ECF-200PO1-21-0126
Revision 0

Groundwater Flow and Migration Calculations for the 2021 Annual Assessment of the Monitoring Networks for the Nonradioactive Dangerous Waste Landfill and Solid Waste Landfill

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

Contractor for the U.S. Department of Energy
under Contract 89303320DEM000030

CPCCo
Central Plateau Cleanup Company

P.O. Box 1464
Richland, Washington 99352

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APPROVED
By Julia Raymer at 8:04 am, Jan 06, 2022

Release Approval Date

ENVIRONMENTAL CALCULATION COVER PAGE

SECTION 1 - Completed by the Responsible Manager

Project: RS&I	**RELEASE / ISSUE** DATE: Jan 06, 2022 HANFORD RELEASE
Date: 11/29/2021	
Calculation Title and Description: Groundwater Flow and Migration Calculations for the 2021 Annual Assessment of the Monitoring Networks for the Nonradioactive Dangerous Waste Landfill and Solid Waste Landfill	

Qualifications Summary

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Degree, Major, Institution, Year: MASc. Civil Engineering (Water), University of Waterloo, 2016

Degree, Major, Institution, Year: BASc. Env Eng (Water Resources), University of Waterloo, 2014

Professional Licenses:

Brief Narrative of Experience: Mr. Chowdhury provides expertise in the application and calibration of numerical groundwater flow models for use in regulatory hydrogeological assessments and remediation studies. He has experience working with large sites characterized by complex hydrogeology and interpreting data from hydrogeological investigations.

Checker(s):

Name: Xiaomin Wang

Degree, Major, Institution, Year: PhD, Earth & Env Sciences, University of Waterloo, 2012

Degree, Major, Institution, Year: Msc, Water Res Eng & Mgmt, University of Stuttgart, 2007

Degree, Major, Institution, Year: Bsc, Env Eng, Dalian University of Technology, 2004

Professional Licenses: Professional Engineer of Ontario, Ontario, Canada

Brief Narrative of Experience: Dr. Wang’s expertise is in water-resource management and hydrogeology and the application of business and finance concepts in multi-disciplinary research. Her work has been focused on groundwater flow modeling for water resources development and protection and to support the designs of remedial measures; environmental data analysis. Her PhD work focused on the development of approaches to assist decision-makers and developers in assessing risks and benefits of a project from both environmental/engineering and financial perspectives. This research involved soil-vapor pathways simulation, data-worth analysis, and risk pricing. Dr. Wang's areas of expertise include: groundwater flow and solute transport modeling; interpretation of hydrogeologic data; soil vapor transport modeling; data assimilation and geostatistics; particle tracking simulation; and landfill design and finite mass analysis.

Senior Reviewer(s):

ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

Name: Alex Spiliotopoulos

Degree, Major, Institution, Year: PhD, Civil & Environmental Eng., University of Vermont, 1999

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Professional Licenses:

Brief Narrative of Experience: Dr. Spiliotopoulos' expertise is analysis to support water resources management. He has developed and applied analytical and numerical models for groundwater flow and contaminant transport, focusing on pump-and-treat system operations, reactive-transport modeling, and optimization applications for least-cost remediation designs. He has extensive experience in assessing water-resources management in support of inter- and intra-state water-resource allocation and conflict resolution, assessment of water quantity and quality data, development and application of statistical tools and numerical interpolation techniques for mapping water-level and water-quality data, and the application of advanced parameter estimation techniques for model calibration. At Hanford, he has designed RPO and RI/FS remedial alternatives, including large-scale pump-and-treat networks and/or MNA and other in-situ treatment technologies for the River Corridor OUs, conducted sitewide multi-constituent plume delineation, and co-authored Remedial Design and Remedial Action Work Plans. He has provided technical support on system performance evaluations and modifications, characterization of plume migration patterns, aquifer test data interpretations as well as practical and theoretical aspects of aquifer hydraulics and their applications. He developed and contributed to numerous presentations to stakeholders, illustrating elements of the proposed remedies, and their impacts on containment and recovery performance.

