1993) and several others exhibiting pH around 5. Operational conditions are considered to be potential drivers for the areal extent of the strontium-90 plume estimated at 100-N. Concentrations of

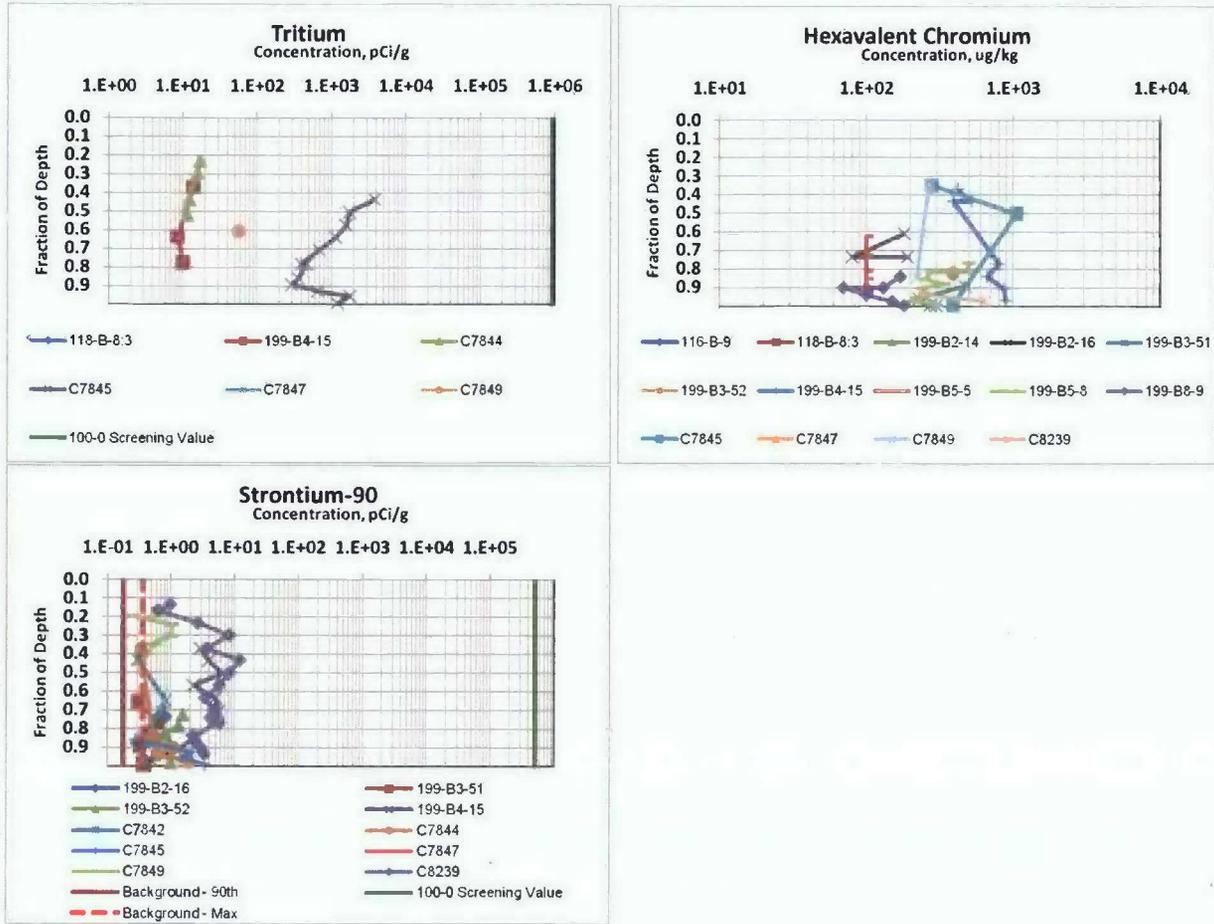
other less-mobile contaminants generally decrease with depth below the disposal structure. The available data indicate that residual concentrations of strontium-90 and tritium remain in the VZ (DOE/RL-2008-46-ADD5).

3.3.2 RI/FS Borehole Data

Several contaminants have been identified in the 100 Area Groundwater OUs. Table 3-15 lists the contaminants of interest for the Groundwater OUs in the 100 Area. As part of developing the RI/FS, VZ samples were collected from a variety of locations within the 100 Area. The selection of the locations was biased towards high-risk waste sites in order to increase the likelihood that existing contamination could be located. At the time of publishing this report, 33 soil borings with samples in the VZ were available. Borings in this dataset were taken from the 100-D, 100-H, 100-K, 100-F, and 100-BC geographic areas. Figure 3-17 through Figure 3-21 consist of scatter plots of observed contaminant concentrations versus fraction of depth below ground surface to the observed water table. The figures also include indicators of the background concentrations (DOE/RL-92-24, *Hanford Site Background*; PNNL-18577, *A Review of Metal Concentrations Measured in Surface Soil Samples Collected on and Around the Hanford Site*; ECF-Hanford-11-0038, *Soil Background Data for Interim Use at the Hanford Site*) and regulatory levels (ECF-Hanford-11-0063, *STOMP 1-D Vadose Zone Modeling for Determination of Preliminary Remediation Goals for 100 Area D, H, and K Source Operable Units*) for comparison purposes. Only analytical results for which detectable levels of contaminants were found were included in the figures. In most cases where background values were available, more than half of the measurements for all geographic areas were measured below this level, however, concentration of some contaminants exceed the background levels. In the case of strontium-90, the majority of detectable measurements were above background; however, the concentration levels of strontium-90 are orders of magnitude below SSLs and PRGs (when calculated) in all geographic areas. The details of SSL and PRG calculations are presented in Section 5.2. The zone of contamination for most contaminants, including Cr(VI), extends through lower half of the VZ thickness.

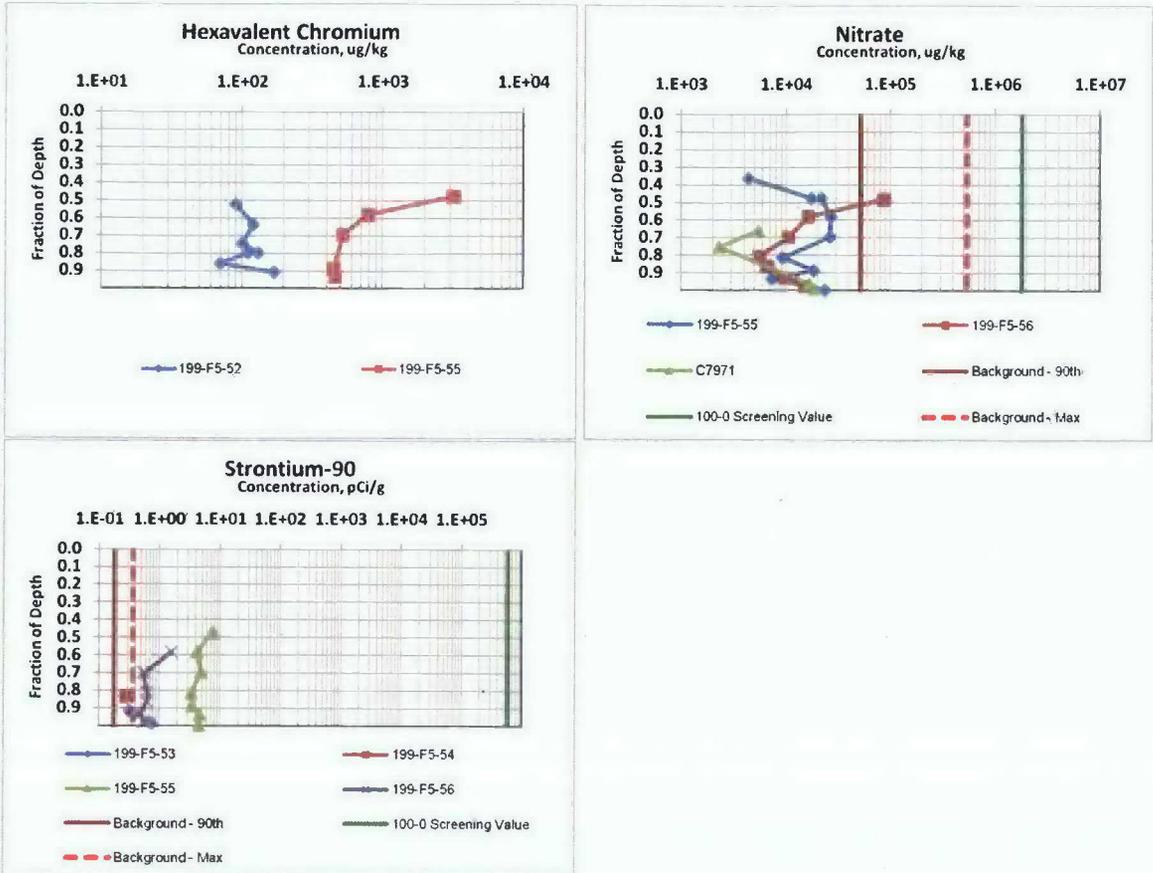
Table 3-15. Contaminants of Interest In the 100 Area Groundwater OUs

Contaminant	100-HR-3			100-BC-5	100-FR-3
	100-KR-4	100-D Source Exposure Area	100-H Source Exposure Area		
Carbon tetrachloride					X
Carbon-14	X				
Chromium	X	X			
Hexavalent chromium	X	X	X	X	X
Manganese					X
Nitrate	X	X			X
Nitrite					
Strontium-90	X	X	X	X	X
Sulfate		X			
Trichloroethene					X
Tritium	X			X	



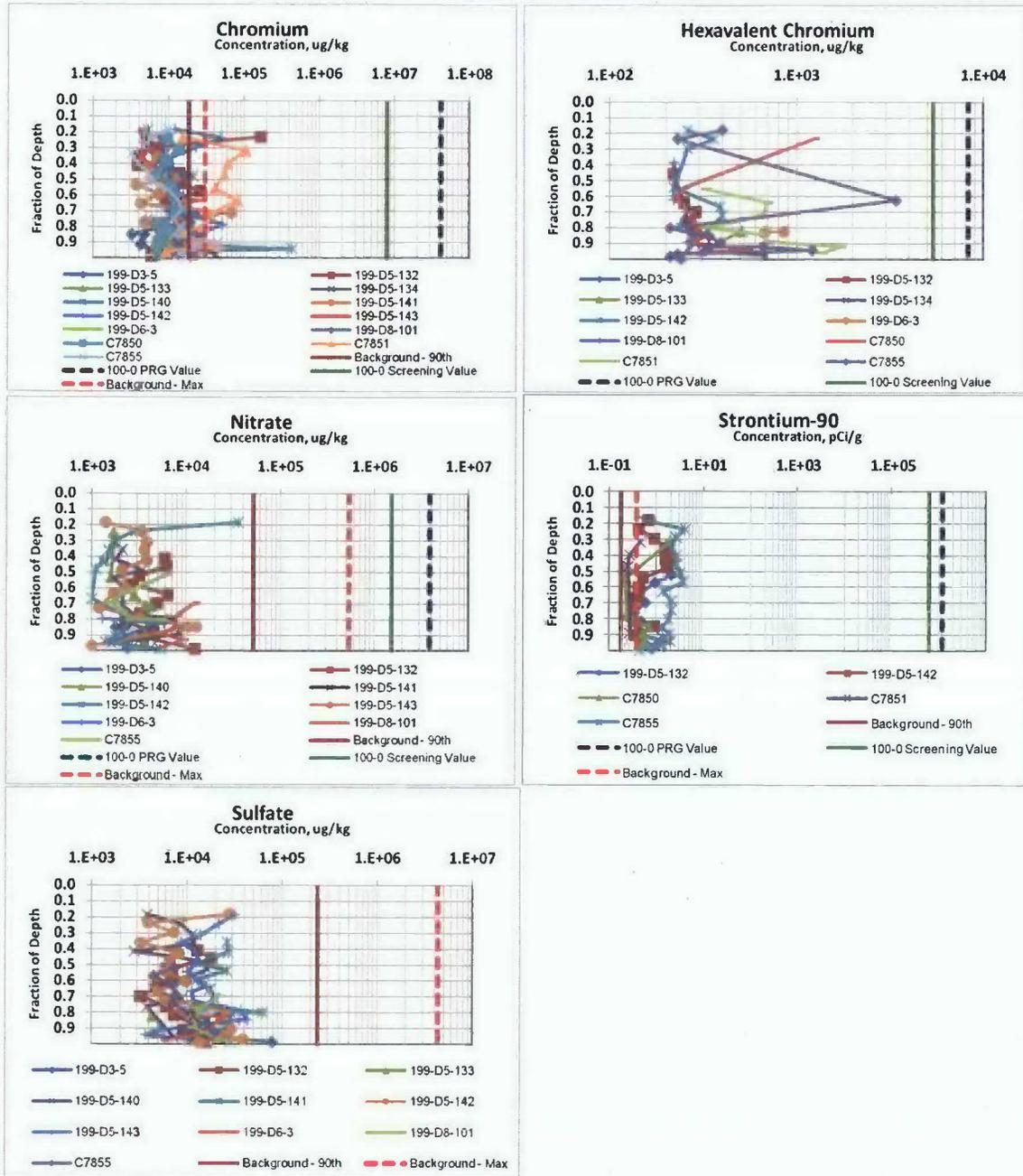
Note: SSL and PRG values, wherever shown, are based on smaller of the surface water and groundwater PRG values. These values may have changed in the latest revision of the environmental calculations.

Figure 3-17. Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-BC Geographic Area where a Detectable Concentration was Registered



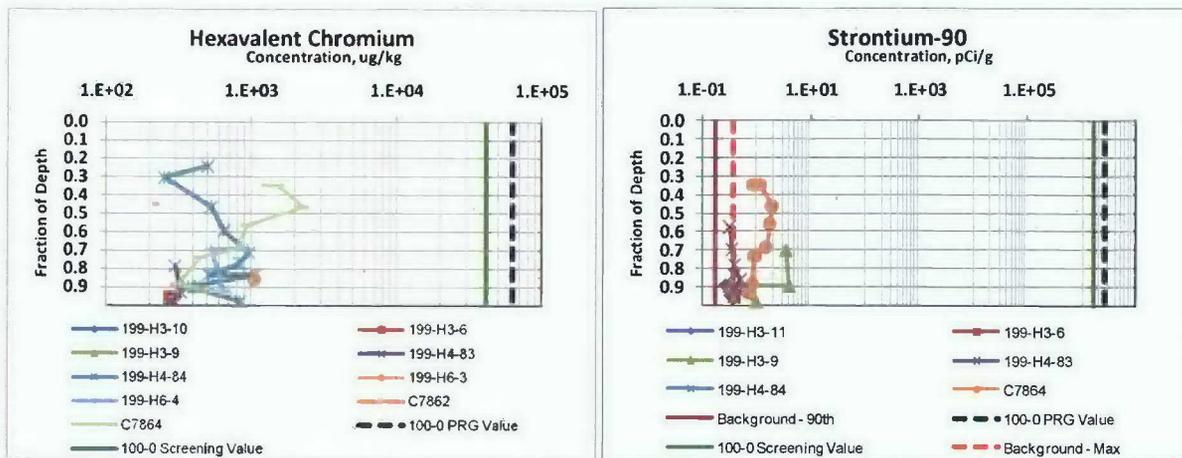
Note: SSL and PRG values, wherever shown, are based on smaller of the surface water and groundwater PRG values. These values may have changed in the latest revision of the environmental calculations.

Figure 3-18. Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-F Geographic Area where a Detectable Concentration was Registered



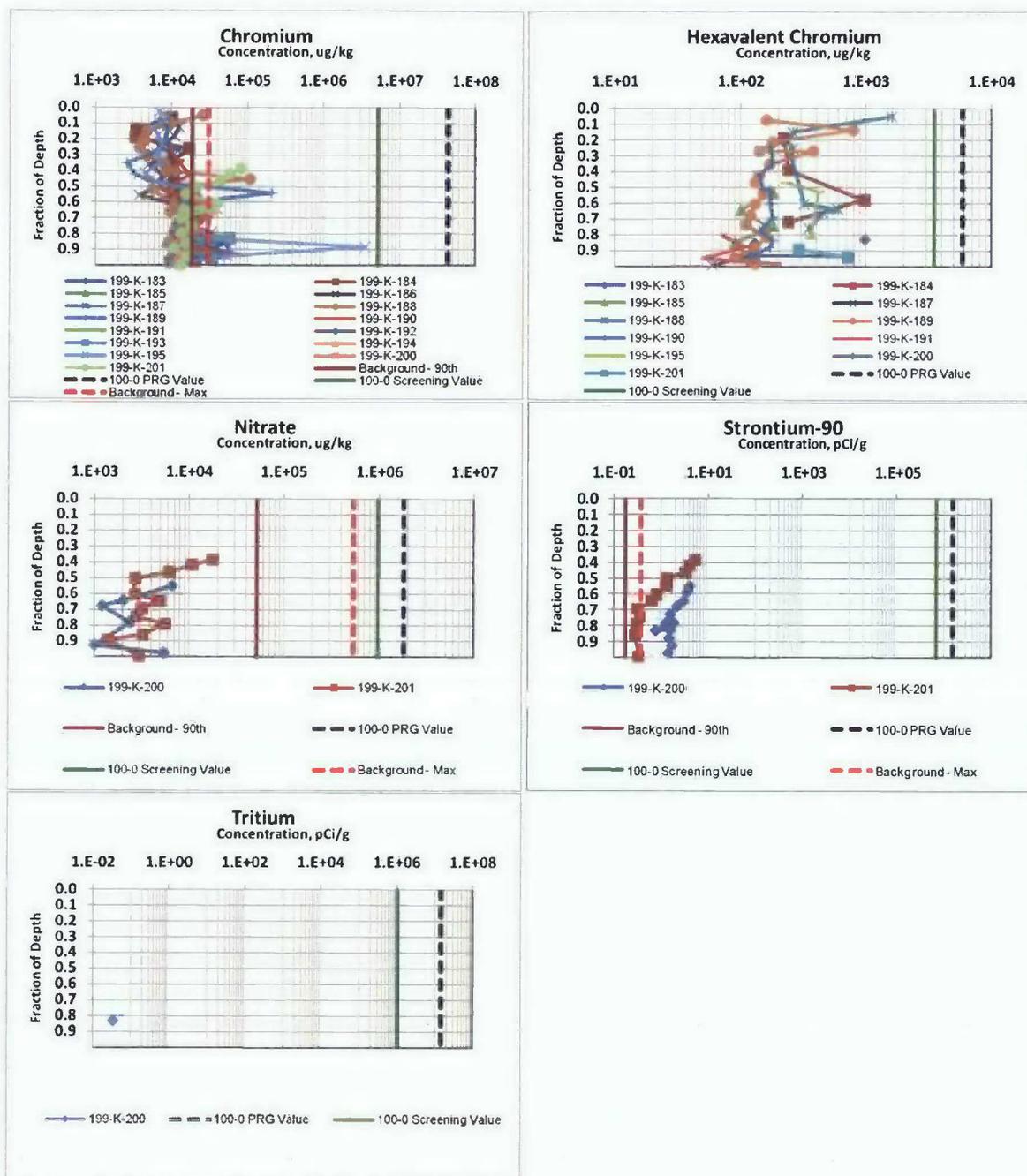
Note: SSL and PRG values, wherever shown, are based on smaller of the surface water and groundwater PRG values. These values may have changed in the latest revision of the environmental calculations.

Figure 3-19. Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-D Geographic Area where a Detectable Concentration was Registered



Note: SSL and PRG values, wherever shown, are based on smaller of the surface water and groundwater PRG values. These values may have changed in the latest revision of the environmental calculations.

Figure 3-20. Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-H Geographic Area where a Detectable Concentration was Registered



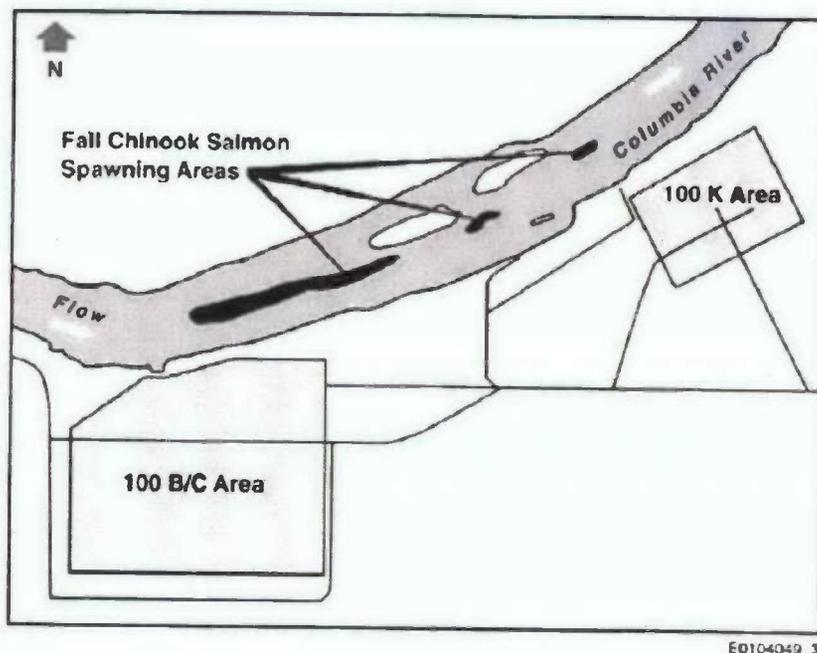
Note: SSL and PRG values, wherever shown, are based on smaller of the surface water and groundwater PRG values. These values may have changed in the latest revision of the environmental calculations.

Figure 3-21. Contaminant Concentrations Plotted against the Fraction of the Depth within the VZ for all Wells in the 100-K Geographic Area where a Detectable Concentration was Registered

3.3.3 Cr(VI) Distribution in Vadose Zone and Aquifer

Cr(VI) is a common contaminant in the subsurface at reactor operations locations in the 100 Areas along the Columbia River. It is present because the compound sodium dichromate was routinely added to reactor cooling water to inhibit metal corrosion of the piping system. The significance of this contaminant is linked to concern for salmon and other aquatic life in the Columbia River. Fall Chinook salmon

spawning areas have been observed near 100-BC (Figure 3-22). Shoreline areas provide rearing habitat for young salmon and steelhead, as well as for many of the other species of fish in the river (DOE/RL-2005-40, *100-BC Pilot Project Risk Assessment Report*). Historical records show that Cr(VI)-bearing materials (mostly liquids) were released into the subsurface during the addition of sodium dichromate to cooling water for use in the reactors and after cooling water use in the reactors. Cr(VI) concentrations in cooling water were set at maximum levels (about 700 µg/L) during early operations because the concentration needed for adequate corrosion inhibition was not well understood. Over time, reactor operations determined that lower concentrations (about 350 µg/L) were adequate. After a single pass through these reactors, the cooling waters were discharged to the surrounding environment by various routes.



Source: DOE/RL-2005-40

Figure 3-22. Approximate Location of Fall Chinook Spawning Areas

The low concentrations of residual Cr(VI) in the VZ soils and the widespread groundwater distribution of Cr(VI) show that the great majority of Cr(VI) passed entirely through the VZ and into the unconfined aquifer or the Columbia River. Estimates of travel time to the Columbia River from 100 Area facilities were on the order of weeks during operations. Despite the clear indications of highly efficient transport through the VZ, a small residual amount remains, suggesting other chemical or physical mechanisms that influenced the transport of a small fraction of the total discharged inventory. The summary discussion of the distribution of the residual contamination of Cr(VI) in both the groundwater and the VZ follows.

3.3.3.1 Groundwater Hexavalent Chromium Distribution

Cr(VI) concentrations in the groundwater plumes near the 100 Area are summarized each year by the Hanford Area Groundwater Monitoring Report (DOE/RL-2010-11, *Groundwater Monitoring and Performance Report for 2009: Volumes 1 and 2*). Chromate contamination is found at levels above drinking water standards (100 µg/L) in the 100-K Area, 100-D Area, and 100-H Area, and at lower concentrations in the 100-B Area, 100-N Area, and 100-F Area (Hartman et al., 2007). The highest

groundwater concentrations are found in the 100-D Area, with concentrations greater than 1,500 µg/L in 2006. Concentrations considerably less than the drinking water standard are also of concern because the Washington State ambient WQS for chronic exposure is 11 µg/L for aquatic biota. Groundwater pump-and-treat systems are active for chromate remediation in the 100-K, 100-D, and 100-H Areas. At the 100-D Area, chromate contamination is also being treated by ISRM (PNNL-16346. *Hanford Site Groundwater Monitoring for Fiscal Year 2006*). Groundwater chromate concentrations found in the 100-D Area at levels greater than that in the cooling water and the contaminant distribution in the 100-D, 100-K, and other areas implicate dichromate leaks or spills and/or liquid waste disposal facilities as likely sources for some of the groundwater contamination (PNNL-16346; BHI-00917, *Conceptual Site Models for Groundwater Contamination at 100-BC-5, 100-KR-4, 100-HR-3, and 100-FR-3 Operable Units*; BHI-01309, *The Chromium Groundwater Plume West of the 100-D/DR Reactors: Summary and Fiscal Year 1999 Update*). Figure 3-23 illustrates the extent of Cr contamination in the 100 Areas based on the recent groundwater monitoring report.

3.3.3.2 Vadose Zone Hexavalent Chromium Distribution

Cr(VI) is the most significant contaminant at each of the 100 Area OU's with the exception of 100-N. Due to the low propensity of Cr(VI) to adsorb to soil in the VZ, the majority of the Cr(VI) has likely passed through the VZ into the groundwater. Results from leachability tests (see next section) indicate that this is the case. The highest soil contaminant concentrations are expected within and near the point of release. Sufficiently high volumes of liquids discharged into a waste site can increase the vertical extent of contamination in the VZ. Where little or no liquid effluents were discharged to a waste site, soil contamination is expected to remain within and only slightly below the point of release. The available data indicate residual concentrations of Cr(VI) remain in the VZ where remedial actions have been completed. However, few data are available to quantify total VZ Cr(VI) quantities and distribution. Soil samples collected and analyzed during interim remedial actions (Borehole B8786 at 116-DR-1&2) indicate that residual contamination is located above the water table and the periodically re-wetted zone. The profiles of the 116-F-4 crib and 116-F-14 retention basin show that contaminant concentrations generally decrease with depth, with the exception of total Cr. Higher concentrations are generally present between 1.5 to 3 m (10 ft.) bgs and are associated with the bottom of the engineered structure. Total Cr concentrations increase with depth at the 116-F-4 crib toward the bottom of the borehole.

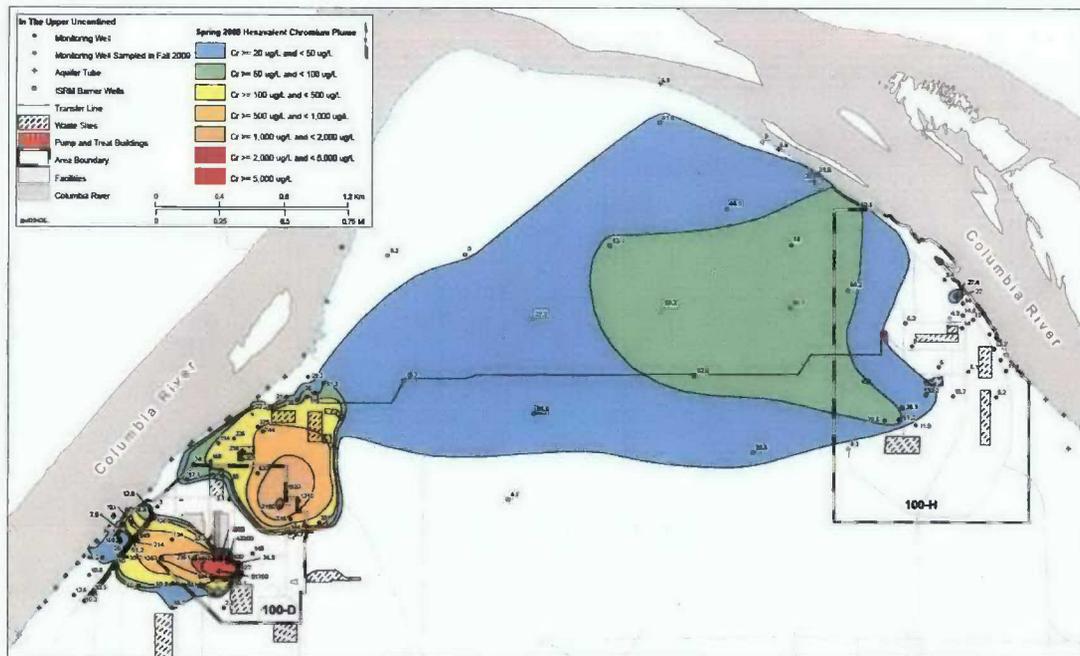
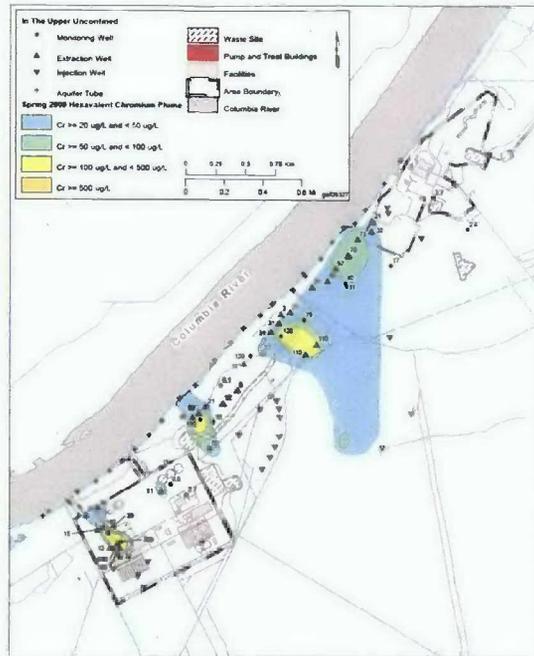


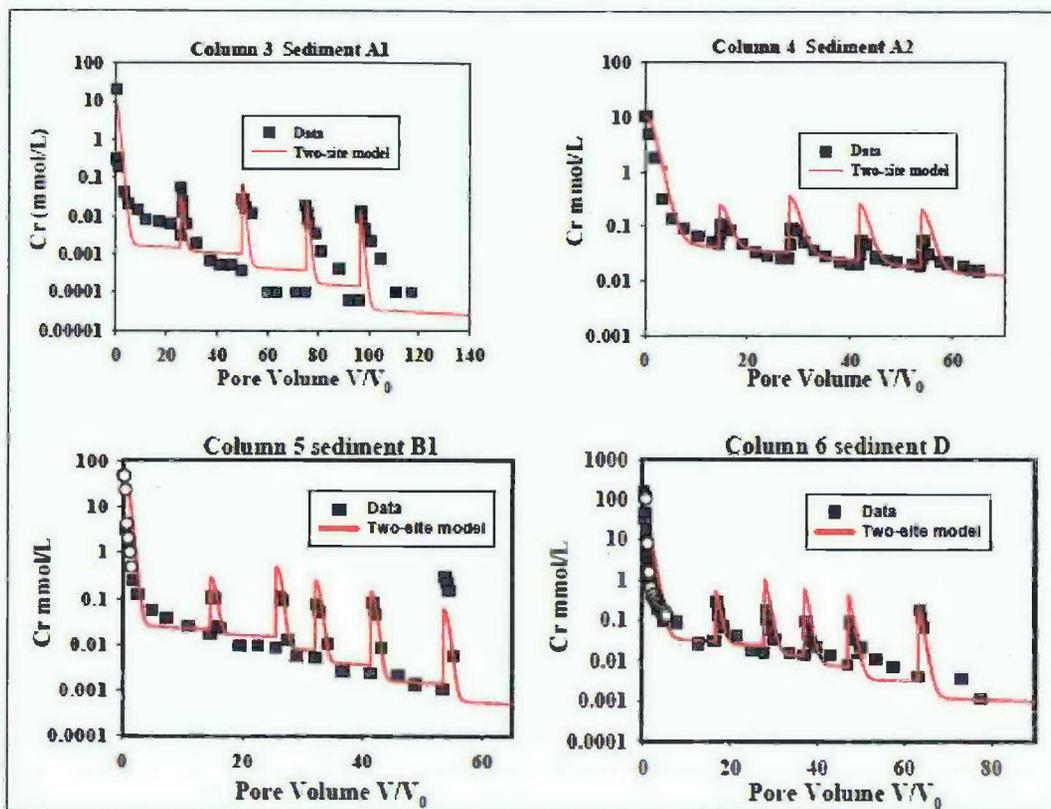
Figure 3-23. Extent of Cr(VI) Contamination in the 100 Areas

3.3.4 Cr(VI) Leachability

Leaching tests have been conducted on Cr-contaminated soils collected under retention basins at 100-D and 100-H geographic areas and under the liquid discharge trench 1301-N in the 100 N Area. In all cases, the leachable fraction of Cr(VI) was less than 1% for a variety of experimental conditions. A detailed description of leaching experiments in soils retrieved below the 116-D-7 retention basin is provided in a remediation description document for that facility (CVP-99-00007, *Cleanup Verification Package for 116-D-7 Retention Basin*). Total Cr concentrations were about 177 mg/kg including a Cr(VI) portion of about 6 mg/kg. It should be noted that the authors put forth the possibility that the measured Cr(VI) could have been Cr(III) that was oxidized to Cr(VI) by the sample preparation process. In standard batch leaching tests with several soil samples, Cr(VI) was detected at very low concentrations (about 2 to 20 $\mu\text{g/L}$) or could not be measured. In the flow through column tests, steady state concentrations from 1 to 2 $\mu\text{g/L}$ were measured by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and about 11 $\mu\text{g/L}$ by colorimetry. The authors considered the ICP-MS measurements to be more accurate. After 12 pore volumes, less than 0.1% of the initial Cr(VI) had passed through the column assuming ICP-MS measurements.

A detailed leaching and characterization study has also been completed using near surface soils (less than 3 m [10 ft] bgs) collected near sodium dichromate storage tanks and railroad tracks in the 100-BC geographic area (PNNL-17674, *Geochemical Characterization of Chromate Contamination in the 100 Area Vadose Zone at the Hanford Site*). Unlike the leaching sediments described above, these soils were only leached by natural infiltration. In this study, two types of leaching behavior were observed. First, large fractions of Cr(VI) in the contaminated soil were eluted in the first pore volume (about 65%) and about 4% of the initial mass was released in the next five pore volumes. After five pore volumes, the leachate concentration had decreased about three orders of magnitude. For example, in one soil sediment initially containing Cr(VI) concentrations of about 550 mg/kg, the first pore volume concentration was greater than 8,000 $\mu\text{g/L}$. After five pore volumes, the concentration was approximately 2 $\mu\text{g/L}$.

As part of the leachability tests (PNNL-17674), modeling using the CXTFIT code (Parker and van Genuchten, 1984, "Determining Transport Parameters from Laboratory and Field Tracer Experiments"; Toride et al., 1999, *The CXTFIT Code for Estimating Transport Parameters from Laboratory or Field Tracer Experiments*) was performed to calculate transport parameters. This code includes a two-site model for adsorption, including a kinetic model and an equilibrium model. Parameter estimation for the CXTFIT model was completed for dispersivity, Peclet Number, K_d (kinetic and equilibrium), and equilibrium site fraction. The two-site model fit Cr(VI) desorption profiles well for columns 3, 4, 5, and 6 (Figure 3-24). The modeling exercise indicated that the majority of the mass of Cr(VI) can be described using the equilibrium model, while a small portion is kinetically controlled with percent equilibrium sites of 97.5, 95, 98.7, and 97 for columns 3, 4, 5, and 6, respectively. Table 3-16 indicates a K_d of 0 or close to 0 is appropriate for equilibrium controlled Cr(VI). The calculated values of dispersivity were close to or within the range of typical values observed in packed laboratory columns (dispersivity less than 2 cm) (Jury et al., 1991, *Soil Physics*). The values of the Peclet number ($\text{PN} = L/\lambda$, where L is the column length) varied between 2.8 and 12.4 (Table 3-17). Generally, the majority of the Cr(VI) mass present in the sediment was removed during the initial leaching phase. A small fraction of the total mass exhibited time-dependent desorption. This fraction released Cr(VI) with reaction half-lives that varied from 76.1 to 126 hours represented a small portion of the total mass of Cr(VI) in the column.



Source: PNNL-17674

Figure 3-24. The Results from Fitting the Two-Site (Two-Region) Model to Experimental Data for Column Experiments 3, 4, 5, and 6

Table 3-16. Results from Modeling the Cr(VI) Desorption Data Using a Two-Site Equilibrium and Kinetic Model (Source: PNNL-17674)

Parameters	Column 3 Sediment A1	Column 4 Sediment A2	Column 5 ^c Sediment B1	Column 6 ^c Sediment D
K _d – kinetic (ml g ⁻¹)	0	45	13	4.8
K _d – equilibrium (ml g ⁻¹)	0	0.33	0	0
Equilibrium site fraction (%)	97.5	95	98.7	97
Rate constant (kinetic site fraction) (h ⁻¹)	0.0082	0.0055	0.0091	0.0068
Reaction half-life ^a (h)	84.5	126	76.1	101.9
Reaction characteristic time ^b (h)	121.9	181.8	109.8	147.1

^aReaction half-life: [ln(2)/rate constant].

^bReaction characteristic time: (1/rate constant).

^cData from other columns were included in these simulations to better represent Cr(VI) effluent concentrations in the first pore volumes.

Table 3-17. Selected Measured and Calculated Physical Properties in Column Experiments 1, 2, 3, 4, 5, and 6
(Source: PNNL-17674)

Column	1 Sediment D	2 Sediment B2	3 Sediment A1	4 Sediment A2	5 Sediment B1	6 Sediment D
Pore Volume ^b (cm ³)	26.51	19.12	19.79	20.89	19.19	19.70
Water Content ^b (cm ³ cm ⁻³)	0.47	0.52	0.37	0.41	0.38	0.37
Residence Time ^b (h)	2.41	2.46	1.13	1.77	1.65	1.32
Bulk Density ^b (g cm ⁻³)	1.40	1.25	1.68	1.57	1.65	1.66
Flow Rate ^a (cm ³ min ⁻¹)	0.183 ± 0.011	0.197 ± 0.014	0.333 ± 0.015	0.196 ± 0.008	0.194 ± 0.012	0.248 ± 0.035
Water Flux (cm min ⁻¹)	0.034	0.037	0.065	0.039	0.039	0.048
Pore Water Velocity (cm h ⁻¹)	4.32	4.26	10.56	5.76	6.24	7.92
Dispersion Coefficient (cm ² h ⁻¹)			27.3	10.1	5.21	29.3
Dispersivity (cm)			2.58	1.75	0.83	3.69
The Péclet number			4.1	5.9	12.4	2.8

^aThe average flow rate was calculated from experimental measurements (the standard deviation is given in squared brackets, more than 100 experimental measurements were taken in each column to determine the average flow rate).

^bPore volume, water content, residence time and bulk density were calculated based on the amount of sediments added in each column and the mass of water used to saturate the columns.

Considered collectively, these experimental results suggest that after Cr(VI) is discharged to the soil column, two primary chemical stages of Cr reactivity occur, which influence its transport characteristics. First, the majority of Cr(VI) remains mobile, transports readily, and contributes groundwater concentrations commensurate with source term strength. Second, some Cr(VI) is sequestered by a variety of mechanisms on some sorption sites that retard further migration. The effectiveness of these sequestration processes increases over time. In the retention basin soil, it appears that the initial highly mobile component of discharged Cr(VI) has already been flushed from the sampled soil. This is expected, given the high leakage volume from the retention basins during operations. Conversely, the reactor area soil has been contacted by much smaller volumes of water since the contaminating event. Therefore, extensive flushing of the soil has not been completed in the natural setting.

The number of pore volumes of groundwater passed through contaminated soil in the 100 Area VZ is not well understood. Additionally, the experimental column soil conditions present a highly idealized environment for groundwater contact and transport with regard to the irregular subsurface features found in the local 100 Area geology. These features could harbor concentrated dichromate solutions or limit contact with groundwater and introduce more complex release mechanisms than those observed in the column tests. Therefore, studies and data collection focused on understanding the long-term hydrology, geological influences, and spatial distribution of Cr(VI) at work in various locations may be needed.

Batch leaching studies have been performed on the soil samples (<2 mm size) taken underneath various waste sites as part of the River Corridor remedial investigation efforts. The results of the batch leach tests are summarized in ECF-Hanford-11-0165 (*Evaluation of Hexavalent Chromium Leach Test Data Conducted on Vadose Zone Sediment Samples from the 100 Area*). A total of 509 samples from 58 locations were analyzed. Only 39 samples from 15 locations had detectable Cr(VI) in the soil and only 10

samples from 4 locations had detectable Cr(VI) in both the soil and leachate. For each sample, analyses were performed using three ratios of soil to leachant (1:1, 1:2.5, and 1:5) by weight. One of the three ratios was selected randomly to run as a duplicate analysis totaling four analyses for each soil sample. The Cr(VI) concentration in the soil samples ranged from 4.31 mg/kg to undetectable levels and the pH of the leachant added to the soil sample was held at pH of 5 to simulate the rain water. Quadruplicate analyses were conducted for each soil sample and if the sorbed mass on any of the quadruplicate samples was flagged as a non-detect then they were excluded from analysis and considered unreliable for K_d determination. However, if the leachate concentration was flagged as a non-detect, the K_d was calculated as a greater than value by assuming the practical quantitation limit (PQL) as the solute concentration. An empirical cumulative distribution function (ECDF) is created from the resulting K_d values (after adjusting for the dilution factors). The ECDF indicates a 90th, 50th, and 10th percentile exceedance of approximately 0.8 mL/g, 9 mL/g, and 29 mL/g, respectively. For the purpose of PRG and SSL calculations the K_d of 0.8 mL/g was chosen as a conservative value (equivalent to the 90th percentile exceedance; that is, 90 percent of the distribution from which these data were developed exhibited higher sorption values). Note that this K_d value pertains only to the residual Cr(VI) in the soil profile; it does not apply to the more mobile fraction that has already migrated out of the vadose zone.

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4. Model Implementation

Numerical predictions of groundwater concentrations from soil contamination are founded on a conceptual model of solute fate and transport for the Hanford Site VZ. Numerous characterization and modeling efforts have yielded ample information with which to construct the conceptual model. Important conceptual model components include the hydrologic driving forces, especially recharge, waste discharges, and aquifer flow; the interaction between the flowing fluids and the sediments of the different hydrostratigraphic units; the interactions between the sediments and the solutes; and the initial distributions of water pressure and solute concentration. The conceptual model also provides an understanding of the uncertainties about model components (e.g., hydraulic properties) and a context for evaluating the relative conservatism of different modeling assumptions.

Peak groundwater concentrations were simulated using 1-D STOMP numerical fate and transport simulations under variably saturated conditions. Simulated transport processes included sorption to sediments and contaminant degradation from radioactive decay. Each model domain comprised a VZ and an underlying aquifer, wherein the peak groundwater concentration was determined. Recharge, gravity, and matric potential gradients were assumed to drive water downward through the VZ's contaminated interval into the aquifer, where a hydraulic gradient was assumed to drive water horizontally towards the simulated monitoring well screen. Two- or three-dimensional STOMP simulations could also be used, but would require greater resources and would yield less-conservative (lower) peak groundwater concentrations. The STOMP code was selected to perform the simulations because of its ability to provide an adequate simulation of the VZ FEPs relevant to calculating PRGs for the Hanford Site and to satisfy the other code criteria and attributes (DOE/RL-2011-50). Model development was completed under a plan written to implement EPA guidance on model planning (EPA/QA/G-5M. *Guidance for Quality Assurance Project Plans for Modeling*).

4.1 Governing Equations

STOMP was used to solve the Richards equation (the water mass conservation equation in PNNL-12030) and the Advection-Dispersion equation (the solute mass conservation equation in PNNL-12030) that govern water flow and solute transport, respectively, under variably saturated conditions beneath the waste sites.

4.1.1 Flow and Solute Transport Equations

The governing equation for variably saturated flow through porous media was simulated using STOMP's single-phase, water-only mode (STOMP-W). As such, the principle processes that drive water flow are gravity and gradients in pressure or volumetric water content. No momentum is transferred from the liquid phase to the vapor phase. The overall equation governing liquid phase flow for STOMP (termed the water mass conservation equation in PNNL-12030) is written as:

$$\frac{\partial}{\partial t} (n_D \rho s) = \frac{\rho k_r k}{\mu} (\nabla P + \rho g z_g) + \tau n_D \rho s \frac{M^w}{M} D^w \nabla X^w + \dot{m}^w \quad (\text{Eqn. 4-1})$$

where t is time (T), n_D is diffusive porosity ($L^3 L^{-3}$), ρ is liquid density (ML^{-3}), s is saturation (-), k_r is relative permeability (-), k is the permeability tensor (L^2), μ is dynamic viscosity ($ML^{-1}T^{-1}$), P is pressure ($ML^{-1}T^{-2}$), g is gravitational acceleration (LT^{-2}), z_g is the unit vector for the z axis (-), τ is tortuosity (-), M^w is molecular weight of water (M/mole), M is molecular weight of the liquid phase (M/mole), D_w is the self-diffusion coefficient of water (L^2T^{-1}), X^w is the mole fraction of water in the liquid phase (-), and \dot{m}^w

is the mass source rate (MT^{-1}), i.e., aggregate rate of sources and sinks. As the gradient of the mole fraction of water in water is zero, the second term on the right-hand side is zero, leaving the well-known Richards equation:

$$\frac{\partial}{\partial t} (n_D \rho s) = \frac{\rho k_r k}{\mu} (\nabla P + \rho g z_g) + \dot{m}^w \quad (\text{Eqn. 4-2})$$

Solving Equation 4-2 requires stipulation of appropriate boundary conditions, initial conditions, and parameter values. Net infiltration was represented as a specified flux boundary condition along the top boundary of the numerical model domain. Lateral groundwater flow was simulated using specified pressure boundaries on the upgradient and downgradient edges of the aquifer portion of the numerical domain. Initial conditions were specified for pressure throughout the model domain. Parameter values were taken from approved Hanford Site databases and reports.

Solute transport in a variably saturated liquid is governed by water movement, diffusion, dispersion, sorption, decay, and chemical reactions. STOMP employs the advection-dispersion equation (termed the solute mass conservation equation in PNNL-12030) as the governing equation for transport of solute mass in the aqueous phase:

$$\frac{\partial C}{\partial t} = -(\nabla C \cdot V) + \dot{m}^c - R^c C + \nabla[(\tau n_D s D^c + n_D s D_h) \nabla C] \quad (\text{Eqn. 4-3})$$

where C is solute concentration (ML^{-3}), V is the seepage velocity vector (LT^{-1}), \dot{m}^c is the solute source rate (MT^{-1}), R^c is the solute decay rate (T^{-1}), D^c is the solute diffusion coefficient for variably saturated media (L^2T^{-1}), D_h is the hydraulic dispersion coefficient (L^2T^{-1}), and all other variables are defined as above. Sorption, which is the interchange of solute molecules between the dissolved phase and the adsorbed phase onto the geologic material, can be linear or nonlinear, equilibrium or non-equilibrium. STOMP calculates equilibrium distribution of the solute molecules between the dissolved and sorbed phases with a general equation of the following form:

$$C_T = n_D s C_l + (1 - n_T) C_s \quad (\text{Eqn. 4-4})$$

Here C_T is the total concentration of the contaminant in a given pore volume, C_l is the dissolved phase concentration (solute concentration), C_s is the sorbed phase concentration, and n_T is total porosity (L^3L^{-3}). STOMP can handle nonlinear equilibrium sorption isotherms such as the Freundlich and Langmuir isotherms, but the linear equilibrium sorption isotherm is the only sorption behavior considered in this report. It is defined as:

$$K_d = \frac{C_s}{C_l} \quad (\text{Eqn. 4-5})$$

where K_d is the distribution coefficient (L^3M^{-1}). Solving the advection-dispersion governing equation and the linear sorption equations above requires stipulation of appropriate boundary conditions, initial conditions, and parameter values. The seepage velocity V in Equation 4-3 is taken from a solution of the Richards equation (Equation 4-2), so the flow system at each time step must be solved prior to solving for concentration in the same time step. Boundary conditions for concentration were typically specified as zero flux or zero concentration. For example, the net infiltration water or aquifer water entering the domain were each assumed to have a zero contaminant concentration. Initial conditions were specified for contaminant soil concentration, C_s , in Equations 4-4 and 4-5, by the user. Values for the dispersivity, diffusion coefficient, and K_d parameters were taken from approved Hanford Site databases and reports.

4.1.2 Constitutive Relations

Solving the Richards Equation (Section 0) requires adequately defined soil-moisture retention and relative permeability functions. The VZ and aquifer sediments were assumed to follow the van Genuchten (1980) moisture retention constitutive relation and the Mualem (1976) relative permeability constitutive relation. The moisture retention constitutive relation defines the relationship between volumetric water content and matric potential, $\theta(\psi)$, and is also known as the pore-pressure-saturation curve or the characteristic curve. According to van Genuchten (1980), the relationship is defined as:

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)(1 + |\alpha\psi|^n)^{-m} \quad (\text{Eqn. 4-6})$$

for which α is proportional to the inverse of the air-entry matric potential (L^{-1}), θ_s is saturated volumetric water content (L^3L^{-3}), θ_r is the residual volumetric water content (L^3L^{-3}), and n and m are dimensionless fitting parameters with $m = (n-1)/n$. In terms of STOMP's state variables and parameters, volumetric water content is the product of water saturation and diffusive porosity, $\theta = s n_D$, and matric potential ψ is the ratio of gas-aqueous capillary pressure to the product of liquid density and the gravitational acceleration constant.

The Mualem-van Genuchten relative permeability in terms of matric potential, $K(\psi)$, is defined as:

$$K(\psi) = K_s + (1 + |\alpha\psi|^n)^{-m\beta} \{1 - [(1 + |\alpha\psi|^n)^{-1}]^m\}^2 \quad (\text{Eqn. 4-7})$$

where K_s is the saturated hydraulic conductivity (LT^{-1}) and β is Mualem's dimensionless fitting parameter. Solving the characteristic equation for matric potential and substituting the result into the above equation yields the relative permeability in terms of volumetric water content:

$$K(\theta) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^\beta \left\{ 1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{m}} \right]^m \right\}^2 \quad (\text{Eqn. 4-8})$$

The n parameter is an index of the pore size variability, which is commonly taken as the inverse of the pore size standard deviation, for the Mualem-van Genuchten parameterization, whereas β represents the tortuosity and the partial correlation in pore radius between two adjacent pores at a given saturation (Mualem, 1976).

4.2 Software Used

STOMP (PNNL-11216; PNNL-12030; PNNL-15782) was selected to simulate the transport of contaminants in the vadose zone of the 100 Area because it fulfills the following specifications:

- The STOMP simulator operational modes needed for implementation of this model is available free for government use under a limited government-use agreement.
- The STOMP simulator solves the necessary governing equations (see Section 4.1 above).
- It is capable of directly simulating the principal FEPs that are relevant (see Section 3.2 above).
- The STOMP simulator is well documented (PNNL-11216; PNNL-12030; PNNL-15782).
- The STOMP simulator development is compliant with DOE O 414.1c requirements (PNNL-SA-54022, *STOMP Software Test Plan Rev. 1.0*; PNNL-SA-54023, *STOMP Software*

Configuration Management Plan Rev. 1.3; PNNL-SA-54079, Requirements for STOMP Subsurface Transport Over Multiple Phases).

- The STOMP simulator is distributed with source code, enhancing transparency.
- The modeling team implementing this model has expertise in use of this simulator.
- There is an extensive history of application of STOMP at Hanford and elsewhere including verification, validation, and benchmarking (see Appendix C, *CHPRC Fact Sheet: STOMP: Validation and Extent of Application*).
- Use of STOMP is in keeping with DOE direction for simulation of VZ flow and transport at the Hanford Site (*Hanford Groundwater Modeling Integration* [Klein, 2006]).

The software used to implement this model and perform calculations was approved under the requirements of, and use was compliant with, PRC-PRO-IRM-309, *Controlled Software Management*. This software is managed under the following software quality assurance documents consistent with PRC-PRO-IRM-309:

- CHPRC-00222, *STOMP Functional Requirements Document*
- CHPRC-00176, *STOMP Software Management Plan*
- CHPRC-00211, *STOMP Software Test Plan*
- CHPRC-00515, *STOMP Acceptance Test Report*
- CHPRC-00269, *STOMP Requirements Traceability Matrix*

4.2.1 STOMP Controlled Calculation Software

The following describes the STOMP controlled calculation software:

- Software Title: STOMP-W (a scientific tool for analyzing single- and multiple-phase subsurface flow and transport using the integrated finite volume discretization technique with Newton-Raphson iteration).
- Software Version: STOMP-W was provided by PNNL on January 30, 2013, and was tested and approved for use by CHPRC as “CHPRC Build 4.”
- Hanford Information System Inventory Identification Number: 2471 (Safety Software S3, graded Level C).

4.2.2 Software Installation and Checkout

Safety Software (CHPRC Build 4 of STOMP) is checked out in accordance with procedures specified in CHPRC-00176. Source or executable files are obtained from the CHPRC software owner, who maintains the configuration-managed copies in MKS Integrity™. Installation tests identified in CHPRC-00211, are performed and successful installation confirmed, and software installation and checkout forms are required and must be approved for installations used to perform model runs. Approved users are registered in the Hanford Information System Inventory for safety software.

™ MKS Integrity is a trademark of MKS, Incorporated.

4.2.3 Statement of Valid Software Application

Use of the STOMP software for implementing the model described in this report is consistent with its intended use for CHPRC, as identified in CHPRC-00222. A fact sheet that provides a brief overview of work that has validated the STOMP simulator software and the breadth of applications to which this simulator has been applied is presented in Appendix C.

4.3 Spatial and Temporal Discretization

STOMP, or any numerical modeling code, solves the governing equations (see Section 4.1) at user-specified locations and times. For STOMP, the conceptual model's physical domain is discretized into grid blocks within which the governing equations are solved on the centroids at times determined by the code's time-stepping algorithm and, in part, by the user. The governing equations are solved using integral volume finite-difference method. STOMP's inactive node feature, most commonly applied in multi-dimensional models to represent non-uniform surfaces or relatively impermeable regions, was not used. STOMP's optional dynamic domain feature was not utilized because this 1-D model is not computationally demanding, so no advantage would be gained by using this feature.

As described in Section 3, the conceptual model represents a column of sediments that comprise a VZ and an underlying aquifer. Recharge-driven flow moves downward through the VZ, where it encounters contamination that is eventually transported to the aquifer, across which a pressure gradient drives horizontal flow. The conceptual model is represented numerically as a vertical, one-dimensional column of evenly-spaced grid blocks with boundary conditions defined on the grid block faces (see Section 0) and initial conditions defined at the centroids (see Section 4.4.2). The number of grid blocks in this vertical column is varied to match the length of each representative stratigraphic column, and the hydraulic and transport properties assigned to each grid block is changed to match the lithologic composition of each stratigraphic column (see Section **Error! Reference source not found.**). STOMP is inherently a three-dimensional code, but through the specification of a single vertical column of grid blocks and the specification of no-flow (zero flux) boundary conditions on the vertical faces (north, south, east, and west), the model is reduced to functioning as a one-dimensional representation.

Given the differences in the representative stratigraphic columns, each grid block was assigned a constant thickness and length. Grid block thickness was set to 0.25 m to represent the changes in lithology and to avoid large grid-block Courant numbers (see Section 4.3.2). A length of 10 m for the 100-D/H, 100-K, 100-BC, 100-F, 100-IU-2/6, and 100-N geographic areas was selected to avoid large grid-block Courant numbers in the aquifer grid blocks during transport simulations (see Section 4.3.2). The results were scaled down to produce results appropriate for a column of a unit length (1 m).

The simulated time span was divided into two intervals, one that represents the period prior to the year 2010 (pre-2010 period), during which only flow was simulated, and one that represents the period after the year 2010 (post-2010 period), during which both flow and solute transport were simulated (see Section 0).

4.3.1 Representative Stratigraphic Columns

A total of 28 different representative stratigraphic columns were simulated for the five different geographic areas: 100-D/H, 100-K, 100-BC, 100-F, and 100-IU-2/6 (Figure 4-1 and Figure 4-2). Some of the representative stratigraphic columns for 100-BC, 100-F and 100-IU-2/6 may be revised based on reevaluation of extent and thickness of Ringold E unit. The thickness of the representative columns

ranged between 8 and 40 m (Table 3-2 through Table 3-7), with a corresponding range of 32 to 160 grid blocks. Model domain dimensions and discretization were held constant for the pre-2010 and post-2010 simulations.

The thickness of the VZ, excluding the 4.5 m of clean fill at the top, ranges between 3.5 and 35.5 m across all geographic areas. Aquifer thickness was set equal to the observed thickness for each representative column unless that thickness was less than 5 m, in which case the minimum thickness was set to a minimum thickness of 5 m. This was necessitated by the model requirement that groundwater concentrations were representative of a water table monitoring well that was constructed with a 6-m (20-ft) screen in such a way that a 5-m-long span was below the water table. However, it was observed that using 5 m deep SZ instead of deeper SZ did not change the peak concentration at the water table. On the other hand, run time for the simulation reduced significantly because the number of active nodes in the model is less than the model with the deeper SZ. So, a 5-m thick SZ was used for all the representative columns.

Depending on source-area-specific geology, the VZ comprises either Hanford formation alone or a combination of Hanford and Ringold E units (Table 3-2 through Table 3-7 and Figure 4-1, Figure 4-2, and Figure 4-3). At the start of each post-2010 simulation, the VZ spans a cover of clean fill with constant thickness as well as contaminated and uncontaminated sediments of varying thickness. The SZ can comprise of, only Hanford formation, a combination of Hanford formation and Ringold E unit, or only Ringold E unit (Table 3-2 through Table 3-7 and Figure 4-1, Figure 4-2, and Figure 4-3). If present, the contact between the Ringold E unit and the RUM forms the bottom of the unconfined aquifer.

Two sequential STOMP simulations were used to determine peak groundwater concentrations. The first stage model, called the pre-2010 model, simulated flow through the representative columns for a 2,010-year period (an arbitrary long period chosen to allow establishment of pressures in equilibrium with the present day conditions). Results from the pre-2010 simulations provided initial aqueous pressure conditions for the 1,000-year-long second stage simulation, the post-2010 model, which is solved for both flow and solute transport. The post-2010 solute transport simulations track the fate of contaminants with different distribution coefficients (K_d) and decay constants through the VZ and into the aquifer. These results were used to identify the peak groundwater concentrations.

As described below, recharge rates varied with time during the pre-2010 simulations to represent changes in land cover with the start of operations at the Hanford Site in the year 1944. Aqueous pressure and saturation values were reviewed at least every ten years after the start of operations to ensure that the values had reached equilibrium prior to the end of the simulation period.

4.3.2 Grid and Time-Step Constraints

The choice of grid block dimensions and time step intervals can affect solution convergence and mass balance errors. Deleterious effects can be minimized by choosing grid-block and time step sizes that yield acceptable Peclet and Courant numbers for the model. Defined as the product of the seepage velocity and the ratio of the time step and the grid block dimension, dimensionless Courant numbers provide a stability constraint and should ideally be less than 1.0 to minimize convergence and mass balance problems (for example, see page 231 in Celia and Gray, 1992, *Numerical Methods for Differential Equations*). Courant numbers for the aquifer grid blocks, in which flow is horizontal under fully saturated conditions, were all less than 1.00. Courant numbers for the VZ grid blocks, in which flow is vertical under variably saturated conditions, were all less than 1.0 for all recharge scenarios. No grid size constraints were placed based on

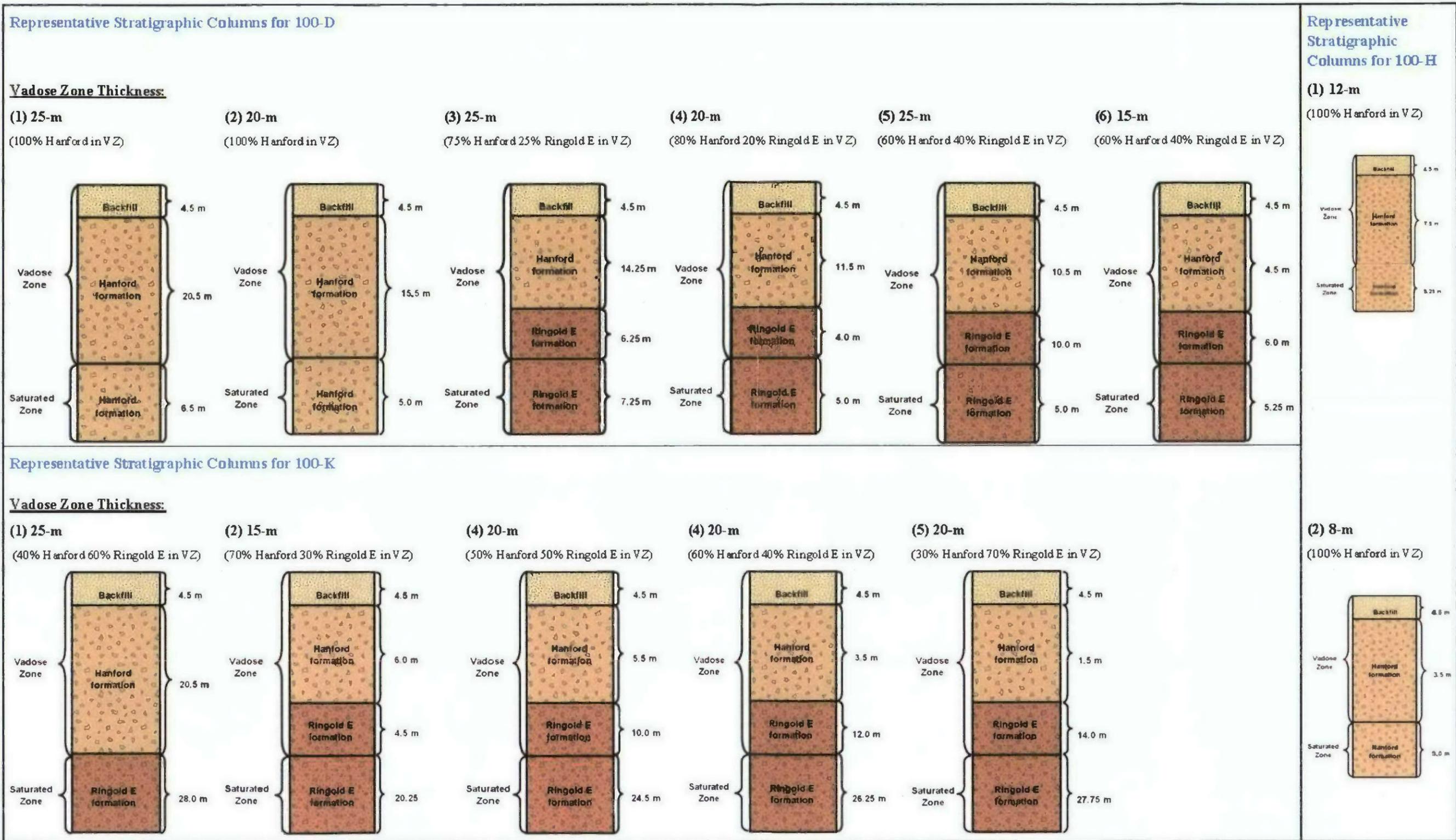
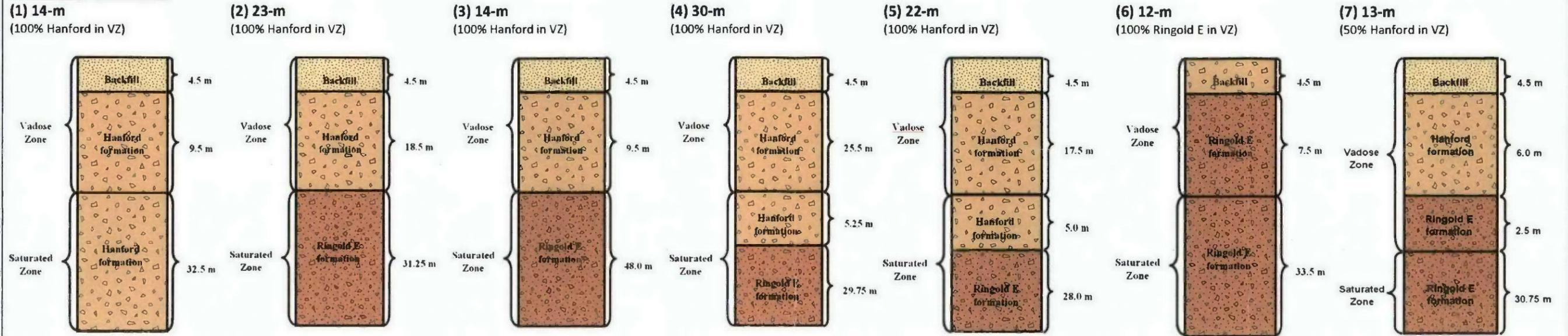


Figure 4-1. Representative Stratigraphic Columns for 100-D, 100-H, and 100-K Geographic Areas

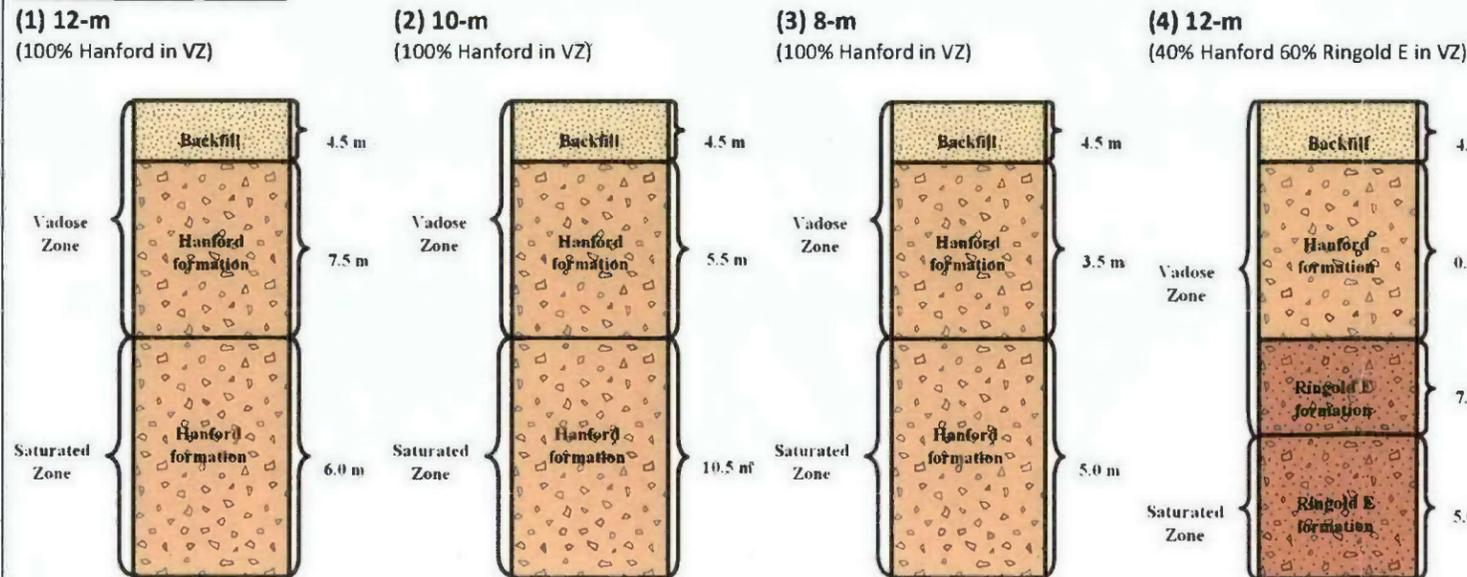
Representative Stratigraphic Columns for 100-BC

Vadose Zone Thickness:

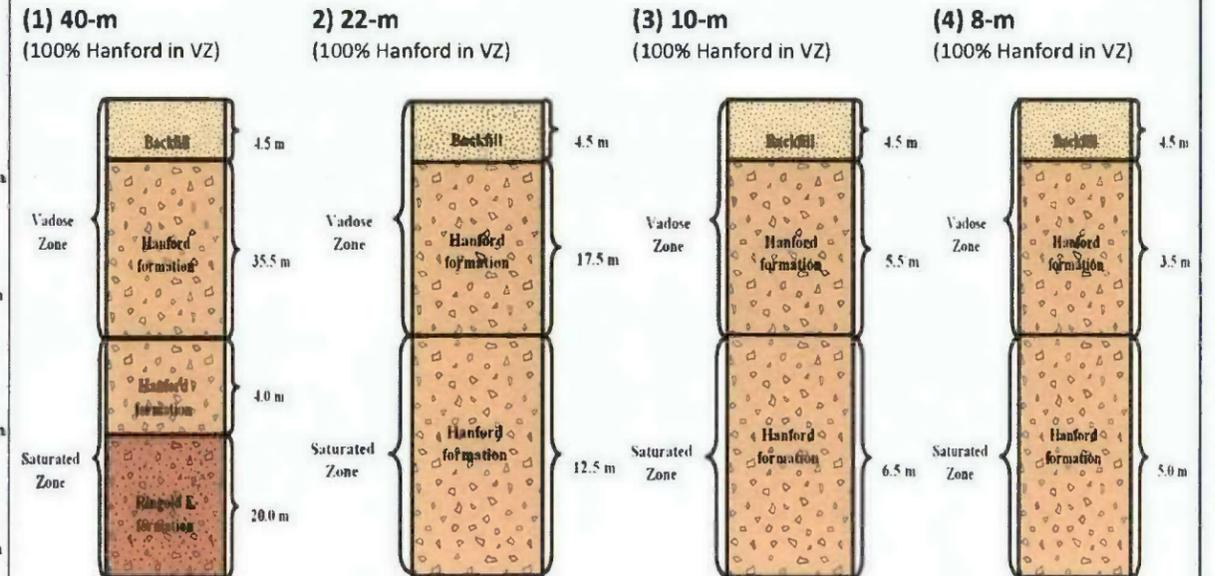


Representative Stratigraphic Columns for 100-F

Vadose Zone Thickness:



Representative Stratigraphic Columns for 100-IU-2 and 100-IU-6



Note: Some representative columns for 100-BF, 100-F, 100-IU-2, and 100-IU are subject to revision based on reevaluation of extent of Ringold E unit.

Figure 4-2. Representative Stratigraphic Columns for 100-BC, 100-IU-2 and 100-IU-6, and 100-F Geographic Areas

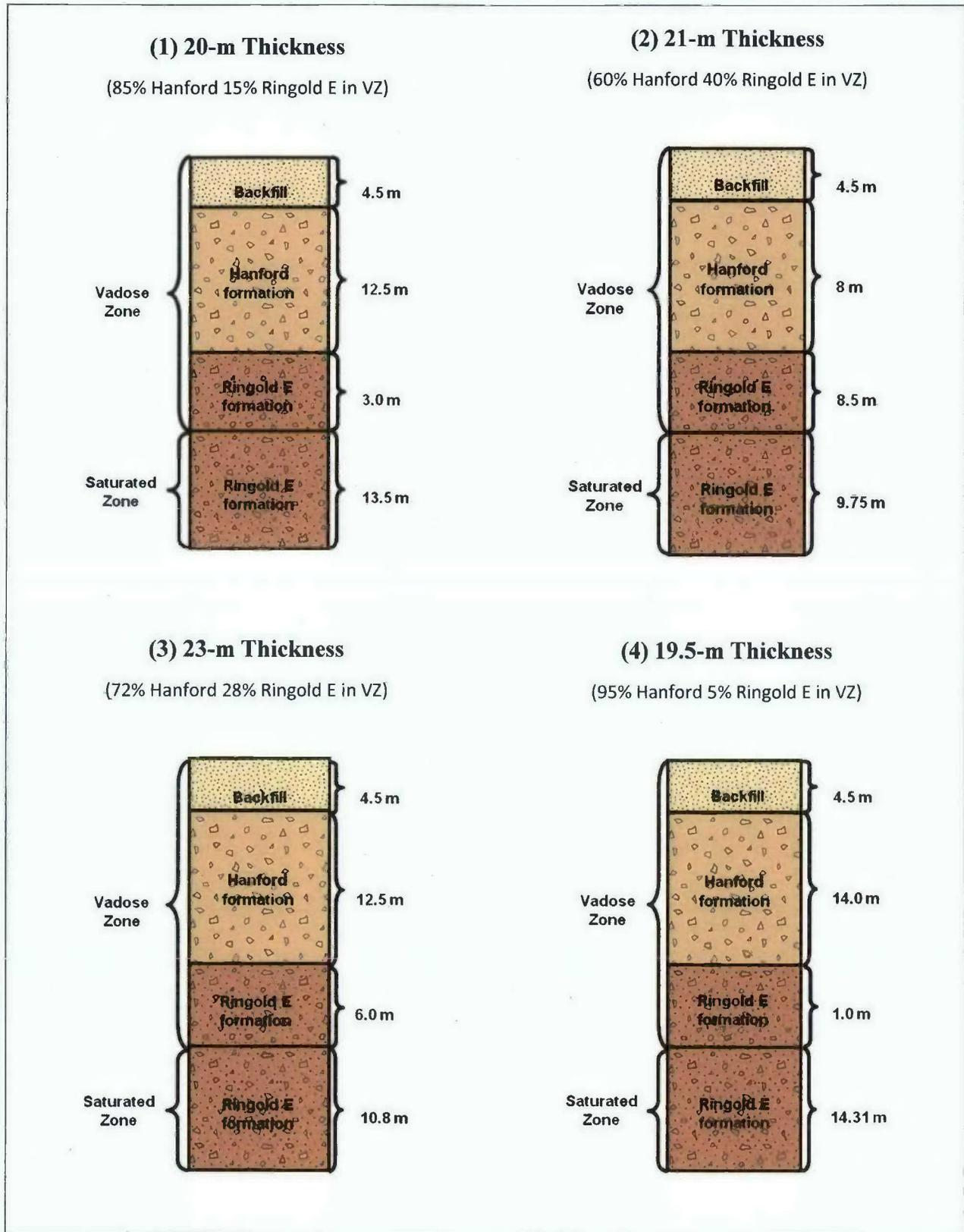


Figure 4-3. Representative Stratigraphic Columns for 100-N Geographic Areas

Peclet numbers because dispersion was assumed negligible (see Section 4.5). The typical grid block size used was uniform in size for each direction, with 10.0 m in the x-direction (representing the horizontal direction parallel to the local direction of groundwater flow), 1.0 m in the y-direction (representing the horizontal direction perpendicular to the local direction of groundwater flow), and 0.25 m in the z-direction (representing the vertical direction).

4.4 Initial and Boundary Conditions

Solving the governing equations for variably saturated flow and transport requires stipulation of boundary conditions and initial conditions. A complete set of boundary and initial conditions must be stipulated for each scenario

4.4.1 Flow and Transport Boundary Conditions

For water flow, boundary conditions are depicted in part (a) of Figure 4-4. No-flow (zero flux) boundary conditions are assigned to all vertical faces of the vadose zone (north, south, east, and west) to reduce the model to one-dimensional representation in the vadose zone (that is, assuming only vertical flow of water). A no-flow boundary is also assigned to the bottom face (the bottom of the aquifer) to truncate the aquifer at a depth of 5 m, representing a 5-meter thick aquifer. The only boundaries open to flow are the top, assigned a specified-flux boundary condition to represent recharge (flux into the top of the model domain) and the east and west faces of the aquifer zone (nodes below the water table), assigned a hydraulic gradient condition to represent aquifer flux from west to east. Thus, the only boundaries across which water flow may occur are the top, representing recharge into the model domain, and the prescribed pressure boundaries assigned to the upstream and downstream faces of the aquifer nodes.

For solute transport, boundary conditions are depicted in part (b) of Figure 4-4. As for the water phase, No-flow (zero flux) boundaries are assigned to all vertical faces of the vadose zone (north, south, east, and west) to reduce the model to a one-dimensional representation of solute transport in the vadose zone. The only source of contamination is imposed by the initial conditions, so a no-flow boundary is also assigned to the top of the domain for the solute phase. The aquifer nodes are assigned no-flow boundaries on the east, north, south faces for solute phases, as well as for the bottom face (again, representing the 5-meter aquifer thickness). Solute flux can only occur at along the east face of the downgradient aquifer nodes. The outflow boundary condition, described on 6.21 of PNNL-12030 and on page 4.4 of PNNL-15782, is assigned to these nodes to transport solute out of the domain according to the advective flux term in the governing equation and does not allow solute to enter into the domain.

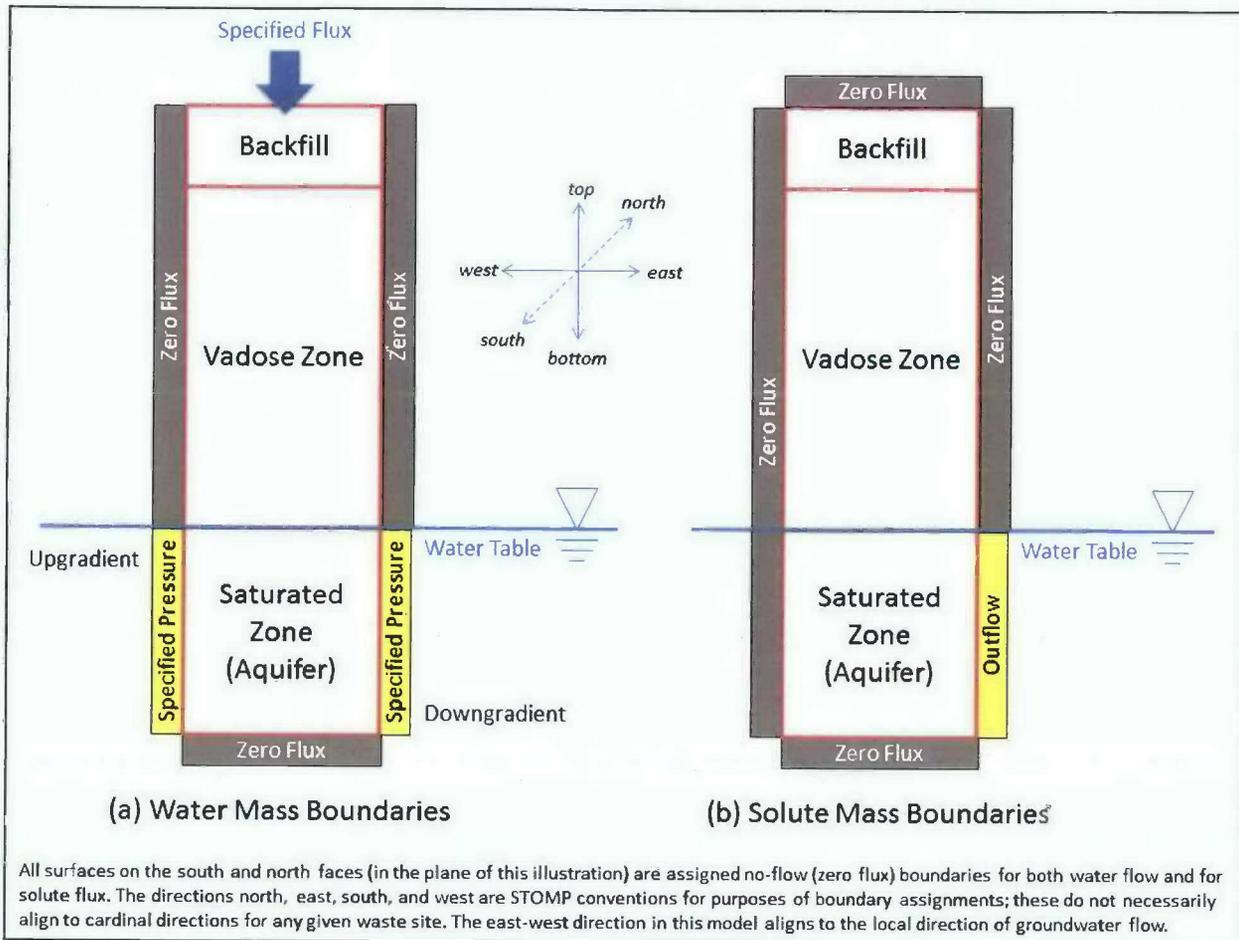


Figure 4-4. Flow Boundary Conditions for (a) Water Mass and (b) Solute Mass Conservation Equations

Recharge

The net infiltration into the VZ, which is used in the model to represent recharge into the aquifer, is driven by the competition between precipitation, potential evaporation, transpiration, run-off, and run-on. In an arid climate, downward fluxes resulting from this competition are episodic and usually infrequent.

A number of studies have been carried out at the Hanford Site to ascertain representative long-term averages of the episodic fluxes, i.e., recharge rates, such as those compiled in PNNL-14702, for the 100 Area. The 100-Area-specific recharge rates provided in PNNL-14702 vary by surface soil type, providing an estimate of the range of recharge rates for various land uses. The four surface soil types were the Ephrata sandy loam, Ephrata stony loam, Burbank loamy sand, and Rupert sand; however, recharge rates for the Ephrata sandy loam and the Ephrata stony loam were described as being identical (PNNL-14702) and have been combined. Thus, the three resulting surface soil types were assumed to represent recharge rate variability. Alternatively, the disturbed soil condition rates may be used as bounding values.

Each calculation of a soil protection level with STOMP requires a pair of simulations; the first is a simulation of water flow only for historic recharge conditions, needed to obtain the soil moisture conditions throughout the model domain at the start time for the second simulation. The second is a coupled simulation of water flow and contaminant transport, starting from the assumed initial contaminant distribution (100:0 or 70:30 models) and the initial moisture distribution provided by the first

simulation. Calendar year 2010 is chosen as the time when the first, historic simulation ends and the second, predictive simulation begins. Recharge rates were conservatively simulated in STOMP as a specified flux boundary condition applied to the top boundary of the model (Figure 4-5) for each recharge scenario and each soil type. Rates were assumed to change over time in step function-fashion for each recharge scenario.

Two recharge scenarios based on differing land use or land cover were evaluated: (1) native vegetation recharge scenario and (2) irrigation recharge scenario. These scenarios represent different future land-use activities that vary over time. The recharge rates for the historic (pre-2010) period are the same for both recharge scenarios, but differ with respect to the recharge rates applied in the predictive (post-2010) period representing different potential future land uses.

The recharge rates for the native vegetation recharge scenario are specified by period in Table 4-1 for the three surface soil types, used to represent variability, and the disturbed soil type. The first period is an arbitrarily long time (from calendar year 0 through 1944) used to attain a steady-state flow condition throughout the model domain at the long-term recharge rate for mature shrub-steppe vegetation conditions. For sites where applicable, a historic irrigation period is specified (for disturbed soil conditions only) from 1880 to 1944 to address the impacts of pre-Hanford agricultural activities, which apply primarily to 100-D and 100-H Areas. The Hanford operations period (1944 to 2010) applies recharge rates applicable to bare soil. For the predictive (post-2010) simulation, vegetation progresses from bare soil, through a cheatgrass phase (for disturbed soil conditions only), to a maturing shrub-steppe vegetation cover through a 30-year transition period (DOE/RL-2011-50) to mature shrub-steppe vegetation cover.

Table 4-1. Recharge Rates for Native Vegetation Recharge Scenario (mm/yr)

Surface Soil Type	Historic Simulation (Pre-2010) (calculation of initial hydraulic conditions)		Predictive Simulation (Post-2010) (calculation of peak groundwater concentration)			
	Pre-Hanford (-1944)	Hanford Operations (1944-2010)	Bare Soil (2010-2015)	Developing Shrub-Steppe (2015-2045)	Mature Shrub- Steppe (2045-)	
Ephrata sandy loam and stony loam	1.5 ^(a)	17.0 ^(a)	17.0 ^(a)	3.0 ^(a)	1.5 ^(a)	
Burbank sandy loam	3.0 ^(b)	52.0 ^(b)	52.0 ^(b)	6.0 ^(b)	3.0 ^(b)	
Rupert sand	4.0 ^(c)	44.0 ^(c)	44.0 ^(c)	8.0 ^(c)	4.0 ^(c)	

Surface Soil Type	Pre-Settlement ^(d) (-1880 or -1944)	Historic Irrigation ^(d) , where applicable (1880-1944)	Hanford Operations (1944-2010)	Bare Soil (2010-2015)	Cheatgrass (2015-2020)	Developing Shrub-Steppe (2020-2050)	Mature Shrub- Steppe (2050-)
Hanford sand, disturbed	4.0 ^(c)	72.4 ^(e)	63.0 ^(f)	63.0 ^(f)	31.5 ^(g)	8.0 ^(h)	4.0 ⁽ⁱ⁾

- a. Source: PNNL-14702 Rev. 1, Table 4-15, Ephrata sandy loam and Ephrata stony loam for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- b. Source: PNNL-14702 Rev. 1, Table 4-15, Burbank loamy sand, for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- c. Source: PNNL-14702 Rev. 1, Table 4-15, Rupert sand for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- d. Irrigated agriculture was prevalent in the 100-D/H Area prior to Hanford Site construction; irrigation therefore was conservatively assumed applicable to all 100-D/H sites from calendar years 1880 through 1944. For areas without historic irrigation, the pre-settlement phase ensures until 1944.
- e. Recharge rates for historic irrigation phase is that from the long-term irrigation rate (Irrigation II) under the irrigation recharge scenario (Table 4-2).
- f. Source: PNNL-14702 Rev. 1, Table 4-15, all areas with soils disturbed by excavations; no vegetation.
- g. Source: PNNL-14702 Rev. 1, Table 4-15, all areas with soils disturbed by excavations; cheatgrass.
- h. Source: PNNL-14702 Rev. 1, Table 4-15, all areas with soils disturbed by excavations; young shrub steppe.
- i. Source: PNNL-14702 Rev. 1, Table 4-15, all areas with soils disturbed by excavations; shrub steppe.

Table 4-2. Recharge Rates for Irrigation Recharge Scenario (mm/yr)

Surface Soil Type	Historic Simulation (Pre-2010) (calculation of initial hydraulic conditions)		Predictive Simulation (Post-2010) (calculation of peak groundwater concentration)			
	Pre-Hanford (-1944)	Hanford Operations (1944-2010)	Bare Soil (2010-2015)	Irrigation I (2015-2045)	Irrigation II (2045-)	
Ephrata sandy loam and stony loam	1.5 ^(a)	17.0 ^(a)	17.0 ^(a)	71.4 ^(g)	69.9 ^(g)	
Burbank sandy loam	3.0 ^(b)	52.0 ^(b)	52.0 ^(b)	74.4 ^(g)	71.4 ^(g)	
Rupert sand	4.0 ^(c)	44.0 ^(c)	44.0 ^(c)	76.4 ^(g)	72.4 ^(g)	
Surface Soil Type	Pre-Settlement ^(d) (-1880 or -1944)	Historic Irrigation ^(d) , where applicable (1880-1944)	Hanford Operations (1944-2010)	Bare Soil (2010-2015)	Irrigation I (2020-2050)	Irrigation II (2050-)
Hanford sand, disturbed	4.0 ^(c)	72.4 ^(e)	63.0 ^(f)	63.0 ^(f)	76.4 ^(g)	72.4 ^(g)

- a. Source: PNNL-14702 Rev. 1, Table 4-15, Ephrata sandy loam and Ephrata stony loam for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- b. Source: PNNL-14702 Rev. 1, Table 4-15, Burbank loamy sand, for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- c. Source: PNNL-14702 Rev. 1, Table 4-15, Rupert sand for reactor along river areas; no vegetation, young shrub-steppe, and shrub-steppe
- d. Irrigated agriculture was prevalent in the 100-D/H Area prior to Hanford Site construction; irrigation therefore was conservatively assumed applicable to all 100-D/H sites from calendar years 1880 through 1944. For areas without historic irrigation, the pre-settlement phase ensures until 1944.
- e. Recharge rates for historic irrigation phase is that from the long-term irrigation rate (Irrigation II phase).
- f. Source: PNNL-14702 Rev. 1, Table 4-15, all areas with soils disturbed by excavations; no vegetation.
- g. Recharge rates for future irrigation phases represent incremental increases over corresponding undisturbed native vegetation recharge rates, based on WDOH guidance (WDOH/320-015, Hanford Guidance for Radiological Cleanup). The recharge increment attributable to irrigation alone is 68.4 mm/yr. This increment is added to the corresponding rate for immature shrub steppe (8.0 mm/yr) and mature shrub steppe (4.0 mm/yr) phases of the native vegetation recharge scenario (Table 4-1) to obtain the total recharge rate.

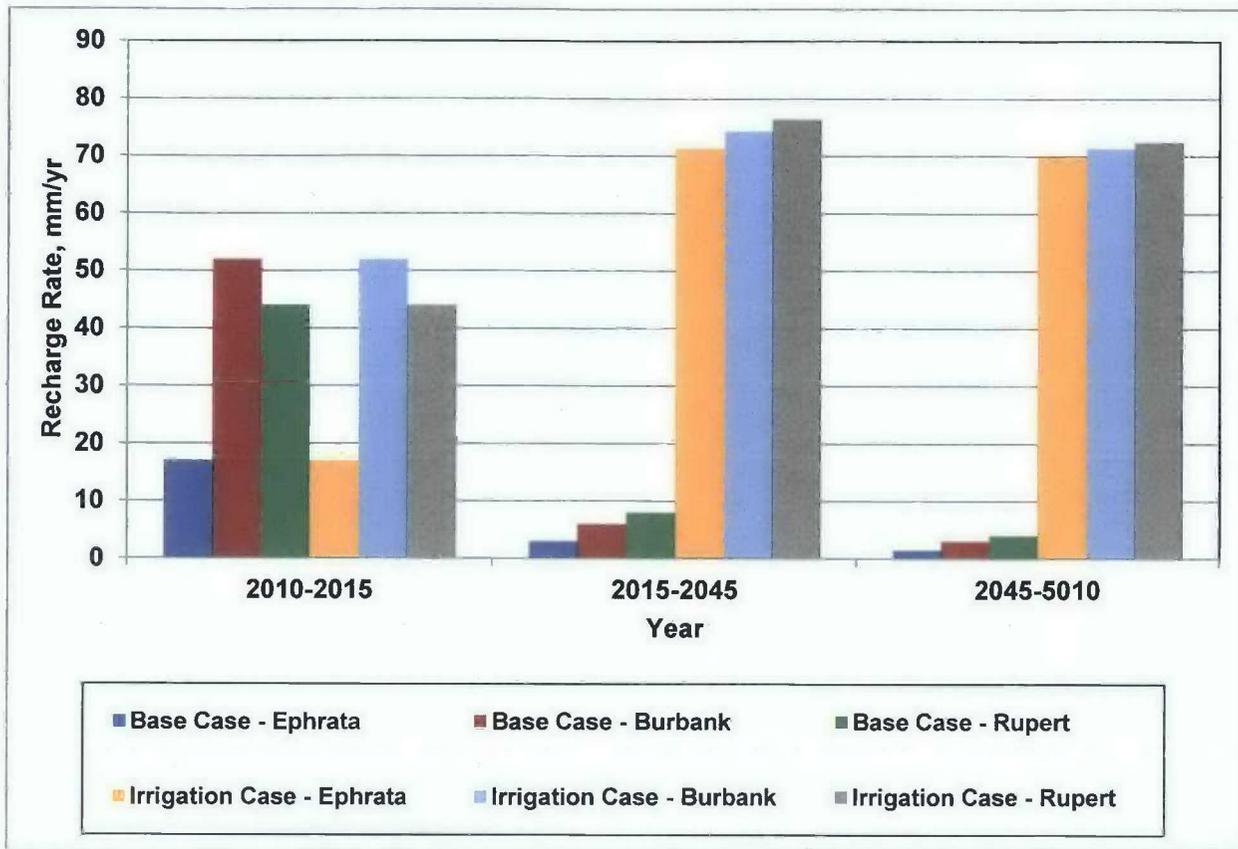


Figure 4-5. Recharge Rates Used for Modeling for Undisturbed Soil Conditions

The recharge rates for the irrigation recharge scenario are specified in Table 4-2 for the three surface soil types used to represent variability and the disturbed soil type. The rates are identical in the historic (pre-2010) periods to those used for the native vegetation recharge scenario. For the predictive (post-2010) simulations, bare soil conditions are assumed to continue for five years (2010 to 2015) as in the native vegetation scenario. Then, irrigation is conservatively assumed to commence in 2016. The recharge rates applied in the “Irrigation I” and “Irrigation II” periods (refer to Table 4-2) were estimated using the same approach employed to assess interim remediation at 100 Area waste sites (DOE/RL-96-17, *Remedial Design Report/Remedial Action Work Plan for the 100 Area*). These site assessments used Remedial Action Goals calculated from RESRAD simulations that assumed total recharge was a combination of irrigation and non-irrigation (base case) recharge rates. As the native vegetation recharge scenario, rates used in the RESRAD simulations were different from those adopted from PNNL-14702, so the RESRAD equation for total recharge was solved to determine the rate attributable to irrigation alone. According to the RESRAD manual, total recharge is a function of precipitation, evapotranspiration, run-off, and applied irrigation, and is defined as

$$I = (1 - C_e)[(1 - C_r)P_r + I_{rr}] \tag{Eqn. 4-9}$$

in which I = annual recharge rate (LT^{-1}), C_e = evapotranspiration coefficient (dimensionless), C_r = runoff coefficient (dimensionless), P_r = annual precipitation rate (LT^{-1}), and I_{rr} = annual irrigation rate (LT^{-1}). Using Equation 4-9 and the RESRAD values for these parameters, $C_e = 0.91$, $C_r = 0.2$, $P_r = 0.16$ m/yr,

and $I_{rr} = 0.76$ m/yr, yielded a total recharge rate of 80 mm/yr. Solving Equation 4-9 with $I_{rr} = 0$ yielded the non-irrigation total recharge rate of 11.6 mm/yr and therefore the recharge attributable to irrigation alone was 68.4 mm/yr, which was then added to the corresponding native vegetation recharge scenario rates to determine a recharge rate for the irrigation recharge scenario for each soil type. For example, the irrigation scenario for the Ephrata soils set the recharge rate to 17 mm/yr from 2010 to 2015, 71.4 mm/yr from 2015 to 2045, and 69.9 mm/yr from 2045 to 5010 (Table 4-2).

Aquifer Flux

The specified pressure values assigned to the edges of the aquifer grid blocks were selected to create a hydraulic gradient across the model domain representative of each geographic area. The hydraulic gradients used for the simulations were based on head data for March 2008 because the greatest number of wells was measured in that month, yielding the greatest number of measurements for all 100 Area source OUs. Additionally, March is midway between low river stage (typically in December) and low river stage (typically in June) for this reach of the Columbia River, and thus can be considered reasonably representative of average conditions over an annual period. Triangulated Irregular Networks (TINs) were developed for the wells using ArcGIS, and hydraulic gradients were computed for each TIN (Table 4-3). This work has been further developed for 100-D, 100-H, and 100-N in ECF-Hanford-14-0028, *Median Hydraulic Gradient Calculation to Support Development of Soil Screening Levels and Preliminary Remediation Goals in the 100 Area*, for a greater time range of hydraulic data (this calculation will be revised to address the remaining geographic areas later). The gradient magnitudes typically varied across two or more orders of magnitude, so the median, a measure of the central tendency of the computed gradients, was selected as a representative value, yielding hydraulic gradients of 0.0014 m/m at 100-D, 0.0035 m/m at 100-H, 0.0039 m/m at 100-K, 0.0019 m/m at 100-BC, 0.0010 m/m at 100-F, 0.0014 m/m at 100-IU-2, 0.0025 m/m at 100-IU-6, and 0.0020 m/m at 100-N.

Table 4-3. Hydraulic Gradients

Geographic Area	Number of Triangular Irregular Networks	Hydraulic Gradient (m/m)				
		Minimum	Maximum	Median	Arithmetic Average	Geometric Average
100-D ^(a)	28	0.00016	0.037	0.0014	0.0023	-
100-H ^(a)	19	0.0011	0.0086	0.0035	0.0037	-
100-K ^(b)	35	0.00085	0.00759	0.00389	0.00379	0.00341
100-F ^(b)	14	0.0002	0.0025	0.0010	0.0011	0.0009
100-IU-2 ^(b)	8	0.0006	0.0024	0.0014	0.0014	0.0013
100-IU-6 ^(b)	14	0.0001	0.0071	0.0025	0.0028	0.0013
100-BC ^(b)	14	0.000012	0.0469	0.0019	0.0018	0.00064
100-N ^(a)	17	0.00025	0.0098	0.0020	0.0022	-

a. Hydraulic gradient calculated in ECF-Hanford-14-0028, *Median Hydraulic Gradient Calculation to Support Development of Soil Screening Levels and Preliminary Remediation Goals in the 100 Area*

b. Hydraulic gradient calculated based on TIN analysis using March 2008 hydraulic data.

Aquifer conditions are dynamic in the 100 Area; the hydraulic gradient, thickness, and in many cases direction of flow vary throughout the year. The use of median gradients for the mid-point month of March is intended to provide a broadly representative value for use in calculation of SSLs and PRGs that will be applicable for the range of locations in each geographic area. This gradient is applied to a model stratigraphy that is based on high-river stage conditions (Section **Error! Reference source not found.**) or the purpose of minimizing the vadose zone thickness as a bounding condition to bound (minimize) transport time

Five representative stratigraphic columns have that include aquifer thicknesses slightly less than 5 m. Specifically, 100-D Columns 4 and 5 (Table 3-2), 100-H Column 2 (Table 3-3), and 100-F Columns 3 and 4 (Table 3-5). It is the aquifer flow rate, rather the aquifer thickness, which determines the dilution rate for vadose zone releases. The aquifer flow rate is determined according to $Q=KAI$, where Q is aquifer flux, K is aquifer conductivity, A is the area perpendicular to flow, and I is the groundwater gradient. Areas for which the representative columns with less than 5-m aquifer thicknesses are representative are subject to the same aquifer flow rate as for upstream locations with greater aquifer thicknesses. Hence, the local hydraulic gradient at these locations must increase in order to maintain the same flux rate through the aquifer as the thickness diminishes. Thus, groundwater dilution rates are similar because the flux is similar. To evaluate this effect in a model would require a more sophisticated modeling effort to apply local hydraulic gradients with seasonal variability, along with seasonally variable aquifer thicknesses, to determine PRGs and SSLs on a waste site by waste site basis. Such refinement is deemed unnecessary to meet the modeling objectives to provide bounding values for SSLs and PRGs; the use of a slightly thicker than actual aquifer (5-m) for these representative stratigraphic columns is offset by the use of the median hydraulic gradient that is lower than it would be for the locations with thinner aquifers.

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4.4.2 Flow and Transport Initial Conditions

For the pre-2010 flow simulations, initial pressure of 86,656.7 Pa, approximately equivalent to -1.5 m matric potential, was assigned to the nodes in the VZ, whereas the aquifer grid blocks were assigned values that matched the boundary condition pressures for the pre-2010 flow simulations. The purpose of the pre-2010 flow simulations is to develop a pressure field that is in equilibrium with the imposed boundary conditions appropriate to the geographic area. Final pressures from the pre-2010 simulations were used as the initial pressures for the post-2010 flow and transport simulations. Thus, the somewhat

arbitrary initial condition selected for the pre-2010 flow simulations does not affect the SSL and PRG calculations.

Based on SGW-51818, *Conceptual Basis for Distribution of Highly Sorbed Contaminants in 100 Areas Vadose Zone*, all contaminants were grouped into two groups, one with lower distribution coefficients ($K_d < 2$ mL/g), and other with the higher distribution coefficients in (≥ 2 mL/g). For the lower K_d contaminants ($K_d < 2$ mL/g), a uniform concentration of 1.0 mg/kg was applied in the entire vadose zone from below the clean backfill down to 0.5 m (two grid blocks) above the water table; this is termed the effective 100:0 initial source distribution (Figure 4-6). Initial concentration in the 0.5 m zone above the water table was not applied due to the physical presence of capillary fringe and water table movement in the periodically rewetted zone that would result from river stage fluctuations. Placing the initial mass at the water table can also result in unrepresentative large peak releases in the simulation start because of the extreme concentration gradients created by the application of this initial condition. According to SGW-51818, for the higher K_d contaminants ($K_d \geq 2$ mL/g) if the soil column is shown to be not contaminated throughout the vertical profile, the most conservative assumption (i.e., contamination throughout the full thickness of the vadose zone) can be considerably relaxed with respect to soil cleanup decisions at waste sites in the 100 Areas. Based on this conclusion, for the high K_d contaminants the upper 70% of the vadose zone below the clean backfill was assumed to be contaminated, while the lower 30% is assumed uncontaminated; this is termed the 70:30 initial source distribution (Figure 4-6). The 70:30 initial source distribution assumption is still conservative for the high K_d contaminants with respect to peak concentration based on observed limited vertical extent (SGW-51818).

A notable exception to the K_d based assignment of an initial source distribution was made for strontium-90. Because field data reveal that this contaminant is found throughout the vadose zone at several sites, use of the 70:30 initial source distribution for this contaminant would clearly be non-conservative. Accordingly, SSL and PRG values were calculated for strontium-90 using the 100:0 initial source distribution at all sites. Strontium-90 is distributed throughout the vadose zone despite its relatively high K_d value for reasons having to do with historic discharge practices that no longer dominate the subsurface. The unit initial concentration is arbitrary, but was chosen only for convenience in calculating PRG values and has no effect on the PRG values since the initial concentration C_i is accounted for in Equation 2-1.

In the calculation methodology, the saturated zone is assumed initially uncontaminated, which may not always be true since plumes can migrate from upgradient locations over time. However, due to several in-built modeling conservatisms, the SSL and PRG calculations are deemed to remain bounding when compared to the results derived from a more sophisticated site-specific predictive model that incorporates all the features and processes relevant at the scale of the model, including any contaminant migration from upgradient locations.

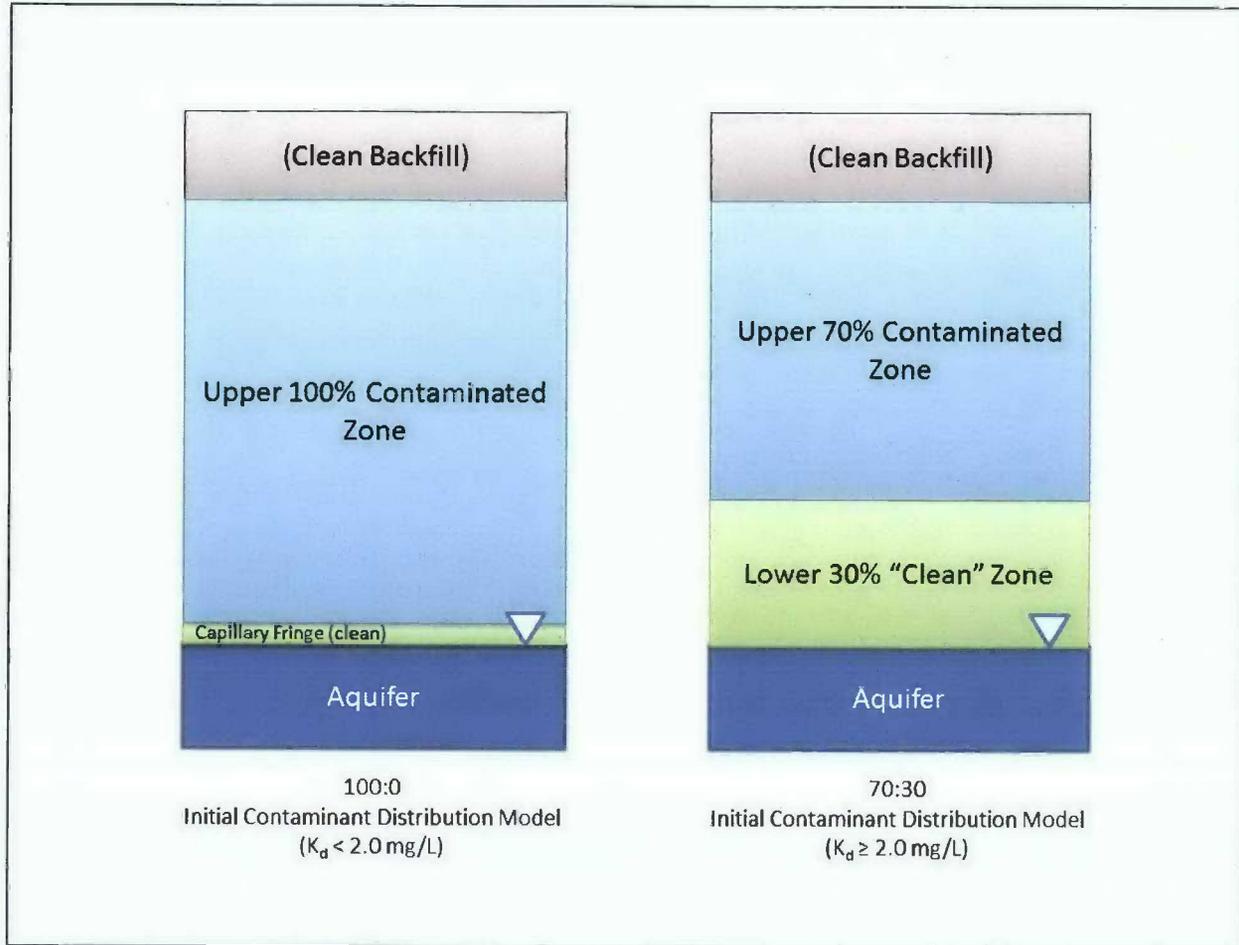


Figure 4-6. Initial Contaminant Distribution Models

4.5 Model Parameterization

Model parameters are presented in this section in terms of hydraulic parameters and ranges (Section 4.5.1) and contaminant transport parameters and ranges (Section 4.5.2).

4.5.1 Hydraulic Parameters and Ranges

To the extent possible, geographic area-specific hydraulic and transport parameter values were used in the STOMP simulations. Based on previous Hanford studies and on the fact that all available measurements of hydraulic properties made the same assumption, the sediments were assumed to follow the van Genuchten (1980) moisture-retention constitutive relation and the Mualem–van Genuchten relative-permeability constitutive relation (Mualem, 1976), thus requiring values to be specified in STOMP for each lithologic unit for:

- Saturated hydraulic conductivity K_s , (LT^{-1}).
- Total porosity n_T (L^3L^{-3}).
- Saturated volumetric water content θ_s , called diffusive porosity n_D in STOMP (L^3L^{-3}).

- Residual saturation s_r (dimensionless), equal to the residual volumetric water content divided by the saturated volumetric water content.
- van Genuchten α (L^{-1}), proportional to the inverse of the air entry matric potential.
- van Genuchten n exponential fitting parameter (dimensionless).

The van Genuchten m parameter was assumed to be fixed and equal to $(n - 1)/n$ and the Mualem β exponent was assumed to be fixed at 0.5 (Mualem, 1976; RPP-20621, *Far-Field Hydrology Data Package for the Integrated Disposal Facility Performance Assessment*).

Hanford and Ringold E units are well to poorly sorted sandy gravels or sandy silty gravels, whereas the backfill consists of poorly sorted sand and gravel with varying fractions of eolian loess and silt (RPP-20621; SGW-44022, *Geologic Data Package in Support of 100-BC-5 Modeling*; SGW-46279, *Conceptual Framework and Numerical Implementation of 100 Areas Groundwater Flow and Transport Model*; PNNL-18564, *Selection and Traceability of Parameters to Support Hanford-Specific RESRAD Analyses Fiscal Year 2008 Status Report*). Within the 100-BC, 100-D, 100-H, 100-K, 100-F, 100-IU-2, and 100-IU-6 geographic areas, the Hanford formation tends to be coarser grained than the Ringold E. The former tends to contain larger gravel clasts than the latter. The Ringold E unit in the 100-BC VZ consists of semi-indurated clay, silt, fine- to coarse-grained sand, and pebble- to cobble-size gravel (SGW-44022). Near the 100-D, 100-H, and 100-K geographic areas the Ringold E unit can locally contain significant amounts of gravel (SGW-40781; SGW-41213; and SGW-46279). The 100-F, 100-IU-2, and 100-IU-6 geographic areas contain larger gravel clasts than the latter, but the Ringold E unit can locally contain significant amounts of gravel (SGW-46279). Where present, the RUM was assumed to act as a lower bound (aquitard) for the aquifer (SGW-46279) and so was not directly included in the STOMP simulations.

Geographic area specific values for several Mualem-van Genuchten hydraulic parameters were obtained for the Hanford formation from data package SGW-46279 (entire 100 Area). This data package cites the data table for the unsaturated hydraulic properties of 15 samples of sandy gravels from the 100 Area, which were originally described in RPP-20621. These 100 Area sediments are dominated by the gravel fraction (> 2 mm size), with gravel clasts accounting for 43% to 75% of the total sample mass (Table 4-4; RPP-20621). Moisture-retention data were measured on the non-gravel sediment fraction (less than 2 mm size) and then corrected for the gravel fraction, whereas hydraulic conductivities were measured on the bulk samples that included the gravel fraction using the constant-head permeameter method for saturated hydraulic conductivity (K_s) and the unit gradient method for unsaturated hydraulic conductivity (RPP-20621). Note that the Hanford formation is the most gravel-rich of the 100 Area lithologies. The K_s measurements were assumed to represent vertical hydraulic conductivity.

Table 4-4. Mualem-van Genuchten Hydraulic Parameters and Fitted Saturated Hydraulic Conductivity Data for 15 Sandy Gravel Samples in the 100 Area Vadose Zone^(a,b)

Sample	HSU ^(c)	Geographic Area	Well Number	Depth (m)	% Gravel	θ_s	θ_r	α	n	K_s
						Saturated Volumetric Moisture Content (cm ³ /cm ³)	Residual Volumetric Moisture Content (cm ³ /cm ³)	van Genuchten Air Entry Fitting Parameter (1/cm)	van Genuchten Exponential Fitting Parameter (-)	Fitted Saturated Hydraulic Conductivity ^(d,e) (cm/s)
2-1307	Ringold	100-HR-3	199-D5-14	18.90	43	0.236	0.0089	0.0130	1.447	1.29E-04
2-1308	Ringold	100-HR-3	199-D5-14	30.64	58	0.120	0.0208	0.0126	1.628	6.97E-05
2-1318	Hanford	100-HR-3	199-D8-54A	15.54	60	0.124	0.0108	0.0081	1.496	1.67E-04
2-2663	Hanford	100-BC-5	199-B2-12	8.20	61	0.135	0.0179	0.0067	1.527	6.73E-05
2-2664	Ringold	100-BC-5	199-B2-12	24.84	73	0.125	0.0136	0.0152	1.516	1.12E-04
2-2666	Hanford	100-BC-5	199-B4-9	21.49	71	0.138	0.00	0.0087	1.284	1.02E-04
2-2667	Hanford	100-BC-5	199-B4-9	23.93	75	0.094	0.00	0.0104	1.296	1.40E-04
3-0570	Hanford	100-KR-1	116-KE-4A	3.50	60	0.141	0.00	0.0869	1.195	2.06E-02
3-0577	Hanford	100-FR-3	199-F5-43B	7.16	66	0.107	0.00	0.0166	1.359	2.49E-04
3-0686	Hanford	100-FR-1	116-F-14	6.49	55	0.184	0.00	0.0123	1.600	5.93E-04
3-1702	Hanford	100-DR-2	199-D5-30	9.78	68	0.103	0.00	0.0491	1.260	1.30E-03
4-1086	Ringold	100-K	199-K-110A	12.77	65	0.137	0.00	0.1513	1.189	5.83E-02
4-1090	Hanford	100-K	199-K-111A	8.20	50	0.152	0.0159	0.0159	1.619	4.05E-04
4-1118	Hanford	100-K	199-K-109A	10.30	66	0.163	0.00	0.2481	1.183	3.89E-02
4-1120	Ringold	100-K	199-K-109A	18.90	63	0.131	0.0070	0.0138	1.501	2.85E-04

Table 4-4. Mualem-van Genuchten Hydraulic Parameters and Fitted Saturated Hydraulic Conductivity Data for 15 Sandy Gravel Samples in the 100 Area Vadose Zone^(a,b)

Sample	HSU ^(c)	Geographic Area	Well Number	Depth (m)	% Gravel	θ_s Saturated Volumetric Moisture Content (cm ³ /cm ³)	θ_r Residual Volumetric Moisture Content (cm ³ /cm ³)	α van Genuchten Air Entry Fitting Parameter (1/cm)	n van Genuchten Exponential Fitting Parameter (-)	K_s Fitted Saturated Hydraulic Conductivity ^(d,e) (cm/s)
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- a. Source: RPP-20621 Rev .0
- b. Moisture retention data were measured on the non-gravel sediment fraction (< 2mm size) and corrected for gravel fraction.
- c. HSU = hydrostratigraphic unit
- d. Assumed to represent vertical hydraulic conductivity
- e. Hydraulic conductivities were measured on the bulk samples that included the gravel fraction using the constant-head permeameter method for saturated hydraulic conductivity (K_s) and the unit gradient method for unsaturated hydraulic conductivity.

Table 4-5 lists the hydraulic parameters used in the STOMP simulations at 100-D and 100-H. Table 4-6 lists the hydraulic parameters used in STOMP simulations in 100-K. Table 4-7 lists the hydraulic parameters used in the STOMP simulations at 100-F, 100-IU-2, and 100-IU-6. Table 4-8 lists the hydraulic parameters used in the STOMP simulations at 100-BC.

The Mualem-van Genuchten hydraulic properties for the Hanford formation in the vadose zone were estimated for each geographic area by averaging the individual parameter values for all samples collected from that geographic area. For example, two samples from borehole 199-D5-14 were selected to provide mean properties for 100-D and 100-H areas for the Ringold Formation, and two samples from boreholes 199-D5-30, and 199-D8-54A (Table 4-4) were selected to provide mean properties for the 100-D and 100-H areas for the Hanford formation (Table 4-5). Vertical saturated hydraulic conductivity of the Hanford formation was obtained by using the geometric mean of the applicable measurements, whereas the other parameters were averaged using the arithmetic mean of the applicable measurements. An exception is the saturated volumetric water content parameter [θ_s in the van Genuchten moisture retention relation, termed diffusive porosity (n_D) in STOMP]. The θ_s values listed in Table 4-4 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, the θ_s values appear to be underestimated and are hard to reconcile with the high K_s values estimated. Therefore, the site-wide estimate of 0.247 was used for Hanford formation (PNNL-18564). There were cases where parameters were unavailable, and the following assumptions were applied to provide needed hydraulic parameters:

- The document and database review did not yield geographic area-specific Mualem-van Genuchten parameter values for the backfill material. Therefore, in the absence of more site-specific data, Hanford site-wide mean parameter values for the backfill reported in Table A.12 of PNNL-18564 were assumed representative for the 100 Area OUs. Mean hydraulic parameters for six samples of backfill and 18 samples of Ringold E gravels that were collected across the Hanford Site (PNNL-18564) were selected to represent these units within the 100 Area (Table 4-5, Table 4-6, Table 4-7, and Table 4-8).
- The document and database review did not yield geographic area specific Mualem-van Genuchten property values for the 100-IU-2 and 100-IU-6 areas. Therefore, the parameters for Hanford formation in the VZ at 100-F were assumed to be representative for the 100-IU-2 and 100-IU-6 (Table 4-7).
- The document and database review did not yield geographic area specific Mualem-van Genuchten property values for the Ringold E unit in the 100-F, 100-IU-2, or 100-IU-6 areas. Therefore, in the absence of more site-specific data, mean hydraulic parameters for 18 samples of Ringold E gravels that were collected across the Hanford Site (reported in PNNL-18564, Table A.12) were selected to represent these units within the 100 Area (Table 4-7).

Geographic area-specific values for Hanford and Ringold E saturated hydraulic conductivities were generally based on parameters reported in the following model data packages for saturated zone modeling: SGW-40781, SGW-41213, and SGW-46279. Horizontal saturated hydraulic conductivity measurements from aquifer (pump) tests and slug tests for the several geographic areas presented in these model data packages were reviewed, and geometric means were calculated for each geographic area from aquifer test measurements only. These are generally the source of the saturated hydraulic conductivity values that are listed in Table 4-5, Table 4-6, Table 4-7, and Table 4-8. Geometric means were used instead of arithmetic means for hydraulic conductivities because the K_s values spanned several orders of magnitude. The following exceptions for assignment of hydraulic conductivity values are noted:

- There were no pumping test data for the Hanford formation in the 100-K geographic area, so the horizontal K_s was set to be ten times the geometric mean vertical K_s for samples from the 100-K geographic area on the basis of an assumed horizontal to vertical anisotropy ratio of 10:1 (Table 4-6).
- The horizontal K_s value for the Hanford unit in the aquifer at 100-F (Table 4-7) was taken from the 100 Area groundwater flow and transport model calibrated value at the time these parameters were developed, which was about 48.3 m/day at the time these values were collected². The vertical K_s value for Hanford unit in the aquifer is assumed to be ten times smaller than horizontal K_s at 100-F (assumed horizontal to vertical anisotropy ratio of 10:1), which is 4.83 m/day.
- For the Hanford formation at 100-IU-2 and 100-IU-6, saturated hydraulic conductivity data were not available, so the horizontal and vertical K_s values for the Hanford formation in the aquifer (Table 4-7) are assumed to be represented by the corresponding values at 100-H (Table 4-5).
- At 100-F, 100-IU-2 and 100-IU-6, saturated hydraulic conductivity data were not available. Therefore, the corresponding values at 100-D (Table 4-5) are assumed to represent the horizontal and vertical K_s values for Ringold E unit in the aquifer at the 100-F, 100-IU-2, and 100-IU-6 OUs (Table 4-7). There are no measurements of K_s for the Hanford formation in the saturated zone in 100-BC. To estimate a value, the ratio of horizontal K_s for Hanford formation between the SZ and VZ at 100-H was calculated (ratio of 53.8), and this ratio was used to estimate the K_s for Hanford in the SZ at 100-BC. The horizontal K_s for Hanford formation in the VZ at 100-BC is 1.02E-03 cm/s, and the corresponding horizontal K_s for Hanford formation in the SZ is about 47.4 m/day (5.49E-02 cm/s) at 100-BC based on the above ratio (Table 4-8).
- There are no measurements of K_s for the Ringold Formation in the saturated zone in 100-BC. To estimate a value, the calibrated value from the 100 Area Groundwater Model (SGW-40679) was used, which is about 6.2 m/day (7.18E-03 cm/s).

100-NR-1 OU-specific values for several Mualem-van Genuchten hydraulic parameters were obtained for the Hanford formation from DOE/RL-96-11, *1301-N and 1325-N Liquid Waste Disposal Facilities Limited Field Investigation Report* and four additional raw data points obtained from HEIS. The RETC software (EPA/600/2-91/065, *The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils*) was used to analyze the raw data to obtain the unsaturated hydraulic properties. These property values are all gravel corrected. The gravel correction was done using Equation 4 in WHC-EP-0883, *Variability and Scaling of Hydraulic Properties for 200 Area soils, Hanford Site*. There were other eight samples from the 100-N Area reported in DOE/RL-96-11. All the available vadose zone parameter values are listed in Table 4-9. The 100-N Area sediments are dominated by the gravel fraction (> 2-mm size), with gravel clasts accounting for 4 to 82% of the total sample mass (Table 4-9). Moisture retention data were measured on the non-gravel sediment fraction (< 2mm size) and corrected for gravel fraction. The gravel correction was done using Equation 1 (WHC-EP-0883, *Variability and Scaling of Hydraulic Properties for 200 Area soils, Hanford Site*, Equation 4):

$$\theta_{(b,s)} = F_f \theta_{(f,s)} = (1 - F_g) \theta_{(f,s)} \quad \text{Equation 1}$$

² Note that the current version of the 100 Area Groundwater Model has a calibrated value of 100 m/day for this parameter (SGW-46279 Rev. 2).

where $\theta_{(b,s)}$ is the volumetric moisture content of the bulk soil which includes gravel, $\theta_{(f,s)}$ is the volumetric moisture content of the fines (the fraction tested in the laboratory), F_f is the volumetric fraction of the bulk soil sample passing through the No. 10 sieve (< 2mm), and F_g is the volumetric gravel fraction (the complement of F_f). This is well-established procedure for soils with substantial aggregate such as the Hanford Site.

Horizontal saturated hydraulic conductivity measurements from aquifer slug tests for the several areas presented therein were reviewed and geometric means were calculated for aquifer test measurements only (Table 4-10). These mean K_s values ranged from 2.6 to 9.4 m/day (Table 4-10). The geometric mean horizontal K_s values shown in Table 4-10 for the Ringold E in 100-N Area were compared against the range of preliminary calibration values currently in use for the 100 Area groundwater flow and transport model and found to be reasonably consistent. Vertical anisotropy value commonly assumed is 0.1 for Hanford Site sediments (SGW-40781; SGW-41213; and SGW-46279).

The Mualem-van Genuchten hydraulic properties for the Hanford formation were estimated for 100-N Area by averaging the individual parameter values for all samples (Table 4-11). An exception is the saturated volumetric water content, given symbol θ_s in the van Genuchten (1980) moisture retention relation and equivalent to the diffusive porosity n_D in STOMP. The θ_s values in Table 4-9 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2mm fraction. The absence of the gravels may have resulted in underestimation of the void volume available for flow because of the difficulty in reconciling high K_s values with very low porosity values. Therefore, the Hanford site-wide estimate of 0.280 and Ringold site-wide estimates of 0.293 were adopted for the total porosity in these units.

Mualem-van Genuchten parameters for the Hanford formation in the 100-N Area were determined from the six samples taken from the Hanford formation in boreholes 199-N-108A and 199-N-109A. The arithmetic mean from all the available data was calculated for all the hydraulic parameters except for K_s . However, in the case of the K_s value, the geometric mean was calculated for sample identification codes BOGL72, BOGL74, BOGL98, BOGLB0 and BOGLB2. The horizontal aquifer saturated conductivity $K_{s,h}$ was estimated as ten times the vertical saturated hydraulic conductivity ($K_{s,h} = 10 \times K_{s,v}$).

Mualem-van Genuchten parameters for the Ringold Formation in 100-N were determined from the six samples taken from boreholes 199-N-108A and 199-N-109A. The arithmetic mean from all the available data was calculated for all the hydraulic parameters except for K_s . For K_s , the geometric mean was calculated from all the available samples and was used as model input. The horizontal aquifer K_s was also taken to be $10 \times K_{s,v}$.

Table 4-5. Hydraulic Parameters Used for Geographic Areas 100-D and 100-H

Geographic Area	Zone	Unit	n_T	n_D	α	n	s_r	$K_{s h}$	$K_{s v}$
			Total Porosity (cm ³ /cm ³)	Diffusive Porosity (cm ³ /cm ³)	van Genuchten Air Entry Fitting Parameter (1/cm)	van Genuchten Exponential Fitting Parameter (-)	Residual Saturation (-)	Horizontal Saturated Hydraulic Conductivity (cm/s)	Vertical Saturated Hydraulic Conductivity (cm/s)
100-D	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.019 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.029 ^(c)	1.378 ^(c)	0.022 ^(c)	4.66E-03 ^(d)	4.66E-04 ^(d)
	Vadose	Ringold E	0.293 ^(e)	0.267 ^(e)	0.013 ^(f)	1.538 ^(f)	0.057 ^(f)	9.48E-04 ^(g)	9.48E-05 ^(g)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.029 ^(c)	1.378 ^(c)	0.022 ^(c)	6.42E-02 ^(h)	6.42E-03 ^(h)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.013 ^(f)	1.538 ^(f)	0.057 ^(f)	2.59E-02 ⁽ⁱ⁾	2.59E-03 ⁽ⁱ⁾
100-H	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.019 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.029 ^(c)	1.378 ^(c)	0.022 ^(c)	4.66E-03 ^(d)	4.66E-04 ^(d)
	Vadose	Ringold E	0.293 ^(e)	0.267 ^(e)	0.013 ^(f)	1.538 ^(f)	0.057 ^(f)	9.48E-04 ^(f)	9.48E-05 ^(f)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.029 ^(c)	1.378 ^(c)	0.022 ^(c)	1.13E-01 ^(h)	1.13E-02 ^(h)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.013 ^(f)	1.538 ^(f)	0.057 ^(f)	4.28E-03 ⁽ⁱ⁾	4.28E-04 ⁽ⁱ⁾

Table 4-5. Hydraulic Parameters Used for Geographic Areas 100-D and 100-H

Geographic Area	Zone	Unit	n_T Total Porosity (cm ³ /cm ³)	n_D Diffusive Porosity (cm ³ /cm ³)	α van Genuchten Air Entry Fitting Parameter (1/cm)	n van Genuchten Exponential Fitting Parameter (-)	S_r Residual Saturation (-)	$K_{s h}$ Horizontal Saturated Hydraulic Conductivity (cm/s)	$K_{s v}$ Vertical Saturated Hydraulic Conductivity (cm/s)
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- a. Source: arithmetic mean of hydraulic parameters for backfill calculated for six samples that were collected within the Hanford Site (hydraulic conductivity assumed isotropic for backfill) reported in PNNL-18564, Table A.12 (these are also the site-wide values for backfill listed in PNNL-14702 Rev. 1, Table 4.5)
- b. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Hanford gravelly sand (Hgs), site-wide. Note the saturated volumetric moisture content values listed in Table 4-4 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, these values appeared to be underestimated and were inconsistent with the high K_s values estimated, so this site-wide estimate was used.
- c. Source: computed arithmetic mean of values for two Hanford formation samples from 100-D and 100-H (Table 4-4, samples 2-1318 and 3-1702).
- d. Source: computed geometric mean of values for two Hanford formation samples from 100-D and 100-H (Table 4-4, samples 2-1318 and 3-1702) for vertical value; horizontal value computed based on assumed anisotropic ratio of 0.1.
- e. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Ringold gravel (Rg), site-wide.
- f. Source: computed arithmetic mean of values for two Ringold Formation samples from 100-D and 100-H (Table 4-4, samples 2-1307 and 3-1308).
- g. Source: computed geometric mean of values for two Ringold Formation samples from 100-D and 100-H (Table 4-4, samples 2-1307 and 3-1308); horizontal value computed based on assumed anisotropic ratio of 0.1.
- h. Source: vertical saturated hydraulic conductivity for saturated zone units was calculated as the geometric mean of aquifer test measurements for the Hanford formation in the 100-D and 100-H areas of data reported in SGW-40781 Rev. 1, Table 7-1.
- i. Source: vertical saturated hydraulic conductivity for saturated zone units was calculated as the geometric mean of aquifer test measurements for the Ringold formation in the 100-D and 100-H areas of data reported in SGW-40781 Rev. 1, Table 7-1.

Table 4-6. Hydraulic Parameters Used for Geographic Area 100-K

Geographic Area	Zone ^(a)	Unit	n_T	n_D	α_c	n	S_r	$K_{s/h}$	$K_{s/v}$
			Total Porosity (cm ³ /cm ³)	Diffusive Porosity (cm ³ /cm ³)	van Genuchten Air Entry Fitting Parameter (1/cm)	van Genuchten Exponential Fitting Parameter (-)	Residual Saturation (-)	Horizontal Saturated Hydraulic Conductivity (cm/s)	Vertical Saturated Hydraulic Conductivity (cm/s)
100-K	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.019 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.117 ^(c)	1.332 ^(c)	0.021 ^(c)	6.87E-02 ^(d)	6.87E-03 ^(d)
	Vadose	Ringold E	0.293 ^(e)	0.267 ^(e)	0.083 ^(f)	1.345 ^(f)	0.013 ^(f)	4.08E-02 ^(g)	4.08E-03 ^(g)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.117 ^(c)	1.332 ^(c)	0.021 ^(c)	3.60E-01 ^(h)	3.60E-02 ^(h)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.083 ^(f)	1.345 ^(f)	0.013 ^(f)	4.86E-03 ⁽ⁱ⁾	4.86E-04 ⁽ⁱ⁾

- a. Source: arithmetic mean of hydraulic parameters for backfill calculated for six samples that were collected within the Hanford Site (hydraulic conductivity assumed isotropic for backfill) reported in PNNL-18564, Table A.12 (these are also the site-wide values for backfill listed in PNNL-14702 Rev. 1, Table 4.5)
- b. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Hanford gravelly sand (Hgs), site-wide. Note the saturated volumetric moisture content values listed in Table 4-4 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, these values appeared to be underestimated and were inconsistent with the high K_s values estimated, so this site-wide estimate was used.
- c. Source: computed arithmetic mean of values for three Hanford formation samples from 100-K (Table 4-4, samples 3-0570, 4-1090, and 4-1118).
- d. Source: computed geometric mean of values for three Hanford formation samples from 100-K (Table 4-4, samples 3-0570, 4-1090, and 4-1118) for vertical value; horizontal value computed based on assumed anisotropic ratio of 0.1.
- e. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Ringold gravel (Rg), site-wide.
- f. Source: computed arithmetic mean of values for two Ringold Formation samples from 100-K (Table 4-4, samples 4-1086 and 4-1120).
- g. Source: computed geometric mean of values for two Ringold Formation samples from 100-K (Table 4-4, samples 4-1086 and 4-1120); horizontal value computed based on assumed anisotropic ratio of 0.1.
- h. Source: vertical saturated hydraulic conductivity for saturated zone units was calculated as the geometric mean of aquifer test measurements for the Hanford formation in the 100-K areas of data reported in SGW-40781 Rev. 1, Table 7-1.
- i. Source: vertical saturated hydraulic conductivity for saturated zone units was calculated as the geometric mean of aquifer test measurements for the Ringold formation in the 100-K areas of data reported in SGW-40781 Rev. 1, Table 7-1.

Table 4-7. Hydraulic Parameters Used for Geographic Areas 100-F, 100-IU-2 and 100-IU-6

Geographic Area	Zone	Unit	n_T	n_D	α	n	S_r	K_{sh}	K_{sv}
			Total Porosity (cm ³ /cm ³)	Diffusive Porosity (cm ³ /cm ³)	van Genuchten Air Entry Fitting Parameter (1/cm)	van Genuchten Exponential Fitting Parameter (-)	Residual Saturation (-)	Horizontal Saturated Hydraulic Conductivity (cm/s)	Vertical Saturated Hydraulic Conductivity (cm/s)
100-F	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.0190 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.0145 ^(c)	1.480 ^(c)	0.000 ^(c)	3.84E-03 ^(d)	3.84E-04 ^(d)
	Vadose	Ringold E	0.293 ^(e)	0.267 ^(e)	0.0080 ^(f)	1.660 ^(f)	0.097 ^(f)	4.13E-03 ^(g)	4.13E-04 ^(g)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.0145 ^(c)	1.480 ^(c)	0.000 ^(c)	5.59E-02 ^(h)	5.59E-03 ^(h)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.0080 ^(f)	1.660 ^(f)	0.097 ^(f)	2.59E-02 ⁽ⁱ⁾	2.59E-03 ⁽ⁱ⁾
100-IU-2 & 100-IU-6	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.0190 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.0145 ^(c)	1.480 ^(c)	0.000 ^(c)	3.84E-03 ^(d)	3.84E-04 ^(d)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.0145 ^(c)	1.480 ^(c)	0.000 ^(c)	1.13E-01 ^(j)	1.13E-02 ^(j)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.0080 ^(f)	1.660 ^(f)	0.097 ^(f)	2.59E-02 ^(k)	2.59E-03 ^(k)

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- a. Source: arithmetic mean of hydraulic parameters for backfill calculated for six samples that were collected within the Hanford Site (hydraulic conductivity assumed isotopic for backfill) reported in PNNL-18564, Table A.12 (these are also the site-wide values for backfill listed in PNNL-14702 Rev. 1, Table 4.5)
 - b. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Hanford gravelly sand (Hgs), site-wide. Note the saturated volumetric moisture content values listed in Table 4-4 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, these values appeared to be underestimated and were inconsistent with the high K_s values estimated, so this site-wide estimate was used.
 - c. Source: computed arithmetic mean of values for two Hanford formation samples from 100-HR-3 (Table 4-4, samples 3-0577 and 3-0686).
 - d. Source: computed geometric mean of values for two Hanford formation samples from 100-HR-3 (Table 4-4, samples 3-0577 and 3-0686) for vertical value; horizontal value computed based on assumed anisotropic ratio of 0.1.
 - e. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Ringold gravel (Rg), site-wide.
 - f. Source: arithmetic mean of hydraulic parameters for Ringold Formation gravel (Rg) calculated for 18 samples that were collected within the Hanford Site reported in PNNL-18564, Table A.12.
 - g. Source: arithmetic mean of hydraulic conductivities for Ringold Formation gravel (Rg) calculated for 18 samples that were collected within the Hanford Site, with hydraulic conductivity assumed to have anisotropic ratio of 0.1, reported in PNNL-18564, Table A.12.
 - h. Source: the horizontal saturated hydraulic conductivity value for the Hanford formation in the aquifer (saturated zone) at 100-F was assigned the calibrated value from an earlier version of the 100 Area Groundwater Model (~48.3 m/day), with the vertical value computed based on assumed anisotropic ratio of 0.1. [Note that the most recent version of the 100 Area Groundwater Model sets this calibrated value at 100 m/day (SGW-46279 Rev. 2, Table 6.2)].
 - i. Source: the horizontal and vertical saturated hydraulic conductivity values for the Ringold Formation in the aquifer (saturated zone) at 100-F is represented by the corresponding values at 100-D (Table 4-5).
 - j. Source: the horizontal and vertical saturated hydraulic conductivity values for the Hanford formation in the aquifer (saturated zone) at 100-IU-2 and 100-IU-6 are represented by the corresponding values at 100-H.
 - k. Source: the horizontal and vertical K_s values for the Ringold Formation in the aquifer at 100-IU-2 and 100-IU-6 are represented by the corresponding values at 100-D (Table 4-5).
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Table 4-8. Hydraulic parameters used for Geographic Area 100-BC

Geographic Area	Zone ^(a)	Unit	n_T	n_D	α	n	S_r	$K_{s/h}$	$K_{s/v}$
			Total Porosity (cm ³ /cm ³)	Diffusive Porosity (cm ³ /cm ³)	van Genuchten Air Entry Fitting Parameter (1/cm)	van Genuchten Exponential Fitting Parameter (-)	Residual Saturation (-)	Horizontal Saturated Hydraulic Conductivity (cm/s)	Vertical Saturated Hydraulic Conductivity (cm/s)
100-BC	Backfill	Hanford	0.276 ^(a)	0.262 ^(a)	0.0190 ^(a)	1.400 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.009 ^(c)	1.369 ^(c)	0.024 ^(c)	9.87E-04 ^(d)	9.87E-05 ^(d)
	Vadose	Ringold E	0.293 ^(e)	0.267 ^(e)	0.015 ^(f)	1.516 ^(f)	0.052 ^(f)	1.12E-03 ^(g)	1.12E-04 ^(g)
	Saturated	Hanford	0.280 ^(b)	0.247 ^(b)	0.009 ^(c)	1.369 ^(c)	0.024 ^(c)	5.49E-02 ^(h)	5.49E-03 ^(h)
	Saturated	Ringold E	0.293 ^(e)	0.267 ^(e)	0.015 ^(f)	1.516 ^(f)	0.052 ^(f)	7.18E-03 ⁽ⁱ⁾	7.18E-04 ⁽ⁱ⁾

- a. Source: arithmetic mean of hydraulic parameters for backfill calculated for six samples that were collected within the Hanford Site (hydraulic conductivity assumed isotopic for backfill) reported in PNNL-18564, Table A.12 (these are also the site-wide values for backfill listed in PNNL-14702 Rev. 1, Table 4.5)
- b. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Hanford gravelly sand (Hgs), site-wide. Note the saturated volumetric moisture content values listed in Table 4-4 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, these values appeared to be underestimated and were inconsistent with the high K_s values estimated, so this site-wide estimate was used.
- c. Source: computed arithmetic mean of values for three Hanford formation samples from 100-BC (Table 4-4, samples 2-2663, 2-2666, and 2-2667).
- d. Source: computed geometric mean of values for three Hanford formation samples from 100-BC (Table 4-4, samples 2-2663, 2-2666, and 2-2667) for vertical value; horizontal value computed based on assumed anisotropic ratio of 0.1.
- e. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Ringold gravel (Rg), site-wide.
- f. Source: single Ringold Formation sample from 100-BC (Table 4-4, sample 2-2664).
- g. Source: single Ringold Formation sample from 100-BC (Table 4-4, sample 2-2664); horizontal value computed based on assumed anisotropic ratio of 0.1.
- h. Source: there were no measurements of this parameter available for the Hanford formation in the saturated zone. The ratio of horizontal saturated hydraulic conductivities for the Hanford formation between the saturated and vadose zones is about 53.8 at 100-H. This ratio was used to estimate the horizontal saturated hydraulic conductivity for the Hanford formation in the saturated zone at 100-BC. The horizontal saturated hydraulic conductivity for Hanford formation in the vadose zone at 100-BC is 1.02E-03 cm/s, so the estimated horizontal saturated hydraulic conductivity for Hanford formation in the SZ is about 47.4 m/day (5.49E-02 cm/s) at 100-BC, based on scaling by the above ratio.
- i. Source: there are no measurements of horizontal saturated hydraulic conductivity for the Ringold Formation in the saturated zone in 100-BC. To estimate a value, the calibrated value from the 100 Area groundwater flow and transport model (SGW-40679) was used, which is about 6.2 m/day (7.18E-03 cm/s).

Table 4-9. Mualem-van Genuchten Hydraulic Parameters for Sandy Gravels in the 100-N Area Vadose Zone

Sample	Hydro-stratigraphic Unit	Well Number	Depth (m)	% Gravel	θ_s	θ_r	α	n	K_s
					Saturated Volumetric Moisture Content (cm ³ /cm ³)	Residual Volumetric Moisture Content (cm ³ /cm ³)	van Genuchten (1980) Air Entry Head Fitting Parameter (1/cm)	van Genuchten (1980) Exponential Fitting Parameter (-)	Fitted Saturated Hydraulic Conductivity (cm/s)
2-3055 ^(a)	Hanford	199-N-108A	25-26	82	0.063	0	0.00512	1.31866	-
2-3056 ^(a)	Ringold	199-N-108A	46.5-47.5	60	0.129	0.0185	0.0375	1.6767	-
2-3057 ^(a)	Ringold	199-N-108A	53-54	60	0.152	0.0083	0.01805	1.8545	-
2-3058 ^(a)	Ringold	199-N-108A	93.5-94.5	60	0.139	0.0168	0.01388	1.788	-
BOGL72 ^(b)	Hanford	199-N-108A	15-15.5	69	0.1540	0.000	0.0018	1.6482	3.20E-04
BOGL74 ^(b)	Hanford	199-N-108A	24-24.5	4	0.4834	0.000	0.0081	1.4477	2.99E-05
BOGL80 ^(b)	Ringold	199-N-108A	43-43.5	60	0.1700	0.000	0.0032	1.5175	8.21E-04
BOGL85 ^(b)	Ringold	199-N-108A	62.8-63.3	51	0.2130	0.000	0.0024	1.6859	7.38E-04
BOGL98 ^(b)	Hanford	199-N-109A	10.5-11	76	0.0564	0.000	0.0148	1.3475	5.89E-02
BOGLB0 ^(b)	Hanford	199-N-109A	17.5-18	65	0.1070	0.000	0.0213	1.3184	5.80E-02
BOGLB2 ^(b)	Hanford	199-N-109A	24.5-25	72	0.0770	0.000	0.0084	1.3796	6.20E-03
BOGLB7 ^(b)	Ringold	199-N-109A	39.5-40	72	0.0628	0.000	0.0043	1.4565	5.29E-03

a. Source: Hanford Environmental Information System (HEIS), for the sample identification numbers shown.

b. Source: DOE/RL-96-11, 1301-N and 1325-N Liquid Waste Disposal Facilities Limited Field Investigation Report.

Table 4-10. Aquifer Horizontal Saturated Hydraulic Conductivity Data Specific to 100-N Area

Source Area	Aquifer Formation	Number of Tests	Saturated Horizontal Hydraulic Conductivity $K_{s,h}$ ^(a)			
			Minimum (m/day)	Maximum (m/day)	Geometric Mean	
					(m/day)	(cm/s)
100-N	Ringold	8	2.6	9.4	5.0	5.78E-03

a. Source: ECF-100NR2-12-0031, *Analysis of Data Collected from Slug Tests Conducted in Remedial Investigation Boreholes Within the 100-NR-2 Groundwater Operable Unit.*

Table 4-11. Hydraulic Parameters Used for 100-N Source Areas

Source Operable Unit	Zone	Formation	n_T	n_D	α	n	S_r	K_s	
			Total Porosity (cm ³ /cm ³)	Diffusive Porosity (cm ³ /cm ³)	van Genuchten (1980) Air Entry Head Fitting Parameter	van Genuchten (1980) Exponential Fitting Parameter (-)	Residual Saturation (-)	Saturated Hydraulic Conductivity	
							Horizontal	Vertical	
							(cm/s)	(cm/s)	
100-N	Backfill	Backfill	0.276 ^(a)	0.262 ^(a)	0.0190 ^(a)	1.40 ^(a)	0.103 ^(a)	5.98E-04 ^(a)	5.98E-04 ^(a)
	Vadose	Hanford	0.280 ^(b)	0.247 ^(b)	0.00990 ^(c)	1.41 ^(c)	0.000 ^(c)	2.89E-02 ^(d)	2.89E-03 ^(e)
	Vadose	Ringold E	0.293 ^(f)	0.267 ^(f)	0.0132 ^(g)	1.66 ^(g)	0.0272 ^(g)	1.47E-02 ^(d)	1.47E-03 ^(h)
	Saturated	Ringold E	0.293 ^(f)	0.267 ^(f)	0.0132 ^(g)	1.66 ^(g)	0.0272 ^(g)	5.78E-03 ⁽ⁱ⁾	5.78E-04 ^(d)

- a. Source: arithmetic mean of hydraulic parameters for backfill calculated for six samples that were collected within the Hanford Site (hydraulic conductivity assumed isotropic for backfill) reported in PNNL-18564, Table A.12 (these are also the site-wide values for backfill listed in PNNL-14702 Rev. 1, Table 4.5).
- b. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Hanford gravelly sand (Hgs), site-wide. Note the saturated volumetric moisture content values listed in Table 4-9 were determined by applying a gravel correction factor to the values determined in the laboratory on the < 2 mm fraction. However, these values appeared to be underestimated and were inconsistent with the high K_s values estimated, so a site-wide estimate was used.
- c. Source: computed arithmetic mean of values for six Hanford formation samples (Table 4-9, samples 2-3055, BOGL72, BOGL74, BOGL98, and BOGLB0, and BOGLB2).
- d. Source: calculated based on assumed vertical-to-horizontal anisotropy for Hanford Site sediments of 0.1.
- e. Source: geometric mean calculated for five Hanford formation samples (Table 4-9, samples BOG72, BOGL74, BOGL98, BOGLB0, and BOGLB2).
- f. Source: PNNL-18564, Tables 6.3 and 6.4, values for total and effective porosity for Ringold gravel (Rg), site-wide.
- g. Source: computed arithmetic mean of values for six Ringold E Formation samples (Table 4-9, samples 2-3056, 2-3057, 2-3058, BOGL80, BOGL85, and BOGLB7).
- h. Source: geometric mean calculated for three Ringold E Formation samples (Table 4-9, samples BOGL80, BOGL85, and BOGLB7).
- i. Source: ECF-100NR2-12-0031, *Analysis of Data Collected from Slug Tests Conducted in Remedial Investigation Boreholes Within the 100-NR-2 Groundwater Operable Unit*.

For transport simulations, STOMP requires the particle density (ρ_p) values of the backfill, Hanford formation, and Ringold units. The particle density of each unit can be calculated using the bulk density (ρ_B) and dividing it by 1- Total Porosity term. Bulk density is necessary for retardation scaling factor calculations. Estimates of bulk density for Hanford formation and Ringold E unit were obtained from PNNL-14702, which gave 1.91 g/cm³ for the Hanford formation and 1.90 g/cm³ for the Ringold E unit. The bulk density estimate of 1.94 g/cm³ for backfill was obtained from PNNL-18564. Dispersion was conservatively assumed negligible, so dispersivity values were all set to zero. Barring numerical dispersion introduced by the solution method, setting dispersivity values to zero yields higher peak concentrations than setting non-zero values and therefore yields conservative PRG values.

4.5.2 Contaminant Transport Parameters and Ranges

Partition coefficient, K_d , values for sorption were identified in ECF-Hanford-12-0023, *Groundwater and Surface Water Cleanup Levels and Distribution Coefficients for Nonradiological and Radiological Analytes in the 100 Areas and 300 Area*. As described in Section 5, simulations were run to produce peak groundwater concentrations for a subset of the range of distribution coefficients required for all contaminants of interest. Typically, the subset comprised 26 distribution coefficients (Table 4-12) between 0 and 16 mL/g. Dividing the K_d range from 0 to 16 mL/g into 26 distribution coefficients and performing calculations provides enough resolution for interpolation in peak concentration when the K_d for a given contaminant falls between the two values for which simulations were performed. For those contaminants with K_d values greater than 16 mL/g, the peak concentration was calculated by using the scaling methods described in Section 5.

For 100-D, 100-H and 100-N areas, the distribution coefficient for each contaminant was directly simulated. Therefore, no interpolation was needed for obtaining peak groundwater concentration in those areas.

4.6 Implementation Using STOMP

Calculations using STOMP are performed in two modeling steps. The first step, called the pre-2010 model, is used to simulate flow through the representative column up to Year 2010. A long-term transient-state simulation is performed so that near steady state hydrologic conditions are reached in the model domain based on the prescribed boundary conditions. The result of this model is used to set up the initial conditions for the second modeling step where both flow and transport are simulated for a period of 1,000 years (starting from year 2010). A detailed description of the STOMP input files³ for both models is presented in Appendix B for a representative column chosen from 100-D geographic area.

³ The parameter values are presented for the purpose of illustration of the model set-up only and do not necessarily imply that the final calculations were run with this parameter set.

Table 4-12. Distribution Coefficients (K_d) used in STOMP Simulations

Distribution Coefficient (mL/g)
0
0.00001
0.0001
0.001
0.01
0.02
0.04
0.06
0.08
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
2.0
4.0
8.0
10.0
12.0
14.0
16.0

5. Model Results and Application

The peak groundwater concentrations obtained by employing STOMP were used to identify those constituents that pose a significant risk from a fate and transport perspective. The objective was to determine concentration of contaminants in the VZ that will not cause an exceedance of groundwater and surface water regulatory standards for the ranges of conditions observed within the 100 Area. Two sets of residual contaminant concentrations for the VZ were developed: SSL and PRGs, each with its own specific purpose.

The SSL for each analyte is defined as the larger of a background level, a practical quantification limit, or a calculated SSL that was computed using STOMP and a highly conservative set of assumptions on contaminant distribution and recharge rates. SSL are used to separate analytes from COPCs and determine which COPCs warrant further evaluation or investigation (EPA/540/R-96/018; EPA/540/R-95/128; DOE-STD-1153-2002). PRGs are defined as the allowable concentrations or activities of constituents in the VZ that are protective of groundwater and surface water quality. PRGs are calculated for COPCs that failed the screening process. For the lower K_d contaminants ($K_d < 2$ mL/g), a uniform concentration of 1.0 mg/kg was applied in the entire vadose zone below the clean backfill up to 0.5 m (two grid blocks) above the water table for the low K_d contaminants; this is termed the effective 100:0 initial source distribution. Initial concentration in the 0.5 m zone above the water table was not applied due to the physical presence of capillary fringe and water table movement in the periodically rewetted zone that would result from river stage fluctuations. Placing the initial mass at the water table can also result in unrepresentative large peak releases in the simulation start because of the extreme concentration gradients created by the application of this initial condition. According to SGW-51818, for the higher K_d contaminants ($K_d \geq 2$ mL/g) if the soil column is shown to be not contaminated throughout the vertical profile, the most conservative assumption (i.e., contamination throughout the full thickness of the vadose zone) can be considerably relaxed with respect to soil cleanup decisions at waste sites in the 100 Areas. Based on this conclusion, for the high K_d contaminants the upper 70% of the vadose zone below the clean backfill was assumed to be contaminated while the lower 30% is treated as uncontaminated; this is termed the 70:30 initial source distribution. The 70:30 initial source distribution assumption is still conservative for the high K_d contaminants with respect to peak concentration based on observed limited vertical extent (SGW-51818)

5.1 Peak Concentration Calculation and Scaling

Peak concentrations for use in calculating SSLs or PRGs were obtained by running multiple simulations using STOMP for the set of K_d values listed in Table 4-12 for the irrigation recharge scenario in the case of SSLs, and for the native vegetation recharge scenario in the case of PRGs. Peak concentrations are estimated, based on the K_d value of each contaminant from linear interpolation of the results of the STOMP simulations, as follows:

1. For contaminants in the range $K_d \leq 1.0$, the 'FORECAST' function in Excel® that uses a best fit (least squares) linear regression is used to estimate peak concentration.
2. For contaminants in the range $1.0 < K_d < 2.0$, a fitted linear regression equation created by performing a linear regression of STOMP simulated peak concentrations against K_d values in the range $0.5 < K_d < 2.0$. This range is estimated separately from higher K_d values because a different initial solute condition (100:0 initial distribution) is used for $K_d < 2.0$ than for higher values. An example is shown in Figure 5-1 using 100-D representative stratigraphic column 1

with irrigation recharge for Ephrata sandy loam soil. For the contaminants with higher K_d values, the inverse of peak concentrations ($1/CPK$) varies nonlinearly with K_d values.

3. For the contaminants in the range $2.0 \leq K_d \leq 8.0$, the 'FORECAST' function in Excel® that uses a best fit (least squares) linear regression is used to perform a linear regression of STOMP simulated peak concentrations against K_d values over the same range. This range is estimated separately from lower K_d values because a 70:30 distribution is used (in contrast to the 100:0 initial solute distribution applied for lower K_d values).
4. For contaminants in the range $K_d > 8.0$, a fitted linear regression equation created by performing a linear regression of STOMP simulated peak concentrations against K_d values in this range is used. The peak concentrations beyond the simulated K_d values were estimated using regression equation mentioned. An example is shown in Figure 5-2 using 100-D column 1 with irrigation recharge scenario rates for Ephrata sandy loam or stony loam surface soil.

The numerical threshold for breakthrough within 1000 years was set to 1.0×10^{-4} $\mu\text{g/L}$ for non-radionuclide contaminants and 1.0×10^{-4} pCi/L for radionuclide contaminants. If breakthrough above this threshold was not simulated in more than one of the representative stratigraphic columns, then the results were assigned the code "NR" to designate a non-representative result. For SSLs, this condition was observed for contaminants with K_d values greater than 22 mL/g; therefore the SSLs for all contaminants with K_d greater than 22 mL/g were coded "NR." For PRGs, this condition was observed for contaminants with K_d values greater than 1 mL/g; therefore the PRGs for all contaminants with K_d greater than 1 mL/g were coded "NR."

If simulated peak concentrations are very small, application of Equation 2-1 can lead to physically unrealistic soil concentrations (e.g., 10 kg of aluminum per kg of soil) for the SSLs or PRGs. Although not strictly necessary, the maximum PRG value was capped at an estimate of the total contaminant mass that could occupy the void volume within a kg of soil.

The bulk density (ρ_B) of the soil in the 100 Area is 1930 kg/m^3 . For 1 kg of soil, the total volume (V_T) of the soil is:

$$\frac{1 \text{ kg}}{1930 \text{ kg/m}^3} = 5.18 \times 10^{-4} \text{ m}^3$$

The contaminant is assumed to occupy all of the pore space. Thus, the maximum mass of contaminant in the soil is:

$$n \times V_T \times \rho_p$$

where n is the total porosity and ρ_p is the particle density of the contaminant. In the 100 Area, the total porosity of Hanford formation or Ringold E unit is 0.28, and the particle density of the contaminant is assumed to equal the particle density of the soil, 2680 kg/m^3 . The maximum mass of contaminant in 1 kg soil is given by:

$$0.28 \times 5.18 \times 10^{-4} \text{ m}^3 \times 2680 \text{ kg/m}^3 = 0.389 \text{ kg} = 3.89 \times 10^5 \text{ mg}$$

Thus the maximum PRG for non-radionuclides is 389,000 mg per kg of soil. Any non-radionuclide PRG with a larger value was replaced by 389,000 mg per kg of soil.

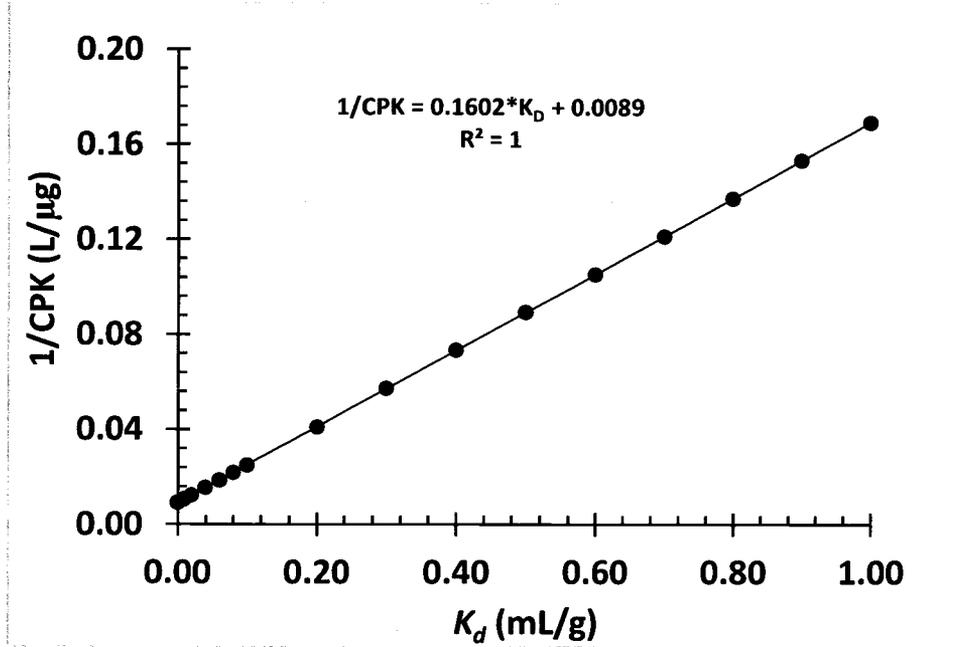


Figure 5-1. Linear Regression Equation for Low K_d Contaminants for 100-D Column 1 and Irrigation Case Recharge with Ephrata Sandy Loam Soil

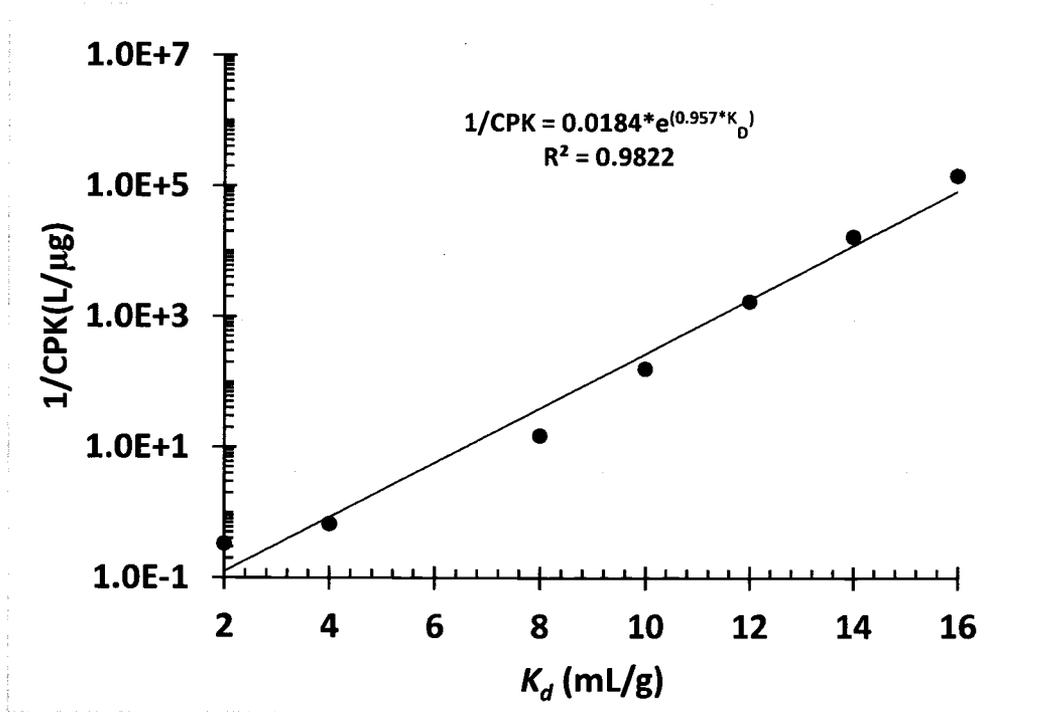


Figure 5-2. Linear Regression Equation for High K_d Contaminants for 100-D Column 1 and Irrigation Case Recharge with Ephrata Sandy Loam Soil

For radionuclides in groundwater, the maximum contaminant mass was transformed into a maximum radionuclide activity using the specific activity of each radionuclide. The specific activity is defined as the amount of radioactivity of a particular radionuclide per unit mass of the radionuclide, which is calculated by:

$$SpA \text{ (pCi/g)} = 3.578 \times 10^{17} / (m_{amu} \times t_{1/2}) \quad (\text{Eqn. 5-1})$$

where SpA is the specific activity (pCi/g), m_{amu} is the atomic mass unit (amu), and $t_{1/2}$ is the decay rate (yr). The specific activities for nickel-63, tritium, and strontium-90, which were the only radionuclides with very large PRG values, were calculated using Equation 5-1, and the maximum PRG values were obtained by multiplying the specific activity by the maximum contaminant mass (Table 5-1).

Table 5-1. Specific Activity and Maximum PRG Value for Selected Radionuclides

Radionuclide	Atomic mass	Half-life (yr)	Specific Activity (pCi/g)	Maximal PRG (pCi/g)
Nickel-63	58.6934	96	6.35E+13	2.44E+13
Tritium	3.0160492	12.35	9.61E+15	3.69E+15
Strontium-90	89.9	29.12	1.37E+14	5.26E+13

5.2 Soil Screening Level and Preliminary Remediation Level Results

SSL and PRG development captures the effects of geologic variability by simulating flow and transport through a set of representative stratigraphic columns within a given geographic area. The calculations are performed using same modeling assumptions except that the irrigation recharge scenario rates are applied for the SSL calculations while the native vegetation (ambient) recharge scenario rates are applied for the PRG calculations. Peak groundwater concentrations are simulated for each representative column and using Equation 2-1 the SSLs and PRGs are calculated separately for each representative column in the geographic area. The SSLs and PRGs for each representative column are compared for a given contaminant and a minimum value is adopted as the final SSLs and final PRG value for each geographic area.

The SSLs and PRG values are computed separately for the protection of groundwater and surface water (using Equation 2-1) because of different water quality standards. The federal and/or state drinking water standards are used for groundwater protection and aquatic water quality standards are used for surface water protection. The final SSL and PRG values for groundwater and surface water are developed to guide risk assessment decisions and for evaluation of selected remedies.

The STOMP simulations provide predictions of peak groundwater concentration for given recharge rates, sediment types, thicknesses, and properties appropriate to the geographic areas. The peak concentration within the 1000-year simulation was used to calculate the SSL and PRG value. Note that, particularly for contaminants with greater sorption, peaks may occur beyond 1000 years but these are not calculated or reported because a 1000-year limit was established for purposes of PRG calculation by agreement with regulatory agencies. One set of test case simulations were run for selecting the low K_d and high K_d contaminants. Column 1 from 100-D OU was chosen for the test case. The native vegetation recharge

scenario rates for Ephrata sandy loam soil was applied and effective 100:0 distribution was applied for the initial contaminant source distribution. The breakthrough curves for different distribution coefficients are shown in Figure 5-3. Observation of the breakthrough curves in Figure 5-3 reveals that for the distribution coefficients < 2 mL/g the peak concentration occurs within 1000 years and for the distribution coefficients > 2 mL/g the peak concentration occurs after 1000 years. Observe that in the cases of $K_d = 0.9$ and $K_d = 1.0$, the peaks occur before 1000 years in Figure 5-3; these peaks in the first one thousand years are higher than later peaks that occur after 1000 years. In contrast, for the higher K_d cases, the peaks in the first thousand years are less than the peaks that occur after 1000 years. As a result, the contaminants were grouped into two groups, one with low distribution coefficients < 2 mL/g and another one with the high distribution coefficients ≥ 2 mL/g for both SSL and PRG calculation.

For the low K_d contaminants effective 100:0 source distribution was used and for the high K_d contaminants 70:30 source distribution was used. The final SSL and PRG value for each recharge scenario is chosen by selecting the minimum value (lowest PRG calculated) from all of the representative columns for that geographic area. If the minimum value calculated is below the estimated quantitation limit (EQL) for soil then EQL was substituted for SSL or PRG value (as a lower threshold). The soil EQL values represent the lowest concentration that can be reliably measured within specified limits of precision and accuracy during routine laboratory operating conditions. EQLs are normally arbitrarily set rather than explicitly determined; for this calculation EQLs are those specified in Appendix A of DOE/RL-2009-41, *Sampling and Analysis Plan for the 100-K Decision Unit Remedial Investigation/Feasibility Study*, and in Appendix A of DOE/RL-2009-40, *Sampling and Analysis Plan for the 100-DR-1, 100DR-2, 100-HR-1, and 100-HR-3 Operable Units Remedial Investigation/Feasibility Study*.

In the absence of sufficient data to determine the subsurface extent of any contaminant, the contaminated interval was assumed to be full thickness of the vadose zone below the waste site in calculating soil SSLs and PRGs. This is a conservative assumption for many of the 100 Area waste sites, especially for those waste sites where large volumes of liquid wastes were discharged to the vadose zone.

Table 5-2 summarizes the representative 1-D columns evaluated in the calculations along with their composition in terms of geologic units and soil type for each geographic area. The 1-D column chosen for SSL and PRG calculations are listed. Note that the representative columns for 100-F and 100-IU geographic areas are based on preliminary information and may be revised.

Examples of the groundwater SSL and PRG values for three contaminants for the representative Column 1 in 100-D geographic area are shown in Table 5-3. As expected, SSLs for the irrigation recharge scenario are smaller than the PRGs for the native vegetation recharge scenario. As the magnitude of K_d increases, the magnitude of the PRG also increases, all other conditions held constant.

Examination of results reveals that SSL values for the Rupert sand soil type are smaller than those for the Ephrata loam or Burbank loam soils. This behavior is a direct result of the relatively high recharge rates for the Rupert sand under the irrigation recharge scenario compared to the rates for the Ephrata loam and Burbank loam soils. Because recharge rates under the irrigation recharge scenario are all high, the peak groundwater concentration occurs in proportion to the irrigation rates. In contrast, the PRG values for the Burbank loam are the lowest. This is because the peak groundwater concentration for mobile contaminants with $K_d < 1$, such as those shown in Table 5-3, occurs quickly, within the first five years of the simulation when the recharge rates are highest under the native vegetation recharge scenario. Table 4-1 shows that the recharge rate for this period represents a bare soil condition for five years, with subsequent periods subject to lower recharge as vegetation develops. The combination of a 100:0 initial

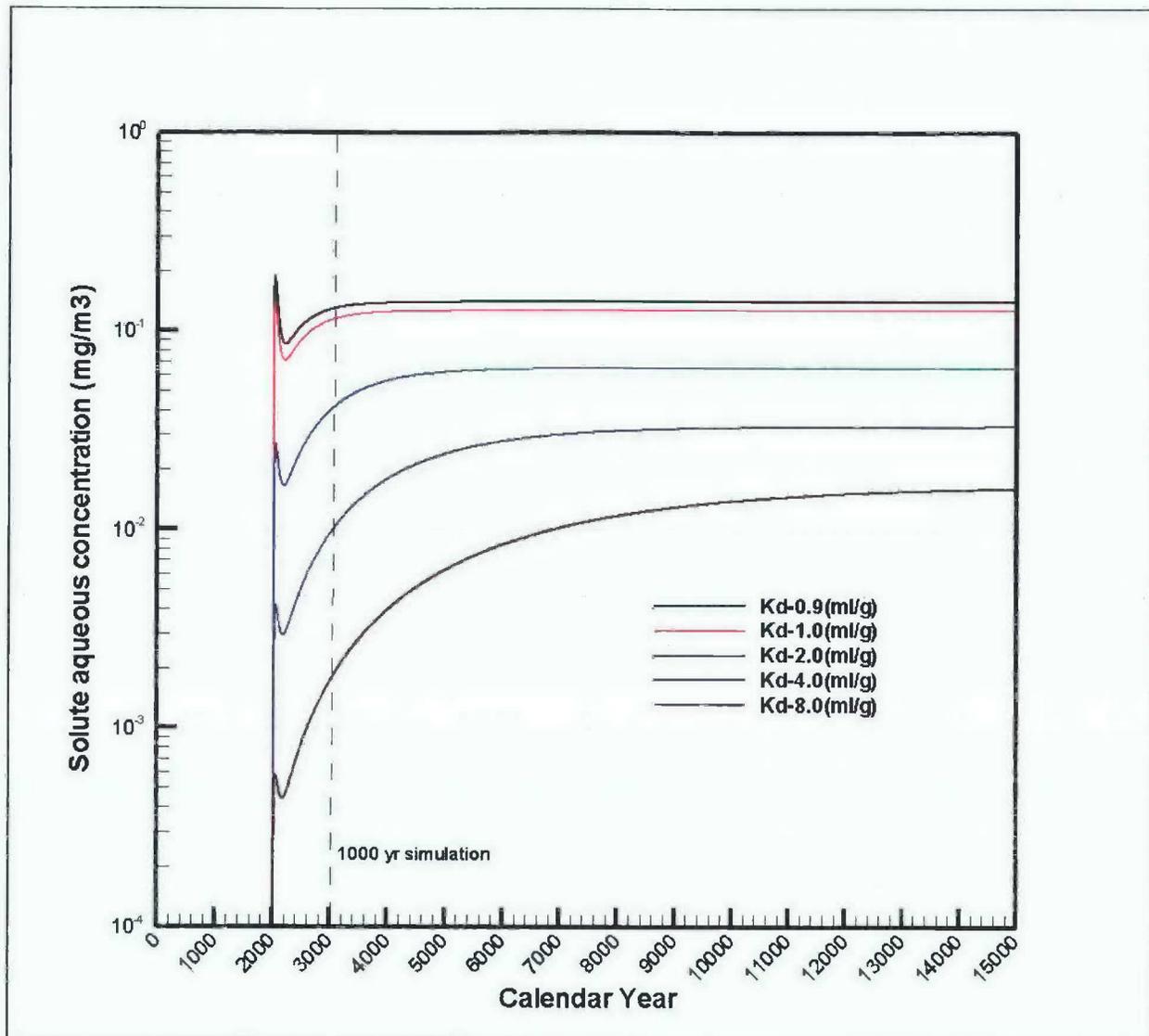


Figure 5-3. Breakthrough Curves for Different Distribution Coefficients with Native Vegetation Recharge Scenario (Column1 of 100-D OU)

condition that places contamination very near the water table and the highest recharge rate occurring in the first five years results in peak groundwater concentrations becoming a function of the recharge in this five-year period. From Table 4-1, the recharge rate under bare soil conditions is higher for Burbank loam (52 mm/yr) than for Rupert sand (44 mm/yr). Hence, the lowest PRG results from the Burbank loam recharge rate in these cases.

Table 5-2. Representative Soil Column Characteristics and Column Number Used for SSL and PRG Calculation

Geographic Area	Representative Column Index	Representative VZ thickness (m)	Representative VZ Composition	Thickness of Hanford fm. in VZ (m)	Thickness of Ringold E in VZ (m)	SZ Composition	Column Index Used For SSL	Soil Type Used For SSL	Column Index Used For PRG Calculation	Soil Type Used For PRG Calculation
100-D	1	25	100% Hanford	25.0	0.0	100% Hanford	3 and 4	Ephrata sandy loam and Rupert Sand	5	Burbank sandy loam
	2	20	100% Hanford	20.0	0.0	100% Hanford				
	3	25	75% Hanford / 25% Ringold E	20.0	5.0	100% Ringold E				
	4	20	80% Hanford / 20% Ringold E	16.0	4.0	100% Ringold E				
	5	25	60% Hanford / 40% Ringold E	15.0	10.0	100% Ringold E				
	6	15	60% Hanford / 40% Ringold E	9.0	6.0	100% Ringold E				
100-H	1	12	100% Hanford	12.0	0.0	100% Hanford	1	Ephrata sandy loam and Rupert sand	1	Burbank sandy loam
	2	8	100% Hanford	8.0	0.0	100% Hanford				
100-K	1	25	40% Hanford / 60% Ringold E	10.0	15.0	100% Ringold E	2 and 3	Rupert sand	1	Burbank sandy loam
	2	15	70% Hanford / 30% Ringold E	10.5	4.5	100% Ringold E				
	3	20	50% Hanford / 50% Ringold E	10.0	10.0	100% Ringold E				
	4	20	40% Hanford / 60% Ringold E	8.0	12.0	100% Ringold E				
	5	20	30% Hanford / 70% Ringold E	6.0	14.0	100% Ringold E				
100-BC	1	14	100% Hanford	14.0	0.0	100% Hanford	NA	NA	NA	NA
	2	23	100% Hanford	23.0	0.0	100% Ringold E				
	3	12	100% Hanford	12.0	0.0	100% Ringold E				
	4	30	100% Hanford	30.0	0.0	15% Hanford 85% Ringold E				
	5	22	100% Hanford	22.0	0.0	15% Hanford 85% Ringold E				
100-F	1	12	100% Hanford	12.0	0.0	100% Hanford	NA	NA	NA	NA
	2	10	100% Hanford	10.0	0.0	100% Hanford				
	3	8	100% Hanford	8.0	0.0	100% Hanford				
	4	9	80% Hanford / 20% Ringold E	7.2	1.8	100% Ringold E				
	5	12	40% Hanford / 60% Ringold E	4.8	7.2	100% Ringold E				
100-IU	1	40	100% Hanford	40.0	0.0	17% Hanford 83% Ringold E	NA	NA	NA	NA
	2	22	100% Hanford	22.0	0.0	100% Hanford				
	3	10	100% Hanford	10.0	0.0	100% Hanford	NA	NA	NA	NA
	4	8	100% Hanford	8.0	0.0	100% Hanford				
100-N	1	20	85% Hanford, 15% Ringold E	17.0	3.0	100% Ringold E	NA	NA	NA	NA
	2	21	60% Hanford, 40% Ringold E	12.5	8.5	100% Ringold E	NA	NA	NA	NA
	3	23	72% Hanford, 28% Ringold E	17.0	6.0	100% Ringold E	NA	NA	NA	NA
	4	19.5	95% Hanford, 5% Ringold E	18.5	1.0	100% Ringold E	NA	NA	NA	NA

VZ = vadose zone; SZ = saturated zone (aquifer); NA = Information not available currently; SSL = soil screening level; PRG = preliminary remediation goal

Table 5-3. Example Groundwater Protection Concentration Results for the First Representative Column in 100-D Geographic Area Using 100:0 Effective Initial Source Distribution

Contaminant	K_d (mL/g)	Ground Water Standard ($\mu\text{g/L}$)	Soil Screening Level (Irrigation Recharge Scenario) (mg/kg)			Preliminary Remediation Goal (Native Veg. Recharge Scenario) (mg/kg)		
			Ephrata loam	Burbank loam	Rupert sand	Ephrata loam	Burbank loam	Rupert sand
Cr(VI)	0.8	48	66	65	63	1950	311	410
Benzene	0.062	0.8	0.15	0.15	0.15	0.97	0.25	0.30
Trichloro-ethene	0.094	0.49	0.12	0.12	0.11	0.81	0.20	0.24

5.3 Calculating Dilution Factors

As the contaminant mass enters the aquifer from the vadose zone the aqueous concentration reduces due to dilution. Because the SSL and PRG calculations are a function of the peak concentration, it is important to understand the dilution factor within the saturated zone. As defined in the Washington Administrative Code (WAC 173-340-747), the dilution factor is the ratio of the combined aquifer and vadose zone water fluxes to the vadose zone water flux:

$$Df = \frac{Q_{vz} + Q_A}{Q_{vz}} \quad (\text{Eqn. 5-2})$$

for which Df = the dimensionless dilution factor, Q_{vz} equals the volumetric flux from the vadose zone into the aquifer (L^3T^{-1}) and Q_A represents the volumetric flux through the topmost five meters of the aquifer (L^3T^{-1}) representing the screened interval in the borehole. The dilution factors for different recharge scenarios are shown in Figure 5-4. For each scenario, the results are presented for the three soil types indicating minor effects on the dilution factors. Because of the high hydraulic conductivity in the aquifer and low recharge rates the dilution factors vary from $1.0E+02$ to $1.0E+06$, indicating significant dilution of the concentration in the saturated zone. The dilution factors for representative columns with aquifers of Ringold E are smaller than the dilution factors for Hanford aquifers for all recharge scenarios (Figure 5-4).

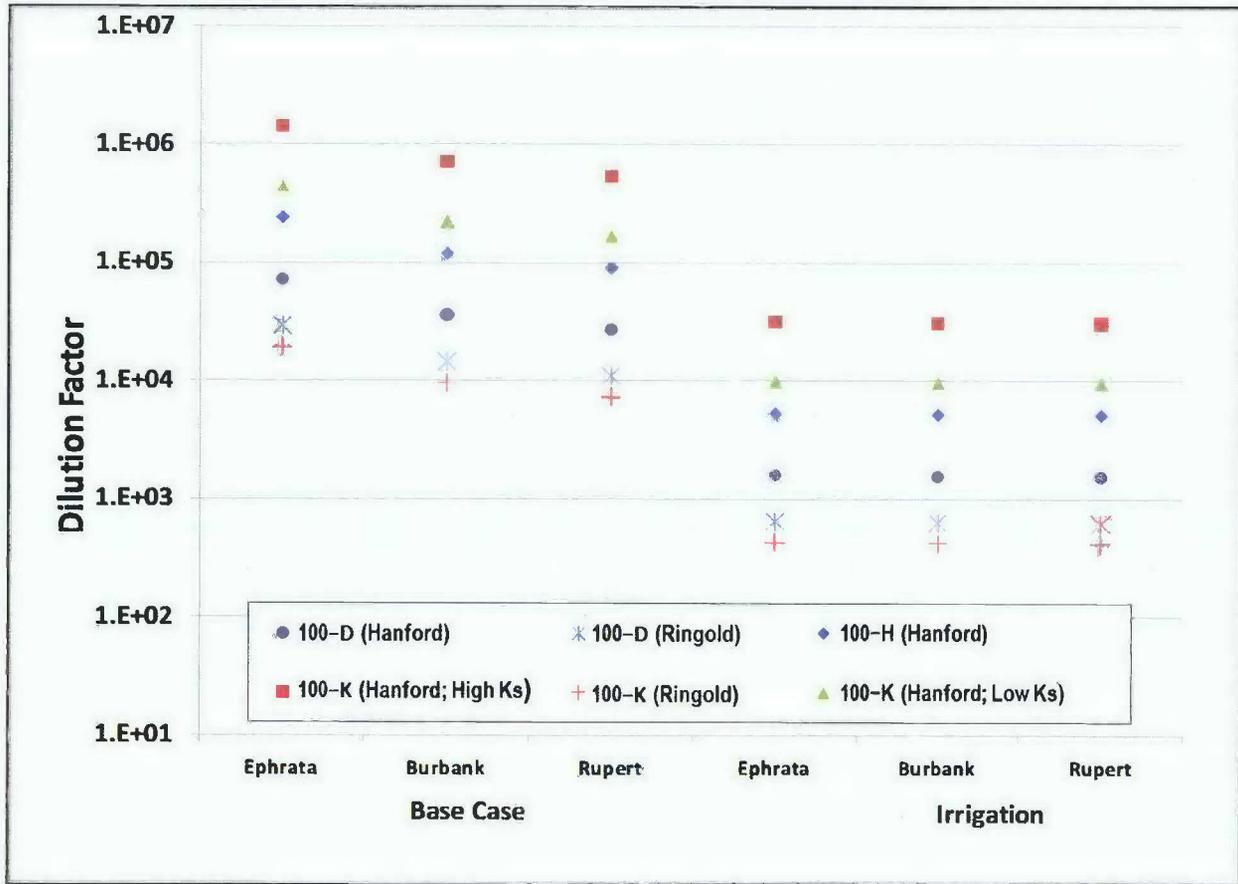


Figure 5-4. Dilution Factors for Representative Stratigraphic Columns (lithology in the saturated zone is listed in parenthesis in legend).

5.4 Application

Detailed tables of SSL and PRG values calculated using the methods described in this report for representative stratigraphic columns in 100-D and 100-H geographic areas are reported in the various attachments of ECF-Hanford-11-0063. The values reported in these tables are used to identify those constituents that pose a significant risk to surface water and groundwater. Table 5-4 provides a list of the contaminants for the 100-D and 100-H geographic areas along with their calculated SSL and PRG values. The values are selected by choosing the lowest value (most conservative) from calculations performed on each representative stratigraphic column (Table 5-2), under various recharge rates for three soil types, for the protection of groundwater and surface water. Final calculations have not been performed on 100-BC, 100-F, 100-K, and 100-IU-2/6 geographic areas.

The PRG values resulting from simulations and back-calculations are only intended to be applied to sites that share the same set of conditions and assumptions underpinning these calculations. The results, in general, should not be applied to other geographic areas. Questions about whether the PRG values are appropriate for a given site should be directed to the CH2M Hill Plateau Remediation Company (CHPRC) lead for modeling and risk assessment. Some waste sites may require a more rigorous investigation of site-specific conditions than those underlying the PRG values. Other simulations and back calculations may be necessary if the assumptions and conditions for a particular site do not match those used in these calculations.

Table 5-4. Preliminary Remediation Goal and Soil Screening Level values for 100-K, 100-D, and 100-H Geographic Areas

Geographic Area	Contaminants of Interest	Preliminary Remediation Goal (PRG) (mg/kg or pCi/g)	Soil Screening Level (SSL) (mg/kg or pCi/g)
100-K	Carbon-14	9.2E+01	4.27E+01
	Chromium (total)	NR ^(a)	NR ^(a)
	Hexavalent Chromium	6.0 ^(b)	6.0 ^(b)
	Nitrate	2.07E+03	9.6E+02
	Strontium-90	NR ^(a)	2.23E+04
	Tritium	1.01E+03	4.27E+02
100-D	Chromium (total)	NR ^(a)	NR ^(a)
	Hexavalent Chromium	6.0 ^(b)	6.0 ^(b)
	Nitrate	3.48E+03	1.65E+03
100-H	Hexavalent Chromium	6.0 ^(b)	6.0 ^(b)
	Strontium-90	NR ^(a)	9.93E+04

(a) Hexavalent chromium soil screening levels and preliminary remediation goals are limited to a maximum value of 6.0 mg/kg because the K_d value used in the model was derived from experiments with soil concentrations less than that value.

(b) "NR" designates a non-representative result for analytes where breakthrough was not simulated to occur in more than one representative stratigraphic column within 1000 years, where breakthrough is defined as concentration exceeding 0.0001 µg/L for nonradionuclide or 0.0001 pCi/L for radionuclides (limit of numerical significance).

6. Model Sensitivity and Uncertainty

This section presents the modeling conservatism and the results of the sensitivity and uncertainty analyses conducted to gain understanding of the important parameters that can affect SSL and PRG calculations.

6.1 Modeling Conservatism

Application of the PRG and SSL values calculated herein requires an understanding of which assumptions and modeling choices were conservative and which were not. Conservative assumptions and modeling choices include:

- The assumption of effective 100:0 source distribution (fully contaminated vadose zone) is likely to be a significant overestimate of the actual source distribution beneath many 100 Area waste sites, even for waste sites where high volume, low concentration discharges occurred during operations.
- PRG and SSL values are selected by taking the minimum SSL or PRG value calculated for all of the representative stratigraphic columns simulated for the particular area.
- Recharge was represented in the numerical model by uniform flux rates specified over particular periods so that vadose zone flow is always downward. In contrast, recharge in an arid vadose zone occurs only as often as the combination of precipitation and antecedent moisture conditions allow, i.e., sporadically or infrequently. Thus, there can be long periods when shallow vadose-zone pore water movement is controlled more by evaporation and transpiration near the surface than gravity, resulting in some upward movement or reduced downward seepage velocity.
- The smallest native vegetation recharge scenario rates are larger than the minimum of the range of rates determined for the Hanford shrub steppe.
- The one-dimensional simulations force all contamination through the vadose zone down to the aquifer, whereas infiltrating water and solutes tend to migrate laterally and vertically as the wetting front redistributes following an infiltration event.
- Dilution upon mixing of groundwater with Columbia River water is assumed negligible. That is to say, the calculation of SSL and PRG values takes no credit for surface water dilution.
- Dispersion is assumed negligible, which leads to larger peak concentrations than if dispersion had been included.
- Volatile organic compounds are assumed to have negligible volatilization so that the resulting peak concentrations are larger than if volatilization had been included.
- Geometric means of measured aquifer horizontal hydraulic conductivity values are lower, and thus more conservative, than arithmetic means because the values typically span several orders of magnitude.
- Initial contaminant mass within the domain is conservatively calculated by assuming that all the sediments, gravels and finer-grained materials (<2 mm size fraction) are active in transporting water and solutes. Majority of the residual contamination is found to be associated with the fine-grained (<2 mm size) portion of the sediments in the vadose zone. However, considerable

uncertainty exists due to the spatial variation in fraction of fine-grained material within the vadose zone. For modeling, the residual contaminant concentration determined in the laboratory on the fine-grained sediments is applied to the bulk volume thereby increasing the initial mass estimate. Under the recharge scenarios considered for the simulations, pore-waters do not have significant interaction with the gravel clasts because pore-waters are mostly restricted to the finer-grained materials due to capillary forces under relatively dry conditions. Thus, the resulting PRG and SSL values are highly conservative because the initial dissolved contaminant concentrations are over predicted.

- Contaminant source mass within the domain is calculated using the bulk density value for gravels and finer-grained materials, whereas laboratory measurements of soil concentrations typically exclude the gravel fraction and measure the concentration of the finer-grained materials only. The bulk density for Hanford formation and Ringold E sediments with gravels is 1.93 g/cm^3 , whereas the bulk density of the $< 2 \text{ mm}$ fraction is lower. Because initial mass loading (applied on a bulk volume basis) is calculated by multiplying the sorbed concentration with the bulk density using a larger bulk density is conservative, as it will lead to larger peak concentration.
- The simulations do not explicitly represent the alternation of thin intervals of finer-grained material with thicker intervals of coarser-grained materials commonly observed in the 100 Area, even though such alternations create local capillary impedances to downward transport through the juxtaposition of intervals with large pores below intervals with small pores. The alternations can lead to spreading of the plume thereby reducing the peak concentration.

Assumptions that may or may not be conservative include:

- The median hydraulic gradient value for each source area may be too small for waste sites near the Columbia River (at certain times of the day) and may be several times too large for waste sites that are far inland from the river. Because volumetric flux through the SZ is a function of hydraulic gradient and affects the dilution factor the peak concentrations will be impacted based on value chosen.
- The assumption of a 5-meter-thick aquifer may or may not be conservative for those 100 Area locations with aquifer thicknesses less than five meters.

The calculations are performed with numerous conservative assumptions. Due to conservative choice of modeling inputs and boundary conditions, the SSL and PRG concentrations are deemed to be bounding estimates (i.e., lead to the lowest threshold concentrations).

In the calculation methodology, the saturated zone is assumed initially uncontaminated, which may not always be true since plumes can migrate from upgradient locations over time. However, due to several in-built modeling conservatisms mentioned above, the SSL and PRG calculations are deemed to remain bounding when compared to the results derived from a more sophisticated site-specific predictive model that incorporates all the features and processes relevant at the scale of the model, including any contaminant migration from upgradient locations. Stated differently, groundwater is not expected to remain contaminated above cleanup levels (or discharge to the Columbia River above ambient water quality standards) any longer because former waste sites are closed with the SSL or PRGs calculated using this methodology.

6.2 Sensitivity Analyses

Sensitivity analyses provide information on how PRGs and SSL might be affected by changes in input parameters. The stratigraphic columns used for performing the sensitivity analyses, when not specified, are restricted to 100-BC and 300 geographic areas in order to reduce the number of calculations. The calculations are further restricted to certain selected stratigraphic columns. Column 2 was selected for 100-BC area and Column 5 was selected for the 300 Area. Results are presented for the native vegetation recharge scenario for Burbank sandy loam when not specified in the sensitivity analysis.

6.2.1 Evaluation of K_d Influence on Contaminant Breakthrough

In order to evaluate the influence of K_d on contaminant breakthrough behavior, the 100-D column 1 was run with irrigation recharge case for Ephrata sandy loam with effective 100:0 source distribution. Figure 6-1 shows the breakthrough curves for different K_d values ranging from 0.8 to 9.0 mL/g. Observation of the break through curves from Figure 6-1 reveals that all the peak concentrations occur within 1000 year simulation time. As the irrigation recharge is so high, it flushes the contaminants very fast through the vadose zone even with higher K_d values. The irrigation recharge scenario does not represent actual site conditions; it is used as a limiting conservative (bounding) condition for calculating screening values only.

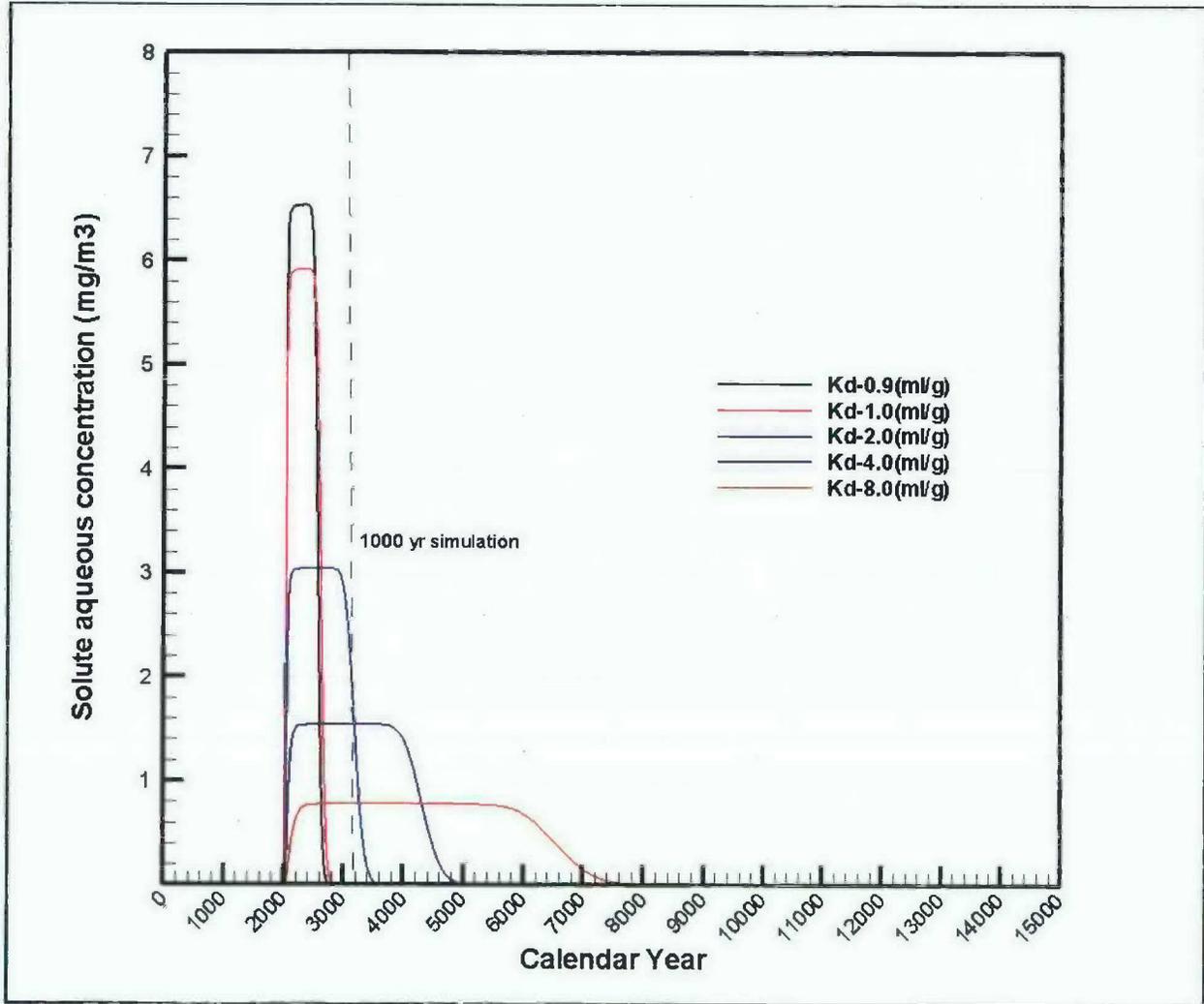
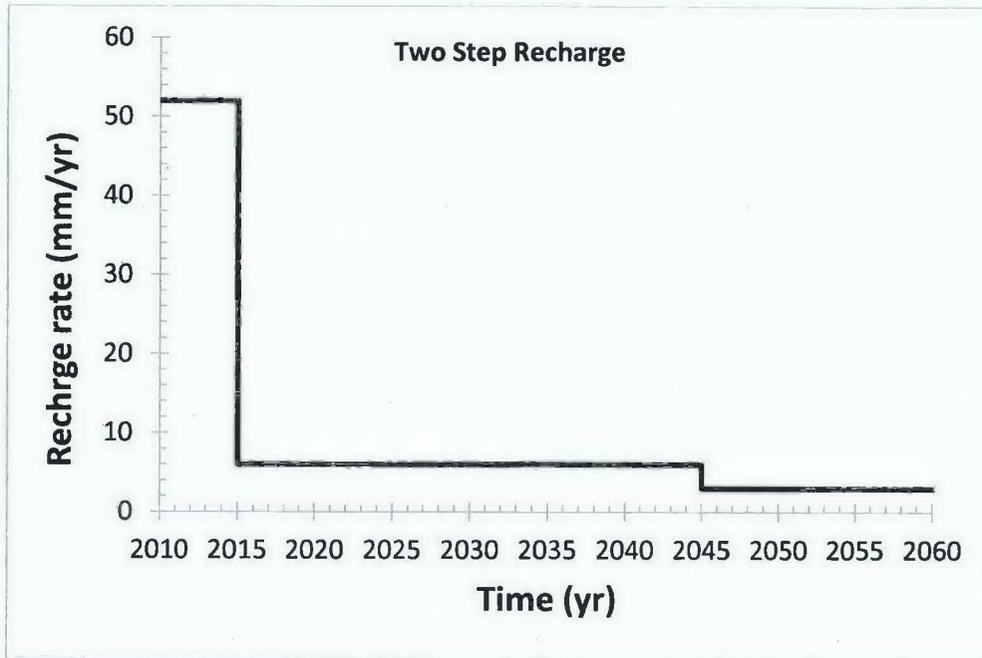


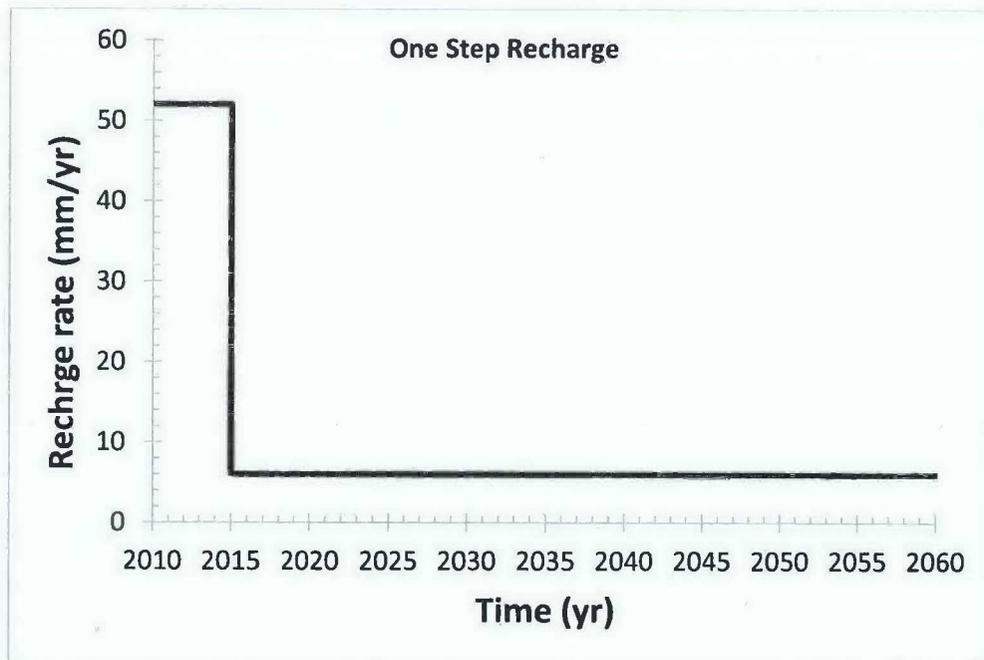
Figure 6-1. Breakthrough Curves for Different Distribution Coefficients with Irrigation Recharge Rate

6.2.2 Sensitivity to Long Term Recharges

Sensitivity to long-term recharge is presented by ignoring the step change in recharge due to establishment of mature shrub steppe vegetation. Because of the frequent occurrence (a once-a-decade cycle) of natural fires on the Hanford reservation, it is possible that mature shrub steppe may not get established. To evaluate the impact of this on the base case, a sensitivity analysis is conducted where the two-step change in recharge imposed in the base case is changed to a one-step change, essentially assuming that immature shrub steppe is the dominant land cover condition. Figure 6-2 shows the change in recharge for Burbank sandy loam. The change in PRG for Cr(VI) is presented in Table 6-1 and graphically presented in Figure 6-3. As the peak concentration occurs before the Year 2045 there is no or negligible change in PRG values in the two recharge scenarios.



(a)



(b)

Figure 6-2. Long-Term Recharge Rate for Burbank Sandy Loam: (a) Two-Step Recharge; (b) One- Step Recharge

Table 6-1. Surface Water PRG for Cr(VI) for Two Step vs. One Step Change in Recharge

Area	Column No	Soil Type	Recharge	Surface Water PRG (mg/Kg)
100-BC	2	Burbank sandy loam	Two Step	17.7
			One Step	17.7
300	5	Burbank sandy loam	Two Step	971.0
			One Step	971.0

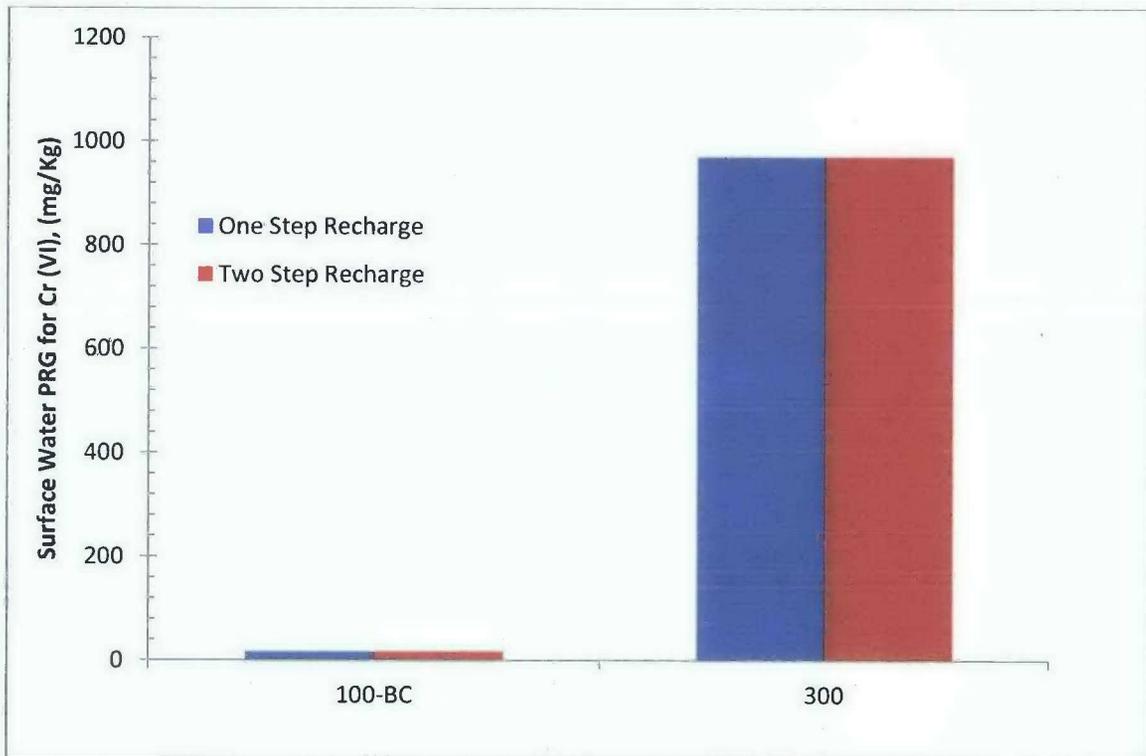


Figure 6-3. Surface Water PRG for Cr(VI) for Different Long-Term Recharge

6.2.3 Effects of Different Source Distribution

This sensitivity analysis focuses on discerning the effects of different source distributions on PRGs. Using the base case recharge, five new source distributions (50:50, 60:40, 70:30, 80:20, and 90:10) were simulated and compared to the PRG values for the effective 100:0 source distribution already computed. A 60:40 source distribution indicates that the top 60% of the VZ thickness beneath the clean cover (backfill) was contaminated with a uniform concentration of 1.0 mg/kg soil, whereas the remaining 40% contained no contamination.

Figure 6-4 shows the final PRG values of Cr(VI) in surface water from the six source distributions in the 100-BC and 300 geographic areas. This sensitivity analysis was performed for Column 2 and 5 for 100-BC and 300 Areas, respectively. As expected, stepwise decreases in the source distribution from 100% to

50% of the VZ thickness beneath the clean cover yields decreasing peak groundwater concentrations and increasing PRG values. Although the source distribution decreased linearly from effective 100:0 to 50:50, the PRG values do not appear to follow a linearly increasing trend.

The VZ thickness for the 300 Area column (16.5 m) chosen for the sensitivity analysis is smaller than 100-BC column (23 m) and SZ is made of Hanford fm. as compared to the Ringold E unit leading to higher hydraulic conductivity. Because of these differences, the initial mass in the 300 Area column is smaller and dilution factor is higher in the SZ compared to the 100-BC column used in the sensitivity analysis. This results in lower peak concentration for the 300 Area column and therefore higher PRG values and relatively larger sensitivity to the source distribution particularly when the source extent is reduced.

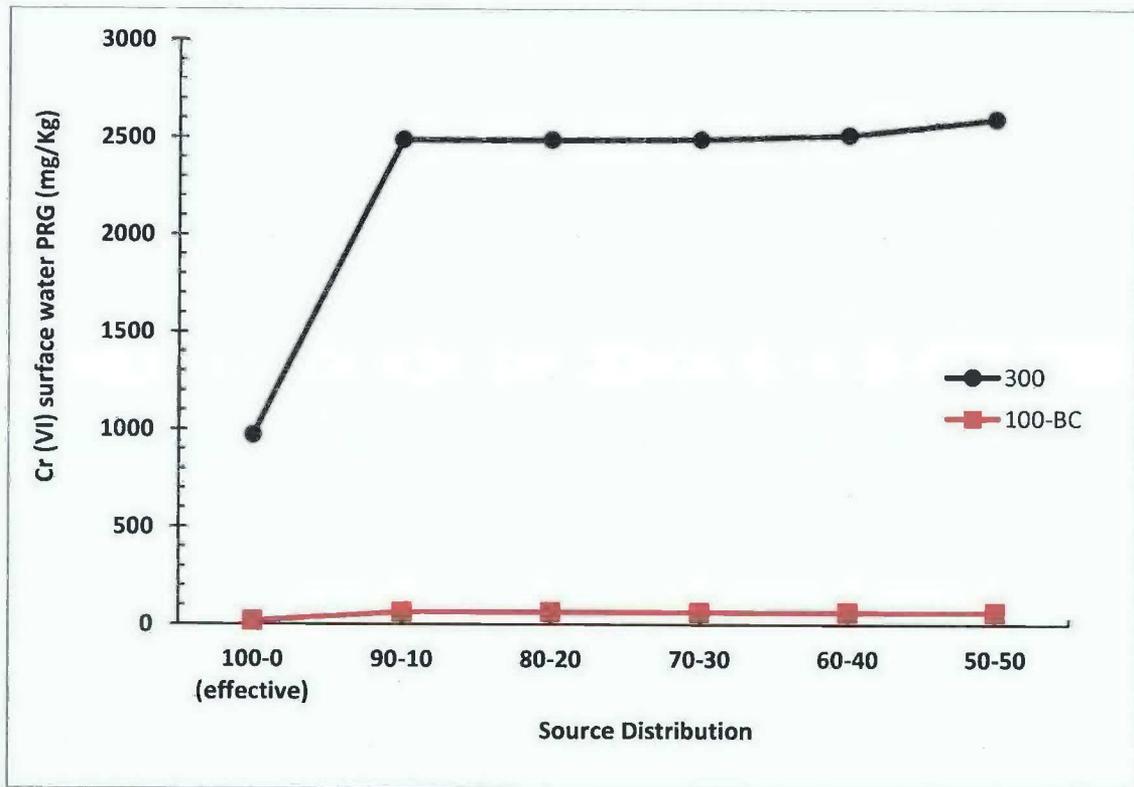


Figure 6-4. Surface Water PRG for Cr(VI) for Different Source Distributions in Soil

6.2.4 Effects of Extending Bare Soil Recharge Period

For the base case scenario, bare soil is assumed to be the land cover between Year 2010 and 2015 (Table 4-2), after which time grasses and shrubs are expected to colonize the bare soil. Accordingly, the recharge rate associated with bare soil is higher than those associated with immature and mature shrub-steppe cover. The effect of extending the bare soil recharge period on surface water PRG for Cr(VI) is evaluated for the base case. Two sensitivity analyses were conducted with the bare soil recharge rate extended to Year 2020 and Year 2030, thereby resulting in application of the bare soil recharge rate for 10 and 20 years, respectively. Simulation time remained at 1,000 years and the duration of the second recharge period, which simulated an immature shrub-steppe cover, remained at 30 years. Significant difference in PRG values has been found for both 100-BC and 300 Areas, as the peak concentration occurs after the bare soil period. The extended bare soil recharge scenario caused more mass arrival to the SZ and

eventually, increased the peak groundwater concentration. Extending the bare soil recharge scenario from 2010-2015 to 2010-2030 caused 3 to 5 times decrease in PRG values for both 100-BC and 300 Areas (Figure 6-5).

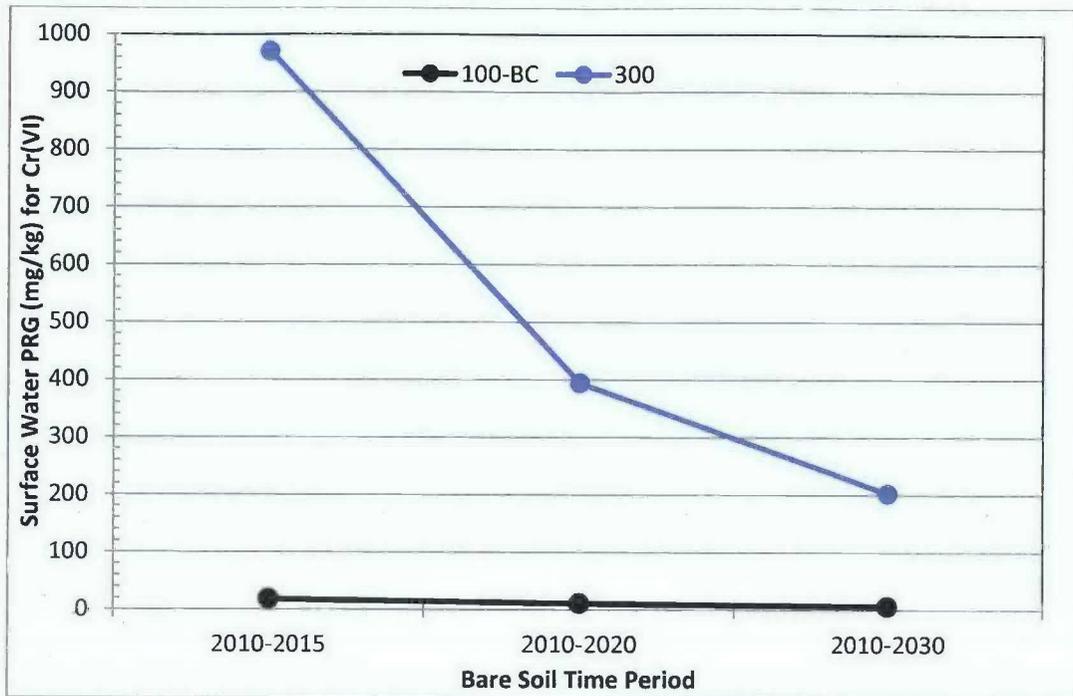


Figure 6-5. Surface water PRG for Cr(VI) for Different Bare Soil Periods under the Base Case Scenario

6.2.5 Sensitivity to Solute Transport Solution Methodology

In STOMP, the governing mass transport equations can be solved either with the power-law scheme of Patankar (1980) or with a third-order scheme using Total Variation Diminishing (TVD) criteria. The Patankar solution scheme was employed in the calculations and is based on the fully implicit finite-difference methodology. In an advection-dominated system (characterized by large Peclet number) the Patankar solution scheme can suffer from numerical dispersion that can result in smearing of otherwise sharp concentration fronts and could also lead to artificial oscillations at the concentration front. The smearing is a result of the first-order approximation of the advective term in the transport equation. The third-order TVD solution methodology does not suffer from numerical errors and can avoid the artificial oscillations with appropriate flux limiting function even for advection-dominated system. A sensitivity analysis was performed to compare the results of the two solution methodologies in terms of peak concentration and the timing of the peak concentration. The calculations were performed for Column 2 in 100-BC geographic area using the effective 100:0 distribution of contaminants for Burbank sandy loam and base case recharge. The K_d for the contaminant simulated was set to zero. Figure 6-6 shows the solute concentration for a node that is located at the water table. The magnitude of peak concentration and the time to peak concentration is nearly identical for both solution methods.

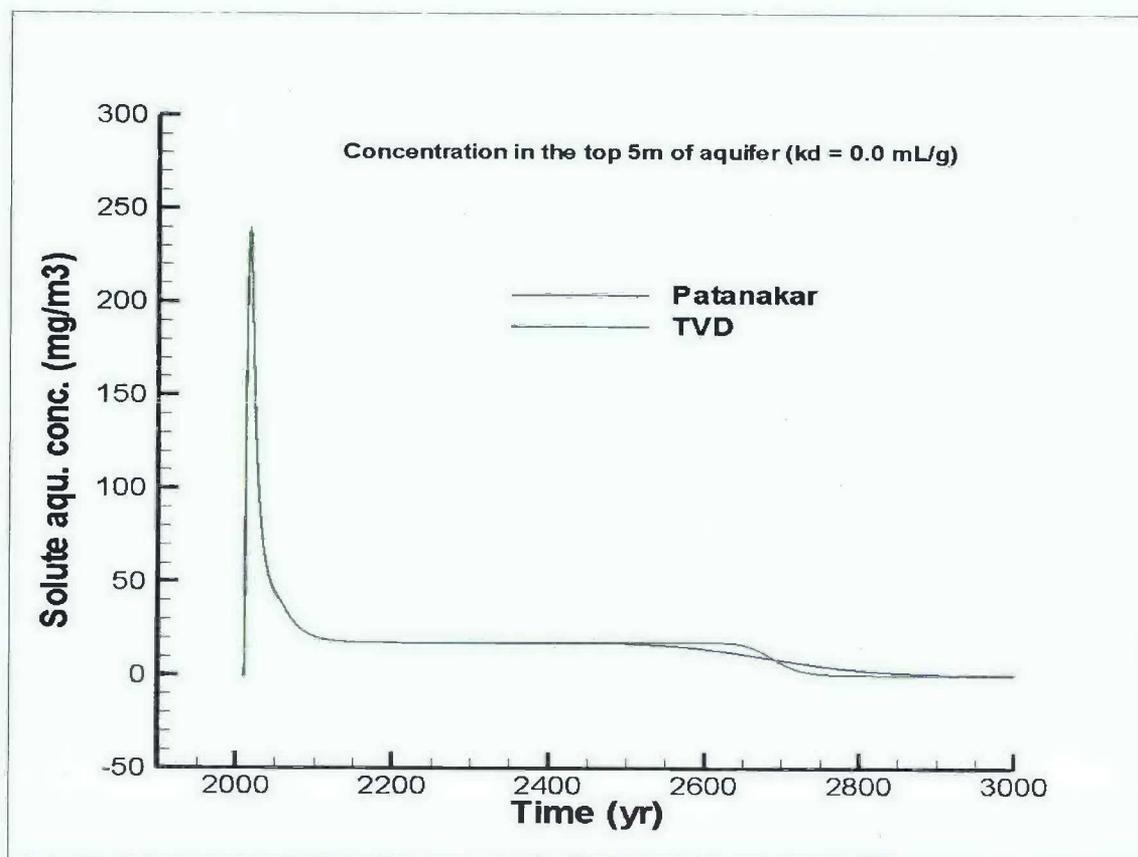


Figure 6-6. Comparison of Non-sorbing Solute Concentration using Patankar and TVD Solution Methodologies for Column 2 of 100-BC Geographic Area with Burbank Sandy Loam recharge and effective 100:0 Contaminant Distribution

6.3 Uncertainty Analyses

The vadose zone models described in this modeling report were developed in order to calculate cleanup levels necessary for the protection of groundwater and surface water. To do this the models predict concentration levels in groundwater and surface water resulting from soil contamination in the vadose zone. As all models are approximations of the real world, it is a given that uncertainty exists within these predictions. Methods have been developed for estimating the contribution to total uncertainty in a prediction from each model parameter. One qualified support software that includes algorithms for estimating the relative contribution to uncertainty is PEST (Doherty, 2010). PEST is graded as support software and was used under the guidance of the software management plan CHPRC-00258, *MODFLOW and Related Software Codes Software Management Plan*. Based on the model inputs and outputs generated and read by PEST, parameters values that best fit observed data can be estimated in an automated fashion. Beyond parameter estimation, the most recent versions also include algorithms for working with predictive uncertainty with model predictions. These algorithms can combine uncertainty introduced by the variability in observed data and uncertainty introduced by the numerical model itself. This section of the report summarizes an application of linear predictive uncertainty analysis (Moore and Doherty, 2005), implemented using PEST, to two of the alternative conceptual models (ACM) described in this document, specifically, the 100-BC column 2 and 100-F column 3. These columns were picked randomly from Table 5-2. First, a discussion of the definition of contribution to prediction uncertainty,

and how it is calculated, is presented. Then, the setup of the model files and parameter values and statistics used in uncertainty analysis are discussed. Finally, relative contribution to prediction uncertainty is presented in the results section.

6.3.1 Contribution to Prediction Uncertainty

All numerical models are approximations of the real world. Predictions made using these models are not exact. Predictive uncertainty of numerical simulation results can be developed by investigating the effect of changing model input parameters on the model predictions. One method for quantifying the uncertainty of predictions comes from frequentist statistical techniques for calculation of the mean and variance of distribution. Figure 6-7(a) shows a normal distribution curve fitted to a set of field parameters. The normal distribution is used to approximate the field observed data over the range of values expected to exist for the given phenomena using a continuous function. The same method can be used to describe a prediction from a numeric model shown in Figure 6-7(b). The most likely simulated result and the variance describe the mean and range of values that may be simulated given the variation in the input parameters. In frequentist statistics, the mean and variance are estimated from a discrete number of field observed measurements. The distribution of the prediction uncertainty is estimated from the results of a discrete number of numerical simulations based on the perturbation of model inputs and fitting a mean and variance distribution to the range of simulated results. Moore and Doherty (2005) illustrated that this type of conceptual framework can be used to combine statistical measures for field data with the uncertainty introduced through the numerical modeling to develop an estimate of predictive uncertainty including both types of data. In this manner, the uncertainty from the field data and uncertainty introduced by the model calculations can be combined into a final prediction and variance that describe the certainty of a prediction.

PEST includes algorithms to estimate relative contribution of model input parameters to the uncertainty in a prediction produced from a numerical model. This is accomplished by perturbing model inputs in a systematic fashion and recording sensitivity of the value of the prediction to changes in model inputs. In this case, PEST will be run using the linear predictive error estimator documented in the PEST manual (Doherty, 2010). Other methods for estimating uncertainty in the prediction exist. However, given the domain of the models (1-D), the linear predictive error estimator was deemed adequate for this analysis. For the linear predictive error analysis, PEST required two STOMP simulations for every model input parameter investigated as part of the analysis. In each of these simulations one parameter is perturbed from its original (initial) value, once above and once below the initial value, hence the need for two simulations per parameter. Based on the sensitivity of the prediction to the change in the parameter value a covariance matrix of model parameters and the prediction can be created. At this point, the uncertainty in the model prediction based on parameter inputs can be estimated by PEST.

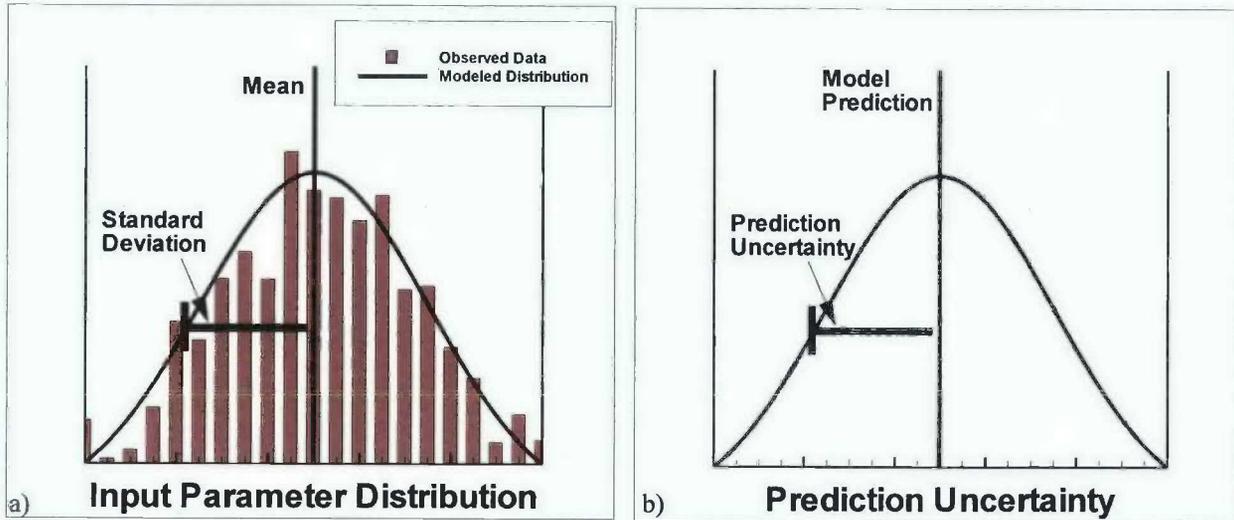


Figure 6-7. Illustration of how Statistical Distributions for Model Input Parameters and Simulated Predictions can be approached with Similar Methods

The PEST documentation notes that the algorithms for this type of analysis depend on model linearity. However, they may be applied to non-linear models (i.e., vadose zone models) for ranking parameters and their ability “to reduce the potential wrongness of a key model prediction” (Doherty, 2010). In line with this observation, the results presented in this analysis are relative contribution of each parameter on the total uncertainty in the prediction rather than presenting the absolute value of uncertainty.

6.3.2 Model Files and Parameters

Two separate analyses are conducted using stylized conceptual model so that the epistemic uncertainty (uncertainty due to lack of knowledge) in model input parameters can be evaluated. For this purpose, two different soil columns with different vertical extent of contaminated zones (100:0 and 50:50) and recharge conditions are selected to evaluate the relative effect of different model input parameters on the resulting soil concentrations used in calculating SSLs and PRGs. The first analysis is based on selecting Column 2 from 100-BC geographic area [Figure 6-8(a)] using Ephrata loam soil cover under irrigation recharge scenario and assuming 100:0 extent of contamination. The second analysis is based on choosing Column 3 from 100-F geographic area [Figure 6-8(b)] using Burbank sandy loam soil cover under base recharge scenario and assuming 50:50 extent of contamination in the vadose zone.

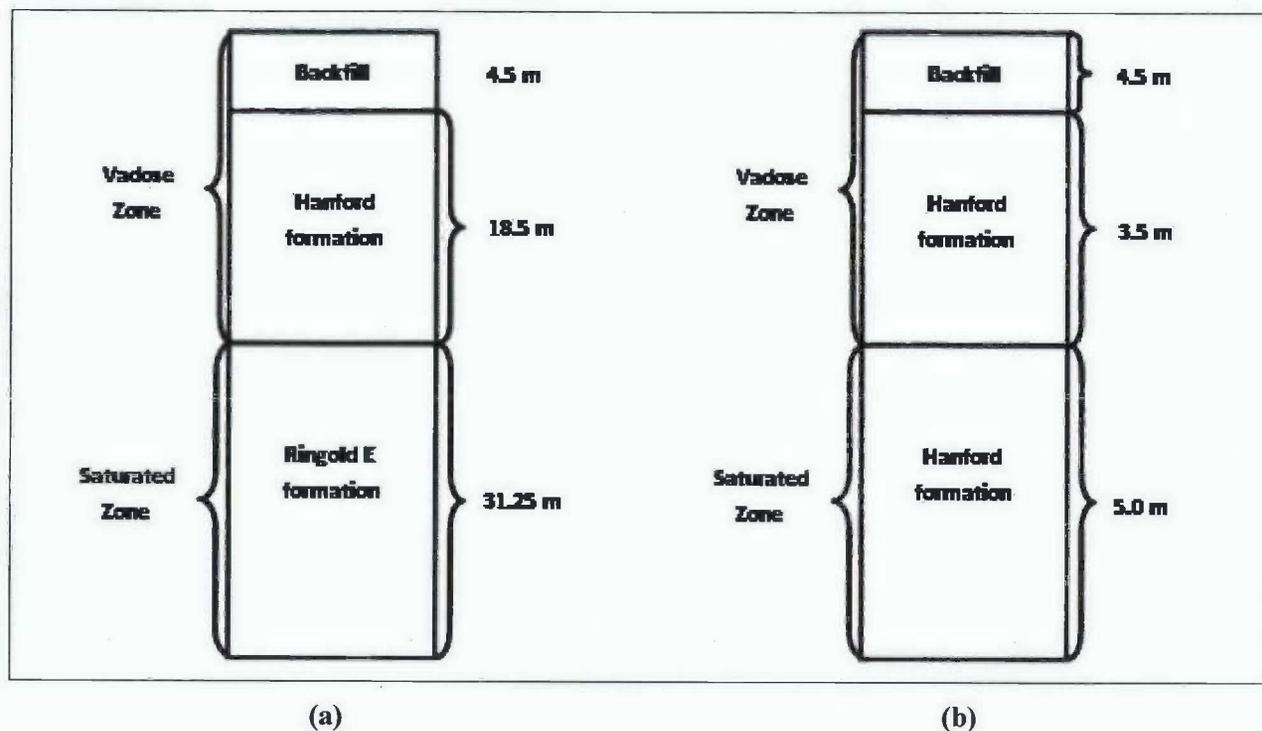


Figure 6-8. (a) Column 2 of 100-BC Geographic Area and (b) Column 3 of 100-F Geographic Area

Once the above soil columns along with the soil type are selected in the model, the basic structure of the stylized conceptual model is ready for evaluation of epistemic uncertainty. Some of model parameters, and their ranges for 100 Area soils, were derived from the available experimental data: these are presented in Table 6-2. Other parameter values were derived from other sources (e.g., PNNL-14702). Table 6-2 shows the list of parameters included in the uncertainty analysis. The table includes the parameter values used in developing the model, the range of values, and the standard deviations for each parameter. Sources for these data are also included in the tables. PEST execution required STOMP simulations to be carried out for two times the number of parameters in the uncertainty file. Therefore, 28 numerical simulations were required for developing the predictive uncertainty distributions for each ACM.

The vadose zone fate and transport calculations were performed using the STOMP Version 3.2 code, Hanford Information System Inventory (HISI) identification number 2471. STOMP and PEST were executed on the RANSAC Linux⁴ Cluster (ransac-0.pnl.gov) that is managed by Pacific Northwest National Laboratory (PNNL). The computer property tag for the frontend node is WD56054 (PNNL Property System). The frontend hardware (controller node) is a Dell[®] PowerEdge[®] 2550 with dual 3.00-GHz (Intel[®] Xeon^{®5}) processors and 2 GB of RAM loaded with the Red Hat^{®6} Enterprise Linux[®] Client release 5.5 (Tikanga) operating system.

The results of CHPRC acceptance testing (CHPRC-00515) demonstrate that the STOMP software is acceptable for its intended use by the CHPRC. Installations of the software are operating correctly, as demonstrated by the RANSAC Linux[®] Cluster system producing the same results as those presented for

⁴ Linux is a registered trademark of Linux Tovalds in the United States and other countries.

⁵ Intel and Xeon are registered trademarks of Intel in the United States and other countries.

⁶ Red Hat is a registered trademark of Red Hat, Inc.

selected problems from the STOMP Application Guide (PNNL-11216). PEST is graded as support software for MODFLOW and related codes, and was used consistent with requirements of the software management plan (CHPRC-00258).

6.3.3 Results Summary

Figure 6-9 and Figure 6-10 show charts of the relative uncertainty with respect to predicted groundwater contaminant concentration for each of the parameters listed in Table 6-2. The relative minimized error variance is calculated by dividing the minimized error variance for a given parameter by the sum of all values for minimized error variance for all parameters. The error variance in output for a parameter perturbation is calculated with respect to the results obtained from initial parameter value (base case).

Figure 6-9 illustrates results for Column 2 from 100-BC geographic area and Figure 6-10 shows results from Column 3 from 100-F geographic area. Uncertainty contributions vary significantly from one another. Hydraulic gradient is the largest contributor to uncertainty in 100-BC simulation while van Genuchten parameters play the largest role in the 100-F simulation. The van Genuchten parameters also contribute significantly to predictive uncertainty in the 100-BC simulation. The difference can be explained in the differences in model setup. The 100-F simulation contaminant concentration only covers top half of the vadose zone and the recharge is from the native vegetation recharge scenario. In contrast, the 100-BC contaminant distribution covers the entire vadose zone and has a much larger recharge due to irrigation. The uncertainty estimate illustrates the decreased travel time in the vadose zone to produce the peak groundwater concentration. Because the contaminant in 100-F simulation must travel through the vadose zone for a larger distance above the water table and in much drier conditions, the parameters affecting fate and transport through this portion of the model contribute most to the difference in calculated peak concentrations. In the 100-BC simulation, where contamination exists right above the water table, the uncertainty analysis indicates that travel through the vadose zone is not as important to final predicted concentrations as the amount of clean ground water entering the groundwater system through saturated groundwater flow.

Table 6-2. Model Input Parameters included as Part of the Sensitivity Analysis and their Input Value Ranges and Standard Deviations

Parameter	Units	Formation	Initial	Max	Min	Standard Deviation	Reference
Total Porosity	-	Hanford	0.28	0.40	0.14	7.889E-02	PNNL-14702 Rev.1 via SGW-44022 Rev. 0 Table 8-2
Diffusive Porosity ^(a)	-	Hanford	0.25	0.37	0.11	2.813E-02	SGW-40781 Rev. 1, Table 6.1
Total Porosity	-	Ringold	0.28	0.39	0.19	5.597E-02	PNNL-14702 Rev.1 via SGW-44022 Rev. 0 Table 8-2
Diffusive Porosity ^(a)	-	Ringold	0.28	0.39	0.19	2.813E-02	SGW-40781 Rev. 1, Table 6.1
Hydraulic Conductivity	cm/s	Hanford	1.02E-03	3.89E-02	6.73E-05	2.777E+00	SGW-40781 Rev. 1, Table 6.1
Hydraulic Conductivity	cm/s	Ringold-S	7.18E-03	6.48E-01	4.63E-05	1.916E-03	SGW-40781 Rev. 1, Table 7.1
van Genuchten α	1/cm	Hanford	0.0100	0.2481	0.0067	1.190E+00	SGW-40781 Rev. 1, Table 6.1
van Genuchten n	-	Hanford	1.41	1.62	1.18	1.649E-01	SGW-40781 Rev. 1, Table 6.1
van Genuchten α	1/cm	Ringold	0.080	0.1513	0.0126	1.079E+00	SGW-40781 Rev. 1, Table 6.1
van Genuchten n	-	Ringold	1.66	1.63	1.19	1.632E-01	SGW-40781 Rev. 1, Table 6.1
Recharge	mm/yr	Natural	1.5	2.25	0.75	7.500E-01	PNNL-14702 Rev.1
Recharge	mm/yr	Production	17	25.5	8.5	8.500E+00	PNNL-14702 Rev.1
Recharge	mm/yr	Early Irrigation	71.4	107.1	35.7	3.570E+01	PNNL-14702 Rev.1
Recharge	mm/yr	Late Irrigation	69.9	104.85	34.95	3.495E+01	PNNL-14702 Rev.1
Head Boundary ^(b)	Pa		406148.3	406148.3	406148.3	1.000E+00	Gradient Calculations, ECF-Hanford-11-0063
Head Boundary	Pa		405962.2	406119.3	405589	1.574E+02	Gradient Calculations, ECF-Hanford-11-0063
Dispersivity	m		0.000	1.000	0.000	1.000E+00	PNNL-14702 Rev.1
Distribution Coefficient ^(b)	g/cm ³		0.00	500.00	0.00	1.000E+00	PNNL-14702 Rev.1

a. Parameter was "tied" to the parameter listed above it. Parameters values changed relative to the other.

b. Parameter was set to either "fixed" at the initial value. These parameters were not used as part of the uncertainty analysis.

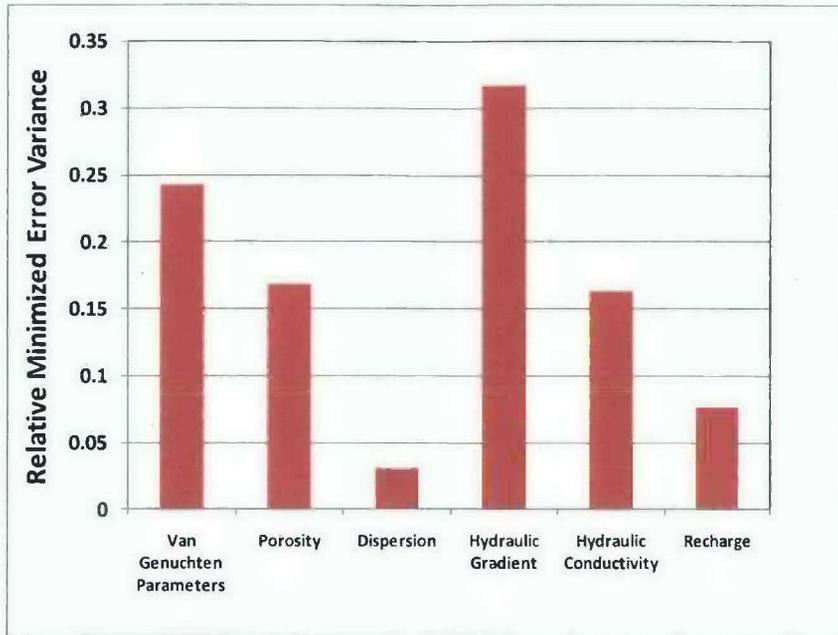


Figure 6-9. Relative Contribution of Parameter Groups to Uncertainty of the Peak Concentration Calculation for Column 2 in the 100-BC Geographic Area

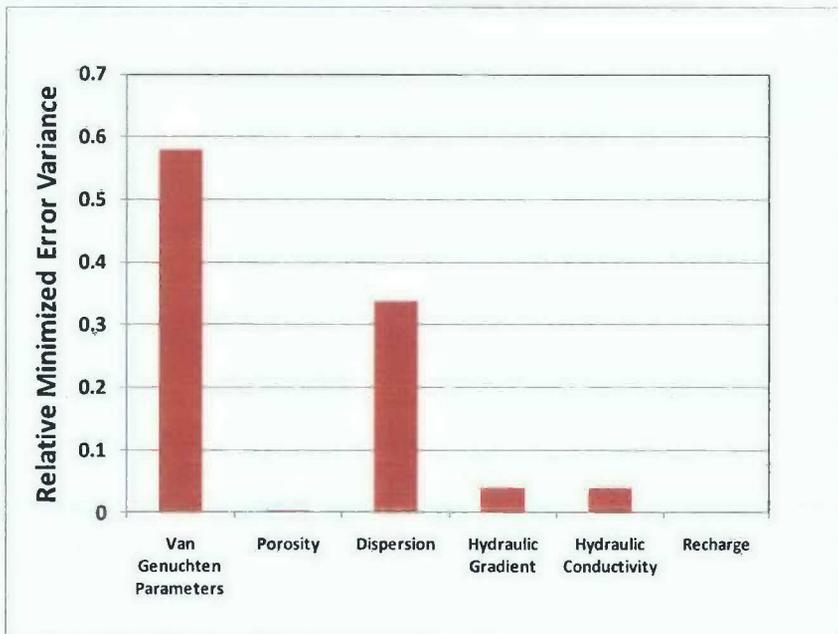


Figure 6-10. Relative Contribution of Parameter Groups to Uncertainty of the Peak Concentration Calculation for Column 3 in the 100-F Geographic Area Ringold Units

6.3.4 Effect of Gravel Correction

Geochemical analysis of soil samples at the Hanford Site are typically conducted on soil with the gravel (particles less than 2 mm in diameter) removed. Analysis of these soil samples are corrected based on the percentage of gravel that is in the sample. One model input parameter that can be affected by this correction is the bulk density. The bulk density directly changes the solute concentration used as the

initial condition in the model. As described in the methodology section of this report, 1 mg/kg of soil contamination is used as the input to the model. However, STOMP does not support soil concentration as an input in the version (STOMP-W) of STOMP used in the analysis. The input parameter used is titled "Solute Volumetric Concentration" (which is the total mass in a grid-block per unit bulk volume of the grid-block). In order to ensure that 1 mg/kg of contamination is entered into the model, the following equation was used to adjust the value of 1 mg/kg of soil contamination to the Solute Volumetric Concentration.

$$C_v = C_s * \gamma_b \quad \text{Eq. 6-1}$$

Where, C_v is the solute volume concentration (mg/m^3), C_s is the soil concentration (1 mg/kg), and γ_b is the bulk density in (kg/m^3). Gravel correction directly changes the concentration used in the STOMP input based on the changes in bulk density.

The bulk density and soil concentration were altered in a series of simulations to illustrate the level of conservatism used in the modeling. The bulk density values were taken based on the gravel percentages listed in Table 4-4. The change in bulk density resulted in a proportional change in the Solute Volumetric Concentration. This in turn resulted in a proportional change to the resulting simulated peak concentration. For example, the gravel correction of 43 percent produces a peak concentration 43 percent smaller than the original result. Not utilizing the gravel correction factor in establishing the initial condition provides a more conservative result for clean-up levels with respect to simulated peak concentration.

7. Model Configuration Management

The models documented in this model package report are collectively identified as the River Corridor Vadose Zone (RCVZ) Models.

All inputs and outputs for the development of the soil SSL and PRG models are committed to the Environmental Model Management Archive (EMMA) to maintain and preserve configuration-managed models. Basis information (that information collected to form the basis for model input parameterization) is also stored in the EMMA for traceability purposes.

The STOMP software is used to implement the models collectively described in this report. These models are configuration managed as discussed in Section 4.2. Safety Software (CHPRC Build 2 of STOMP) is checked out in accordance with procedures specified in CHPRC-00176. Source or executable files are obtained from the CHPRC software owner, who maintains the configuration-managed copies in MKS Integrity™. Installation tests identified in CHPRC-00211 are performed and successful installation confirmed, and software installation and checkout forms are required and must be approved for installations used to perform model runs. Approved users are registered in the HISI for Safety Software.

Use of the STOMP software for implementing the model described in this report is consistent with its intended use for CHPRC, as identified in CHPRC-00222.

7.1 Model Version History

This is the first edition of the RCVZ Models. Future revisions to this report will include a history to date of versions issued for the RCVZ Models collectively described by this model package report.

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Appendix A

Method for Determining Representative Stratigraphic Columns for Various Geographic Areas

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The following are the steps taken to produce the representative geology for each OU.

- 1) Began with data from GRAM, Inc.
 - a. 100 Area RUM and RE elevation master_10-19-10.xls
 - i. Contained borehole location/depth information and elevations of Hanford/RE and RUM contacts.
- 2) Brought data into ArcGIS and used GIS techniques to select “representative” boreholes of the waste sites in each of the 100 D,H,K, BC, F, IU, and N vadose zone OUs.
 - a. Selection Criteria:
 - i. Within 35 m of waste sites (if none then further)
 - ii. Representation to RUM (didn’t use wells that ended mid upper formations)
 - iii. If no borehole representation where needed then used interpolated surfaces to determine formation elevations.
- 3) Calculations
 - a. GIS
 - i. Water Level Jun 2008 elev (m)
 1. surfer grid head elevation file from SSPA’s 100 area groundwater model
 - ii. LiDAR
 1. 2010 terrain/surface elevation ArcGIS grid
 - iii. Vadose Thickness (m)
 1. $VZTHICK = \text{Ground surface (GS)} - \text{Water Table (WT)}$
 - iv. Aquifer Thickness (m)
 1. $AQTHICK = WT - RUM$
 - v. Waste Site Closest to Well
 1. Spatial Join (ArcGIS tool)
 - vi. Distance Well is from Wastesite (m)
 1. Spatial Join (ArcGIS tool)
 - b. Excel—for each representative borehole/location
 - i. Total Thickness (m)
 1. $TOTTHICK = GS - RUMCONTACT$
 - ii. Hanford (%) in Vadose
 1. $VZHF = \text{IF}(WT > HFRECONTACT, 1, (GS - HFRECONTACT) / VZTHICK)$
 - iii. RE (%) in Vadose
 1. $VZRE = 1 - VZHF$
 - iv. Hanford saturated (%)
 1. $SATHF = \text{IF}(VZHF < 1.0, \text{IF}((HFRECONTACT > RUMCONTACT), (WT - HFRECONTACT) / AQTHICK, 1))$
 - v. RE saturated (%)
 1. $SATRE = 1 - SATHF$
 - vi. Total Hanford (%)
 1. $HFTOT = \text{IF}((HFRECONTACT > RUMCONTACT), (GS - HFRECONTACT) / TOTTHICK, (GS - RUMCONTACT) / TOTTHICK)$
 - vii. Total RE (%)
 1. $1 - HFTOT$

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Appendix B

Description of STOMP Input File

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STOMP INPUT FILE

A STOMP input file is composed of cards, some of which are required and others which are optional or unused depending on the operational mode. In the STOMP-W mode following card are necessary for simulating flow and transport.

1. Simulation Control Card
2. Solution Control Card
3. Grid Card
4. Rock/Soil Zonation Card
5. Mechanical Properties Card
6. Hydraulic Properties Card
7. Saturation Function Card
8. Aqueous Relative Permeability Card
9. Initial Conditions Card
10. Boundary Conditions Card
11. Solute/Fluid Interactions Card
12. Solute/Porous Media Interactions Card
13. Surface Flux Card
14. Output Control Card

Descriptions of these cards can be found in STOMP user guide (PNNL-15782) and input file formats can be found in Appendix A of the user guide. For an example of input files⁷ one column (Column 1) from 100-D area is chosen. Figure B-1 shows the column with different zone thickness. Note that only the top five meters of the saturated zone will be represented in the model (less than the saturated thickness shown in Figure B-1). Two sequential STOMP simulations were used. The first stage, called the pre-2010 model, simulated flow through the representative columns for a 2,010-year period. Results from the pre-2010 simulations provided initial aqueous pressure conditions for the 3,000-year-long second stage simulation in a file called "restart". This restart file was used for the post-2010 model, which is solved for both flow and solute transport. Both of the input files are explained below.

⁷ The parameter values in the input file are presented for the purpose of illustration of the model set-up only and do not necessarily imply that the final calculations were run with this parameter set.

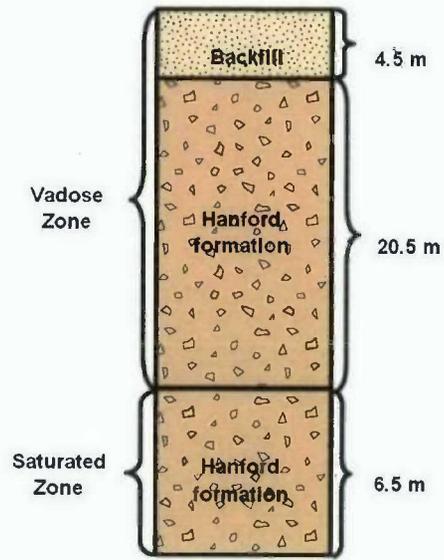


Figure B-1: Stratigraphic columns for 100-D (Column 3).

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
1	~Simulation Title Card	The input that follows provides information about this simulation
2	1,	STOMP version number,
3	100D 1D,	Simulation Title,
4	Amena Mayenna,	User name,
5	Intera Inc.,	Company name,
6	Jan 16 2014,	Input creation date,
7	11:00 PM PST,	Input creation time,
8	1,	Number of simulation note lines,
9	PRG calculation 100D Column1 Native vegetation recharge case with STOMP Version 4.0.	Simulation notes
10		(blank line for readability)
11	~Solution Control Card	The input that follows controls the simulation operational mode, duration, time stepping, and interfacial averaging schemes.

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
12	Normal,	Execution mode option, <i>NOTE: normal simulation begins from the initial conditions specified below in the ~Initial Conditions card</i>
13	Water,,	Operation mode option,
14	1,	Number of execution time periods,
15	0.,yr,2010.,yr,1.0e-09,yr,0.01,yr,1.25,8,1.e-6,	initial time, units, final time, units, initial time step, units, maximum time step, units, time step acceleration factor, maximum number of Newton-Raphson iterations, convergence criteria,
16	500000,	maximum number of time step,
17	0,	number of interfacial averaging variables,
18		(blank line for readability)
19	~Grid Card	The input that follows defines the model grid coordinate system to be used and the number and sizes of nodes.
20	cartesian,	coordinate system option,
21	1,1,120,	number of X-direction nodes, number of Y-direction nodes, number of Z-direction nodes,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
22	0.0, m, 10, m,	X dir surface position, units, surface position, unit,
23	0, m, 1.0, m,	Y dir surface position, units, surface position, unit,
24	88.750000,m,120@0.25,m,	Z dir surface position, units, number of nodes@node width, units,
25		(blank line for readability)
26	~Rock/Soil Zonation Card	The input that follows assigns the nodes defined in the ~Grid Card above to unique rock or soil types.
27	3,	number of rock/soil zone types,
28	HS,1,1,1,1,1,20,	zone name (Hanford formation in saturated zone) , X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, <i>NOTE: These nodes are assigned to the Hanford formation saturated (HS)– that is, the aquifer portion of the model domain.</i>
29	HF,1,1,1,1, 21, 102,	zone name (Hanford formation in unsaturated zone), X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
30	BF,1,1,1,1,103,120,	zone name (Backfill), X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,
31		(blank line for readability)
32	~Mechanical Properties Card	The input that follows assigns mechanical properties to each rock or soil type defined in the ~Rock/Soil Zonation Card above.
33	#Soil name,particle density,units,total porosity,diffusive porosity (theta S),specific storativity - default = 1E-07*diff porosity, #units - default = 1/m, tortuosity function,	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
34	BF,2.68,g/cm^3,0.276,0.262,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment
35	HF,2.68,g/cm^3,0.280,0.247,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
36	HS,2.68,g/cm ³ ,0.280,0.247,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment
37	#Soil name, x-direction hydraulic conductivity, units, y-direction hydraulic conductivity (not used),units, z-direction hydraulic conductivity, units,	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
38		(blank line for readability)
39	~Hydraulic Properties Card	The input that follows assigns hydraulic parameters to each rock or soil type defined in the ~Rock/Soil Zonation Card above.
40	BF,5.98E-04,hc:cm/s,,,5.98E-04,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment
41	HF,4.66E-03,hc:cm/s,,,4.66E-04,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment
42	HS,6.42E-02,hc:cm/s,,,6.42E-03,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment

B-7

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
43		(blank line for readability)
44	#Soil name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
45	~Saturation Function Card	The input that follows assigns water retention parameters for unsaturated flow to each rock or soil type defined in the ~Rock/Soil Zonation Card above.
46	BF,Nonhysteretic van Genuchten,0.019, 1/cm,1.4,0.103,, #ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,
47	HF,Nonhysteretic van Genuchten,0.029, 1/cm,1.378,0.022,, # ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,
48	HS,Nonhysteretic van Genuchten,0.029, 1/cm,1.378,0.022,, # ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,
49		(blank line for readability)
51	~Aqueous Relative Permeability Card	The input that follows assigns method for calculating relative permeability as a function of aqueous saturation for unsaturated zone.
52	BF, Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
53	HF,Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),
54	HS,Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),
56		(blank line for readability)
57	~Initial Conditions Card	The input that follows assigns initial hydraulic conditions to nodes defined in the ~Grid Card above. <i>NOTE: initial conditions are applied at node centers.</i>
58	Aqueous Pressure, Gas Pressure,	initial saturation option A, initial saturation option B, <i>NOTE: gas pressure is unspecified, and therefore defaults to atmospheric pressure throughout the unsaturated zone (101,325 Pa).</i>
59	2,	Number of initial conditions specified,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
60	Aqueous Pressure,1.4906840E+05,Pa,,,,,-9793.52,1/m,1,1,1,1, 20,	<p>For initial condition #1;</p> <p>variable name, magnitude, units, X-dir pressure gradient ,units, Y-dir pressure gradient, units, Z-dir pressure gradient, units, X-dir starting node ,X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p> <p><i>NOTE: Calculation of base pressure in first node: saturated thickness = 5.0 m, Atmospheric pressure = 1.01E+05 Pa, water unit weight = 9793.52 N/m³, node spacing = 0.25m, so base pressure (at the center of bottom node) = 101325 + 9793.52 * (5.0-0.125) = 1.4906840E+05 Pa.</i></p>
61	Aqueous Pressure,86656.7554,Pa,,,,,-100.,1/m,1,1,1,1,21, 120,	<p>For initial condition #2;</p> <p>variable name, magnitude, units, X-dir pressure gradient, units, Y-dir pressure gradient, units ,Z-dir pressure gradient, units, X-dir starting node ,X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p>
62		(blank line for readability)

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
63	~Boundary Conditions Card	<p>The input that follows assigns boundary conditions to exterior node faces; these boundaries may vary in time by assigning multiple times that the boundary variable changes.</p> <p><i>NOTE: Boundary conditions area applied at node faces.</i></p> <p><i>NOTE: direction of boundary fluxes consistent with STOMP conventions (positive is up, east, and north; negative is down, west, and south).</i></p> <p><i>NOTE: any face that is not assigned a boundary condition defaults to a no-flow boundary assignment in STOMP.</i></p> <p><i>NOTE: boundary conditions with more than one time range will transition linearly between the rates at the times prescribed.</i></p>
64	3,	number of boundary conditions specified,
65	top,neumann,zero flux,zero flux,	<p>For boundary condition #1;</p> <p>boundary surface direction, aqueous phase boundary type, (all the rest are zero flux boundaries)</p>

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
66	1,1,1,1, 120, 120,6,	For boundary condition #1 (recharge at top boundary); X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,
67	0.,yr, -4.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #1 (start); boundary time, units, aqueous volumetric flux (recharge rate), units,...
68	1880,yr, -4.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #2 (until 1880); boundary time, units, aqueous volumetric flux (recharge rate), units,
69	1880,yr, -7.2400000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #3 (starting 1880); boundary time, units, aqueous volumetric flux (recharge rate), units,
70	1944,yr,-7.2400000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #4 (until 1944); boundary time, units, aqueous volumetric flux (recharge rate), units,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
71	1944,yr,-6.3000000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #6 (starting 1944); boundary time, units, aqueous volumetric flux (recharge rate), units,
72	2010,yr,-6.3000000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #6 (end); boundary time, units, aqueous volumetric flux (recharge rate), units,
73	# Hydraulic gradient = 1.1E-3 m/m.	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
74	# With 10 m horizontal span of a grid, the head drop from the edge to middle points of	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
75	# the grid is 10m*0.0011 m/m = 0.011m	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
76	# The pressure drop is 0.011m * 9793.52Pa/m = 107.73 Pa.	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
77	west, hydraulic gradient,	For boundary condition #2 (aquifer gradient, upgradient side); boundary surface direction, aqueous phase boundary type,
78	1, 1,1,1,1,20,1,	For boundary condition #2; X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,
79	0.,yr, 1.4906840E+05,Pa,	For boundary condition #2, starting at time #1; boundary time, units, base aqueous pressure, units, <i>NOTE: is the upstream water phase boundary for the aquifer nodes; the condition establishes a fixed hydraulic gradient across the aquifer nodes to simulate aquifer flow.</i>
80	east, hydraulic gradient,	For boundary condition #3; boundary surface direction, aqueous phase boundary type,
81	1, 1,1,1,1,20,1,	For boundary condition #3; X-dir starting, node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
82	0.,yr, 1.4896070E+05,Pa,	<p>For boundary condition #3, starting at time #1; boundary time, unit, base aqueous pressure, unit,</p> <p><i>NOTE: hydraulic gradient 0.0011m was applied from west to east, distance between west and east surface = 10m, so pressure at the east surface = west pressure – $0.0011 * 10 * 9793.52 = 1.711E+05 - 107.73 = 1.7099E+05$ Pa</i></p> <p><i>NOTE: is the downstream water phase boundary for the aquifer nodes; the condition establishes a fixed hydraulic gradient across the aquifer nodes to simulate aquifer flow.</i></p>
83		(blank line for readability)
84	~Output Control Card	The input that follows specifies the output to be reported to the screen throughout the simulation, to the output file throughout the simulation, and to the plot and restart files at prescribed times during the simulation.
85	1,	number of reference nodes at which output will be reported to the screen during simulation run

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
86	1,1,20,	For reference node #1; reference node X index, reference node Y index, reference node Z index,
87	50, 50, yr, m, 6, 6, 9,	reference node screen output frequency (every 50 time step), reference node output file frequency (every 50 time step), time unit, length unit, screen significant digits, output file significant digits, plot file significant digits,
88	8,	number of output files variables
89	aqueous saturation,,	For output variable #1; variable name, units,
90	aqueous matric potential, m,	For output variable #2; variable name, units,
91	aqueous moisture content,,	For output variable #3; variable name, units,
92	xnc aqueous vol, m/yr,	For output variable #4; variable name, units,
93	znc aqueous vol, m/yr,	For output variable #5; variable name, units,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
94	aqueous courant number,,	For output variable #6; variable name, units,
95	total water mass,,	For output variable #7; variable name, units,
96	water mass source int,,	For output variable #8; variable name, units,
97	1,	number of plot/restart files times
98	2010. yr,	For plot/restart file time #1; plot/restart file time, units,
99	8,	number of plot files variables
100	aqueous saturation,,	For plot variable #1; variable name, units,
101	aqueous matric potential, m,	For plot variable #2; variable name, units,
102	aqueous moisture content,,	For plot variable #3; variable name, units,

Example Historic (Pre-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
103	xnc aqueous vol, m/yr,	For plot variable #4; variable name, units,
104	znc aqueous vol, m/yr,	For plot variable #5; variable name, units,
105	aqueous courant number,,	For plot variable #6; variable name, units,
106	total water mass,,	For plot variable #7; variable name, units,
107	water mass source int,,	For plot variable #8; variable name, units,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
1	~Simulation Title Card	The input that follows provides information about this simulation
2	1,	STOMP version number,
3	100D 1D,	Simulation Title,
4	Amena Mayenna,	User name,
5	Intera Inc.,	Company name,
6	Jan 16 2014,	Input creation date,
7	12:00 PM PST,	Input creation time,
8	1,	Number of simulation note lines,
9	PRG calculation 100D Column1 Native vegetation recharge case with STOMP Version 4.0.	Simulation notes
10		(blank line for readability)
11	~Solution Control Card	The input that follows controls the simulation operational mode, duration, time stepping, and interfacial averaging schemes.

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
12	restart,	Execution mode option, <i>NOTE: restart simulation begins from the initial conditions specified below in the ~Initial Conditions card</i>
13	Water w/ transport courant,,	Operation mode option, <i>NOTE: automatic transport time step limit option is selected to force simulation transport time steps to stay within Courant limit.</i>
14	1,	Number of execution time periods,
15	2010.,yr,3010,yr,1.0e-09,yr,0.01,yr,1.25,8,1.e-6,	initial time, units, final time, units, initial time step, units, maximum time step, units, time step acceleration factor, maximum number of Newton-Raphson iterations, convergence criteria,
16	500000000,	maximum number of time step,
17	0,	number of interfacial averaging variables,
18		(blank line for readability)

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
19	~Grid Card	The input that follows defines the model grid coordinate system to be used and the number and sizes of nodes.
20	cartesian,	coordinate system option,
21	1,1,120,	number of X-direction nodes, number of Y-direction nodes, number of Z-direction nodes,
22	0.0, m, 10, m,	X dir surface position, units, surface position, unit,
23	0, m, 1.0, m,	Y dir surface position, units, surface position, unit,
24	88.750000,m,120@0.25,m,	Z dir surface position, units, number of nodes@node width, units,
25		(blank line for readability)
26	~Rock/Soil Zonation Card	The input that follows assigns the nodes defined in the ~Grid Card above to unique rock or soil types.
27	3,	number of rock/soil zone types,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
28	HS,1,1,1,1,1,20,	<p>zone name (Hanford formation in saturated zone) , X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p> <p><i>NOTE: These nodes are assigned to the Hanford formation saturated (HS)– that is, the aquifer portion of the model domain.</i></p>
29	HF,1,1,1,1, 21, 102,	<p>zone name (Hanford formation in unsaturated zone), X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p>
30	BF,1,1,1,1,103,120,	<p>zone name (Backfill), X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p>
31		(blank line for readability)
32	~Mechanical Properties Card	The input that follows assigns mechanical properties to each rock or soil type defined in the ~Rock/Soil Zonation Card above.
33	#Soil name,particle density,units,total porosity,diffusive porosity (theta S),specific storativity - default = 1E-07*diff porosity, #units - default = 1/m, tortuosity function,	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
34	BF,2.68,g/cm ³ ,0.276,0.262,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment
35	HF,2.68,g/cm ³ ,0.280,0.247,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment
36	HS,2.68,g/cm ³ ,0.280,0.247,Pore Compressibility,1e-7,1/Pa,,,Millington and Quirk, # ECF-Hanford-11-0063-r6 Table 7	zone name, particle density, units, total porosity, diffusive porosity, select pore compressibility option, pore compressibility, units, reference pressure (default),units (default), tortuosity function option, #comment
37	#Soil name, x-direction hydraulic conductivity, units, y-direction hydraulic conductivity (not used),units, z-direction hydraulic conductivity, units,	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
38		(blank line for readability)
39	~Hydraulic Properties Card	The input that follows assigns hydraulic parameters to each rock or soil type defined in the ~Rock/Soil Zonation Card above.

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
40	BF,5.98E-04,hc:cm/s,,,5.98E-04,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment
41	HF,4.66E-03,hc:cm/s,,,4.66E-04,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment
42	HS,6.42E-02,hc:cm/s,,,6.42E-03,hc:cm/s, # ECF-Hanford-11-0063-r6 Table 7	zone name, X-direction hydraulic conductivity, units, Y-direction hydraulic conductivity (zero), units, Z-direction hydraulic conductivity, units, #comment
43		(blank line for readability)
44	#Soil name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
45	~Saturation Function Card	The input that follows assigns water retention parameters for unsaturated flow to each rock or soil type defined in the ~Rock/Soil Zonation Card above.
46	BF,Nonhysteretic van Genuchten,0.019, 1/cm,1.4,0.103,, #ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,
47	HF,Nonhysteretic van Genuchten,0.029, 1/cm,1.378,0.022,, # ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
48	HS,Nonhysteretic van Genuchten,0.029, 1/cm,1.378,0.022,, # ECF-Hanford-11-0063-r6 Table 7	zone name, moisture retention function, vG alpha, units, vG n, residual saturation, vG m - default = 1 - 1/n,
49		(blank line for readability)
51	~Aqueous Relative Permeability Card	The input that follows assigns method for calculating relative permeability as a function of aqueous saturation for unsaturated zone.
52	BF, Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),
53	HF,Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),
54	HS,Mualem,,	zone name, permeability function name, van Genuchten m parameter (default =1-1/n),
56		(blank line for readability)
57	~Initial Conditions Card	<p>The input that follows assigns initial hydraulic conditions to nodes defined in the ~Grid Card above.</p> <p><i>NOTE: initial conditions are replaced by contents of the 'restart' file because the Restart execution mode was specified in the ~Simulation Control Card, above.</i></p>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
58	Aqueous Pressure, Gas Pressure,	<p>initial saturation option A, initial saturation option B,</p> <p><i>NOTE: gas pressure is unspecified, and therefore defaults to atmospheric pressure throughout the unsaturated zone (101,325 Pa) EXCEPT for the solute concentration which is specified with an OVERWRITE option to cause this input to be used in place of the 'restart' file contents.</i></p>
59	3,	Number of initial conditions specified,
60	Aqueous Pressure,1.4906840E+05,Pa,,,,,-9793.52,1/m,1,1,1,1, 20,	<p>For initial condition #1;</p> <p>variable name, magnitude, units, X-dir pressure gradient ,units, Y-dir pressure gradient, units, Z-dir pressure gradient, units, X-dir starting node ,X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p> <p><i>NOTE: Calculation of base pressure in first node: saturated thickness = 5.0 m, Atmospheric pressure = 1.01E+05 Pa, water unit weight = 9793.52 N/m³, node spacing = 0.25m, so base pressure (at the center of bottom node) = 101325 + 9793.52 * (5.0-0.125) = 1.4906840E+05 Pa.</i></p>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
61	Aqueous Pressure,86656.7554,Pa,,,,,-100.,1/m,1,1,1,1,21, 120,	<p>For initial condition #2;</p> <p>variable name, magnitude, units, X-dir pressure gradient, units, Y-dir pressure gradient, units ,Z-dir pressure gradient, units, X-dir starting node ,X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p>
62	Solute Volumetric Overwrite,Con100,1930,1/m^3,,,,,,1,1,1,1, 45, 102,	<p>For initial condition #2;</p> <p>variable name, magnitude, units, X-dir pressure gradient, units, Y-dir pressure gradient, units ,Z-dir pressure gradient, units, X-dir starting node ,X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node,</p> <p><i>NOTES:</i></p> <ul style="list-style-type: none"> • <i>OVERWRITE is used to force initial concentration to be applied over the contents of the 'restart' file.</i> • <i>Initial contamination is applied from nodes 45 to 102 (70:30 model)</i> • <i>Particle density = 2.68</i> • <i>Bulk density = (1-porosity)*particle density = (1-0.28)*2.68 = 1.93 gm/cc = 1930 kg/m³</i> • <i>Thus, initial concentration = 1 mg/kg = 1930 mg/m³</i>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
63		(blank line for readability)
64	~Boundary Conditions Card	<p>The input that follows assigns boundary conditions to exterior node faces; these boundaries may vary in time by assigning multiple times that the boundary variable changes.</p> <p><i>NOTE: Boundary conditions area applied at node faces.</i></p> <p><i>NOTE: direction of boundary fluxes consistent with STOMP conventions (positive is up, east, and north; negative is down, west, and south).</i></p> <p><i>NOTE: any face that is not assigned a boundary condition defaults to a no-flow boundary assignment in STOMP.</i></p> <p><i>NOTE: boundary conditions with more than one time range will transition linearly between the rates at the times prescribed.</i></p>
65	3,	number of boundary conditions specified,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
66	top,neumann,zero flux,zero flux,	For boundary condition #1; boundary surface direction, aqueous phase boundary type, ... (all the rest are zero flux boundaries)
67	1,1,1,1, 120, 120,8,	For boundary condition #1 (recharge at top boundary); X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,
68	2010.,yr, -63.00000000,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #1 (start); boundary time, units, aqueous volumetric flux (recharge rate), units,...
69	2015.,yr, -63.00000000,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #2 (until 2015); boundary time, units, aqueous volumetric flux (recharge rate), units,...
70	2015.,yr, -3.1500000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #3 (starting 2015); boundary time, units, aqueous volumetric flux (recharge rate), units,...

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
71	2020.,yr, -3.1500000E+01,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #4 (until 2020); boundary time, units, aqueous volumetric flux (recharge rate), units,..
72	2020.,yr, -8.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #6 (starting 2020); boundary time, units, aqueous volumetric flux (recharge rate), units,...
73	2050.,yr, -8.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #6 (until 2050); boundary time, units, aqueous volumetric flux (recharge rate), units,...
74	2050.,yr, -4.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #7 (starting 2050); boundary time, units, aqueous volumetric flux (recharge rate), units,...
75	3010.,yr, -4.0000000E+00,mm/yr,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	For boundary condition #1, starting at time #8 (until end); boundary time, units, aqueous volumetric flux (recharge rate), units,...
76	# Hydraulic gradient = 1.1E-3 m/m.	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
77	# With 10 m horizontal span of a grid, the head drop from the edge to middle points of	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
78	# the grid is 10m*0.0011 m/m = 0.011m	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
79	# The pressure drop is 0.011m * 9793.52Pa/m = 107.73 Pa.	<i>NOTE: entire line is a comment line that is not read by STOMP – as indicated by use of the “#” symbol in the first column)</i>
80	west,hydraulic gradient,zero flux,zero flux,	For boundary condition #2 (aquifer gradient, upgradient side); boundary surface direction, aqueous phase boundary type,...
81	1, 1,1,1,1,20,1,	For boundary condition #2; X-dir starting node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
82	2010,yr, 1.4906840E+05,Pa,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	<p>For boundary condition #2, starting at time #1; boundary time, units, base aqueous pressure, units,</p> <p><i>NOTE: is the upstream water phase boundary for the aquifer nodes; the condition establishes a fixed hydraulic gradient across the aquifer nodes to simulate aquifer flow.</i></p>
83	east,hydraulic gradient,outflow,outflow,outflow,outflow, outflow,outflow,outflow,outflow,outflow,outflow,outflow,outflow,	<p>For boundary condition #3; boundary surface direction, aqueous phase boundary type,</p>
84	1, 1,1,1,1,20,1,	<p>For boundary condition #3; X-dir starting, node, X-dir ending node, Y-dir starting node, Y-dir ending node, Z-dir starting node, Z-dir ending node, number of boundary times,</p>

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
85	0.,yr, 1.4896070E+05,Pa,	<p>For boundary condition #3, starting at time #1; boundary time, unit, base aqueous pressure, unit,</p> <p><i>NOTE: hydraulic gradient 0.0011m was applied from west to east, distance between west and east surface = 10m, so pressure at the east surface = west pressure – $0.0011 * 10 * 9793.52 = 1.711E+05 - 107.73 = 1.7099E+05$ Pa</i></p> <p><i>NOTE: is the downstream water phase boundary for the aquifer nodes; the condition establishes a fixed hydraulic gradient across the aquifer nodes to simulate aquifer flow. Contaminant mass exits the model domain through the assignment of the outflow boundary condition on the downgradient face of the aquifer nodes.</i></p>
86		(blank line for readability)
87	~Solute/Fluid Interactions Card	The input that follows specifies how dilute solute mass will interact with fluid (diffusion, decay).
88	1,	number of solutes,
89	Con100,conventional,0.0,m^2/s,continuous,100000000.0,yr,	solute name, Effective diffusion calculation method, aqueous molecular diffusion coefficient@20 degree Celsius, units, solute partitioning option, half life, units,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
90	0,	number of chain decay lines (for radioactive solute),
91		(blank line for readability)
92	~Solute/Porous Media Interaction Card	The input that follows specifies the dilute solute mass will interact with the solid phase (retardation).
93	# 1	(comment line to help discern different soil type assignments)
94	BF,0.0,m,0.0,m,	zone name, longitudinal dispersivity, unit, transverse dispersivity, units,
95	Con100, 1950.00000,cm ³ /g,	solute name, solute aqueous partitioning coefficient (Kd), units,
96	# 2	(comment line to help discern different soil type assignments)
97	HF,0.0,m,0.0,m,	zone name, longitudinal dispersivity, unit, transverse dispersivity, units,
98	Con100, 1950.00000,cm ³ /g,	solute name, solute aqueous partitioning coefficient (Kd), units,
99	# 3	(comment line to help discern different soil type assignments)

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
100	HS,0.0,m,0.0,m,	zone name, longitudinal dispersivity, unit, transverse dispersivity, units,
101	Con100, 1950.00000,cm ³ /g,	solute name, solute aqueous partitioning coefficient (Kd), units,
102		(blank line for readability)
103	~Surface Flux Card	The input that follows directs STOMP to record flux of water mass and solute mass across the downgradient nodes of the aquifer cells to a special surface flux output file.
104	2,	number of surface flux inputs,
105	2,gw_conc.srf,	number of surface flux inputs in file, file name,
106	Aqueous Volumetric Flux,m ³ /yr,m ³ ,east,1,1,1,1, 1, 20,	surface flux type,unit,unit(integral),surface orientation,X-dir starting node,X-dir ending node,Y-dir starting node, Y-dir ending node,Z-dir starting node, Z-dir ending node,
107	Solute Flux,Con100,1/yr,,east,1,1,1,1, 1, 20,	surface flux type,unit,unit(integral),surface orientation,X-dir starting node,X-dir ending node,Y-dir starting node, Y-dir ending node,Z-dir starting node, Z-dir ending node,
108		(blank line for readability)

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
109	~Output Control Card	The input that follows specifies the output to be reported to the screen throughout the simulation, to the output file throughout the simulation, and to the plot and restart files at prescribed times during the simulation.
110	1,	number of reference nodes at which output will be reported to the screen during simulation run
111	1,1,20,	For reference node #1; reference node X index, reference node Y index, reference node Z index,
112	50, 50, yr, m, 6, 6, 9,	reference node screen output frequency (every 50 time step), reference node output file frequency (every 50 time step), time unit, length unit, screen significant digits, output file significant digits, plot file significant digits,
113	11,	number of output files variables
114	aqueous saturation,,	For output variable #1; variable name, units,
115	aqueous pressure,Pa,	For output variable #2; variable name, units,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
116	aqueous hydraulic head,m,	For output variable #3; variable name, units,
117	aqueous matric potential,cm,	For output variable #4; variable name, units,
118	aqueous moisture content,,	For output variable #5; variable name, units,
119	xnc aqueous vol,m/yr,	For output variable #6; variable name, units,
120	znc aqueous vol,m/yr,	For output variable #7; variable name, units,
121	aqueous courant number,,	For output variable #8; variable name, units,
122	total water mass,,	For output variable #9; variable name, units,
123	solute aqueous concentration,Con100,1/m^3,	For output variable #10; variable name, units,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
124	solute volumetric concentration,Con100,1/m^3,	For output variable #11; variable name, units,
125	1,	number of plot/restart files times
126	3010. yr,	For plot/restart file time #1; plot/restart file time, units,
127	12,	number of plot files variables
128	no restart,,	For plot variable #1 (option to skip writing restart file at end); variable name, units,
129	aqueous saturation,,	For plot variable #2; variable name, units,
130	aqueous pressure,Pa,	For plot variable #3; variable name, units,
131	aqueous hydraulic head,m,	For plot variable #4; variable name, units,

Example Predictive (Post-2010) Model Annotated Input File

Line	STOMP Input Line	Explanation
132	aqueous matric potential,cm,	For plot variable #5; variable name, units,
133	aqueous moisture content,,	For plot variable #6; variable name, units,
134	xnc aqueous vol,m/yr,	For plot variable #7; variable name, units,
135	znc aqueous vol,m/yr,	For plot variable #8; variable name, units,
136	aqueous courant number,,	For plot variable #9; variable name, units,
137	total water mass,,	For plot variable #10; variable name, units,
138	solute aqueous concentration,Con100,1/m^3,	For plot variable #11; variable name, units,
139	solute volumetric concentration,Con100,1/m^3,	For plot variable #12; variable name, units,

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Appendix C

CHPRC Fact Sheet STOMP: Validation and Extent of Application

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The STOMP (Subsurface Transport Over Multiple Phases) simulator software was developed at Pacific Northwest National Laboratory in the early 1990s and has been subject to extensive use and improvement since that time. The fundamental purpose of the STOMP simulator software is to produce numerical predictions of thermal and hydrogeologic flow and transport phenomena in variably saturated subsurface environments, which are contaminated with volatile or non-volatile organic compounds. Auxiliary applications include numerical predictions of solute transport processes including reactive transport. This fact sheet provides a brief overview of work that has validated the STOMP simulator software and the breadth of applications to which this simulator has been applied.

EXAMPLES OF VALIDATION, BENCHMARKING, AND VERIFICATION FOR STOMP

Document	Validation/Benchmark/Verification Performed
<p><i>STOMP Subsurface Transport Over Multiple Phases: Application Guide</i> PNNL-11216, Nichols et al. 1997, Pacific Northwest National Laboratory, Richland, Washington</p>	<ul style="list-style-type: none"> • Saturated Flow – validation against analytical solution of Theis (1935) • Saturated Flow – validation against analytical solution of the leaky aquifer problem • Saturated Flow – benchmark against numerical solution of Morris and Reddell (1991) for flow to two wells in a non-homogenous domain • Saturated Transport – validation against analytical solution of van Genuchten and Alves (1982) for one-dimensional transport in a uniform steady flow field • Saturated Transport – validation against analytical solution of Cleary and Ungs (1978) for the “patch source” problem for transport in a steady uniform two-dimensional flow field • Sea-Water Intrusion: validation against the analytical solution of Henry’s Problem for steady-state diffused seat water wedging within a confined aquifer balanced against a fresh-water field as revisited by Ségol (1994) • Density-Driven Flow: verification against Elder’s Problem for transient thermal convection in porous media (Voss and Souza 1987). • Flow and Transport in Unsaturated Porous Media: verification against results for infiltration of water into a uniform laboratory scale soil column filled with very dry soils as reported by Haverkamp et al. (1977) • Flow and Transport in Unsaturated Porous Media: verification and benchmark against experimental and numerical simulation results reported by Touma and Vauclin (1986) for two-phase (air and water), one-dimensional infiltration into a soil column • Energy and Phase Mass Conservation: validation against hand calculations to demonstrate conservation of energy and phase mass in multiple phases for single-node system undergoing the following phase changes: evaporation, condensation, and thawing; and for flow from hot, two-phase conditions • Heat Pipe Flow and Transport: validation against the heat pipe problem posed and solved analytically by Udell and Fitch (1985) • Heat Pipe Flow and Transport: verification against the experimental results reported by Jame and Norum (1980) for a freezing/thawing heat pipe problem • Non-Aqueous Phase Liquid Flow and Transport: benchmark against the simulations conducted with the MOFAT code reported by Kaluarachchi and Parker (1989) for infiltration and redistribution of oil in a hypothetical, two-dimensional aquifer • Non-Aqueous Phase Liquid Flow and Transport: verification against experimentally determined fluid saturations during the infiltration and redistribution of a LNAPL and a DNAPL in a partly saturated one-dimensional column reported in Oostrom et al (1995). • Non-Aqueous Phase Liquid Flow and Transport: verification against experimentally determined Trichloroethylene (TCE) gaseous concentrations reported in Lenhard et al. (1985)

Simulation of Unsaturated Flow and Nonreactive Solute Transport in a Heterogeneous Soil at the Field Scale

NUREG/CR-5998 & PNL-8496,
1993, Pacific Northwest
Laboratory, Richland,
Washington

Verification of unsaturated flow and nonreactive solute transport in a heterogeneous soil at the field scale using the Las Cruces trench site in New Mexico.

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), Water
Resources Research 32(3):595-
609

Numerical modeling of hysteretic multiphase flow: 1. Model description and verification and 2. A validation exercise

White et. al (1993) in *EOS Transactions*, 74(16), AGU

Verification conducted to test the hysteretic permeability-saturation-pressure (k-S-P) relations that were embodied in the numerical simulator STOMP. The data used in the validation exercise were measured during a multiphase one-dimensional flow experiment where the elevation of the water table was fluctuated to produce wetting and drying fluid saturation paths. Water and NAPL contents were measured nondestructively at specified flow-cell locations via radiation attenuation. These measurements were compared to simulations of the experiment using STOMP. Close agreement was obtained between the experimental data and the numerical results, except for the highest and lowest measurement elevations. For the highest position, a slight modification to the relative permeability function provided better agreement with the experimental NAPL data. For the lowest position, the discrepancy between experimental data and numerical simulations is attributed to an absence of a nonwetting-fluid entry-pressure concept in the k-S-P model.

Numerical analysis of a three-phase system with a fluctuating water table

White and Lenhard (1993) in
Proceedings of Thirteenth Annual AGU Hydrology Days

Verification against multiphase flow experiment measurements involving subjecting an initially water-drained, three-phase (air-oil-water) to a fluctuating water table to quantify the entrapment of air and NAPL by phases of greater wettability under dynamic conditions.

Measurement and predictions of density-driven vapor flow of trichloroethylene in sandy porous media

Oostrom et al. (1994) in *EOS*,
75(16), American Geophysical
Union

Verification against experimental measurements of spatial and temporal evolution of gaseous-phase trichloroethylene (TCE) in a variably saturated 1-m-high by 2-m-long flow cell.

An experimental and numerical study of LNAPL and DNAPL movement in the subsurface

Oostrom et al. (1994), *EOS*

Verification against experimental measurements of the multiphase transport of LNAPL and DNAPL in a one-m-long glass column.

Models to determine first order rate coefficients from single-well push-pull tests.

Schroth and Istok (2006), *Ground Water* 44(2): 275–283

Validation against analytical solution for a push-pull test (injection and extraction from a single well) used for in situ determination of a variety of aquifer properties. The results of a STOMP based numerical model were in good agreement with the results of the analytical solution.

Intercomparison of Numerical Simulation Codes for Geologic Disposal of CO₂

Pruess et al. (2002), LBNL-51813, Lawrence Berkeley National Laboratory, Berkeley, California

Benchmark with other numerical simulation codes, including the TOUGH2 family of codes, MUFTE_UG, SIMUSCOPP, GEM, FLOTRAN, ECLIPSE 300, and NUFT.

EXAMPLES OF THE BREADTH OF STOMP APPLICATIONS (ASIDE FROM THE HANFORD SITE)

Document(s)	Location / Application
<p><i>Preliminary Total-System Analysis of a Potential High-Level Nuclear Waste Repository at Yucca Mountain</i></p> <p>PNNL-8444, Eslinger et al. (1993), Pacific Northwest National Laboratory, Richland, Washington</p>	<p>Yucca Mountain, Nevada</p> <p>Simulation of long-term gas phase transport of carbon-14 in potential high-level waste repository in unsaturated volcanic tuff</p>
<p><i>Simulation of Two-phase Carbon-14 Transport at Yucca Mountain, Nevada</i></p> <p>White et al. (1992) in <i>Proceedings of Solving Ground Water Problems with Models</i></p>	
<p><i>Numerical Analysis of the In-Well Vapor-Stripping System Demonstration at Edwards Air Force Base</i></p> <p>PNNL-11348, White and Gilmore (1996), Pacific Northwest National Laboratory, Richland, Washington</p>	<p>Edwards Air Force Base near Mohave, California</p> <p>In support of interim cleanup activities, simulation of in-well vapor stripping remediation technology designed to remove dissolved volatile organic compounds from groundwater. The in-well vapor-stripping system comprises an engineered and a hydrologic component that operate in unison to form an in situ recirculation pattern. The engineered system is driven with compressed air, utilizing an air-lift pumping scheme that volatilizes dissolved organic compounds. The volatile vapors are removed from the gas stream above the ground surface and pumped water is infiltrated into the hydrologic system below the ground surface.</p>
<p><i>Performance Assessment of the In-Well Vapor-Stripping System</i></p> <p>PNNL-11414, Gilmore et al. (1996), Pacific Northwest National Laboratory, Richland, Washington</p>	

NAPL Migration in Response to Hydraulic Controls at the Brooklawn Site near Baton Rouge, Louisiana

White and Oostrom (1997) in *Proceedings of Twenty First Annual American Geophysical Union Hydrology Days*

Brooklawn Site, Baton Rouge, Louisiana

Evaluation of the effectiveness of the hydraulic containment strategy being implemented at the Brooklawn Site to control DNAPL migration toward a fresh water aquifer. The investigation comprised experimental and numerical components. Laboratory experiments on soil samples and pumped DNAPL from the Brooklawn site were conducted to determine hydrologic properties of the soils and physical and chemical composition of the liquid. Numerical simulations were conducted using a multifluid simulator for multiple realizations of a two dimensional cross-section through the Brooklawn site transecting the region of known DNAPL contamination. Multifluid flow behavior considered included three-phase retention and relative permeability characteristics, nonwetting fluid entrapment, and multiphase pumping. The principal objective of the simulations was to generate quantitative comparisons between various hydraulic control options, thus providing a stronger scientific rationale for future environmental management decisions at the site. Results indicate that under current conditions the pumping wells peripheral to the DNAPL plume do not significantly contribute to hydraulic control of DNAPL migration or source recovery.

Transport of Carbon-14 in a Large Unsaturated Soil Column

Plummer et al. (2004), *Vadose Zone Journal* 3 (1): 109-121

Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID

Estimation of solid-aqueous distribution coefficient for sediments through inverse modeling of carbon-14 transport data using both a simple gas-diffusion model and STOMP to support work on the Radioactive Waste Management Complex (RWMC) of the Idaho National Engineering and Environmental Laboratory (INEEL) that includes activated metals that release radioactive C-14 as they corrode.

The Ohio River Valley CO₂ Storage Project Final Technical Report

Gupta (2008)

Mountaineer Power Plant, New Haven, West Virginia

A series of numerical simulations of CO₂ injection were conducted as part of a program to assess the potential for geologic sequestration in deep geologic reservoirs, the Rose Run formation and the Copper Ridge formation, at the AEP Mountaineer Power Plant outside of New Haven, West Virginia. The simulations were executed using the H₂O-CO₂-NaCl operational mode of the Subsurface Transport Over Multiple Phases (STOMP) simulator.

Validation of CO₂ Injection simulations with Monitoring Well Data

Bacon et al. (2009), Energy Procedia

Geological sequestration of carbon dioxide in the Cambrian Mount Simon Sandstone: Regional storage capacity, site characterization, and large-scale injection feasibility, Michigan Basin

Barnes et al. (2009), Environmental Geosciences: 16(3), 163-183

Quantification of Microbial Methane Oxidation in an Alpine Peat Bog

Urmann et al. (2007), Vadose Zone Journal 6:705-712

Hydrology and subsurface transport of oil-field brine at the U.S. Geological Survey OSPER site "A", Osage County, Oklahoma

Herkelrath et al. (2007), Applied Geochemistry 22(10):2155-2163

Modeling of Bromide in a Single-well Injection-Withdraw Experiment

Hellerich et al. (1999) in Hazardous and Industrial Wastes, Proceedings of the 31st Mid-Atlantic Industrial and Hazardous Waste Conference.

Thermal Analysis of GCLs at a Municipal Solid Waste Landfill

Hanson et al. (2005), Civil and Environmental Engineering

Phytocapping: An alternative technique to reduce leachate and methane generation from municipal landfills

Venkatraman and Ashwath (2007), The Environmentalist 27(1):1573-2991

Midwest Regional Carbon Sequestration Partnership geologic field test site, Otsego County, Michigan

STOMP used to assess potential carbon dioxide (CO₂) injection rates into saline formations at several sites for the MRCSP. An injection test of approximately 10,000 metric tons into the Bass Islands Dolomite with CO₂ injection rates from 250-500 tons per day, was performed in the test well at the MRCSP geologic field test site. Reservoir simulations were performed to estimate injection parameters, such as bottom hole pressures and pressure response over time in the storage formation, and compared to measurements taken during the test.

Drained but partially regenerated raised peat bog in Eigenthal above the city of Lucerne, Switzerland

STOMP used to simulate a gas push-pull test to quantify methanotrophic activity in situ in the vadose zone above a petroleum-contaminated aquifer.

U.S. Geological Survey OSPER site "A", Osage County, Oklahoma

STOMP used to simulate a subsurface salt plume.

National Chromium, Inc. chromium metal plating facility located in northeastern Connecticut

Mechanisms controlling the transport of bromide in a single-well injection-withdrawal experiment determined through modeling using the STOMP simulator.

An undisclosed solid waste landfill, Michigan

STOMP used to simulate in one dimension heat transfer near the center of the landfill.

Queensland, Australia

Trial use of STOMP to calculate daily water balance to identify suitable plant species and optimize thickness of soil cover for use in phytocapping.

***Numerical Analysis to Investigate
the Effects of the Design and
Installation of Equilibrium Tension
Plate Lysimeters on Leachate
Volume***

Mertensa et al. (2005) 4:488-499

***Degassing of $^3\text{H}/^3\text{He}$, CFCs and SF_6 by
denitrification: Measurements and
two-phase transport simulations***

Visser et al. (2008), Journal of
Contaminant Hydrology 103(3-
4):206-218

Lake Taupo catchment, New Zealand

Applied STOMP to a two-dimensional model for a range of subsurface conditions to examine the effect of the lower boundary condition on solute transport in lysimeters.

The Netherlands

Used STOMP as a two-phase flow and transport model to study reliability of $^3\text{H}/^3\text{He}$, CFCs and SF_6 as groundwater age tracers under agricultural land where denitrification causes degassing.