SECTION 2 - Completed by Preparer

Calculation Number: ECF-200PO1-21-0126 | Revision Number: 0

Revision History

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0	Initial Issue	11/29/2021	ALL

SECTION 3 - Completed by the Responsible Manager

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SECTION 4 - Document Review and Approval

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Xiaomin Wang	Project Hydrogeologist	Per email approval attached	11/29/2021

ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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Responsible Manager(s):			
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SECTION 5 - Applicable if Calculation is a Risk Assessment or Uses an Environmental Model

Prior to Initiating Modeling:

Required training for modelers completed:
Integration Lead:

Print First and Last Name	*Signature / Date*

Safety Software Approved:
Integration Lead:

Print First and Last Name	*Signature / Date*

Calculation Approved:

Risk/Modeling Integration Manager:

Print First and Last Name	*Signature / Date*

Kristen Pekoske

From: Xiaomin Wang
Sent: Monday, November 29, 2021 11:39 AM
To: Mashrur Chowdhury
Cc: Kristen Pekoske
Subject: ECF-200PO1-21-0126, Rev. 0

Mashrur,

The subject ECF, titled "Groundwater Flow and Migration Calculations for the 2021 Annual Assessment of the Monitoring Networks for the Nonradioactive Dangerous Waste Landfill and Solid Waste Landfill" and dated 11/29/2021, was reviewed and updated. I approve it for publication as of today, November 29, 2021.

Regards,
Xiaomin Wang

Contents

Figures

Terms

2D	two-dimensional
ASCII	American Standard Code for Information Interchange
CPCCo	Central Plateau Cleanup Company
CY	calendar year
DWMU	dangerous waste management unit
ECF	environmental calculation file
ESRI	Environmental Systems Research Institute
HHK	horizontal hydraulic conductivity
NRDWL	Nonradioactive Dangerous Waste Landfill
SME	subject matter expert
SWL	Solid Waste Landfill
TRIM	Tikhonov regularized inverse method

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1 Purpose

This environmental calculation file (ECF) describes calculations made to evaluate the continued suitability of the final status groundwater monitoring network for the dangerous waste management unit (DWMU) Nonradioactive Dangerous Waste Landfill (NRDWL). NRDWL is located approximately 5.6 km (3.5 mi) southeast of the 200 East Area of the Hanford Site Central Plateau (Figure 1). This ECF re-evaluates the efficacy of the final status well networks using groundwater flow conditions calculated for calendar year (CY) 2021 to verify the continued suitability of the well locations for monitoring purposes. This ECF describes the conceptual and methodological basis for the calculations performed, the specific methods and codes used to perform the calculations, and presents the calculation results.

In addition, an evaluation of the monitoring well network for the Solid Waste Landfill (SWL) is included in this ECF. SWL, shown on Figure 1, is not a DWMU so it is not subject to the same regulatory requirements. However, because it is adjacent to NRDWL, the same methodology used for NRDWL was used to evaluate the locations of the SWL monitoring wells.

2 Background

This chapter describes the final status groundwater monitoring network for NRDWL and the monitoring network for SWL that are evaluated in this ECF. The network for SWL is not considered final status because it is not in the same regulatory framework as NRDWL. The water-table elevation map used as the basis for the calculations performed to evaluate the network is also described in this chapter.

2.1 Groundwater Monitoring Networks

The final status groundwater monitoring network for NRDWL (Figure 2), was determined in SGW-60589, *Engineering Evaluation Report for the Nonradioactive Dangerous Waste Landfill Groundwater Monitoring*, and consists of three upgradient shallow wells, 699-26-38, 699-26-35A, and 699-26-34A; three downgradient shallow wells, 699-26-33A, 699-25-34F, and 699-25-34B; one upgradient deep well, 699-26-35C; one downgradient deep well, 699-25-33A; and two cross-gradient wells, 699-26-34B and 699-25-34D.

The wells, with the exception of the two deep wells (699-26-35C and 699-25-33A), are screened at the top of the unconfined aquifer in order to detect significant increases in groundwater contamination that would result from a release at NRDWL that reaches the underlying water table from the regulated unit.

The monitoring network for SWL (Figure 2) consists of one upgradient well, 699-24-36; and five downgradient wells, 699-22-35, 699-23-34B, 699-24-34D, 699-24-34E, and 699-25-34E.

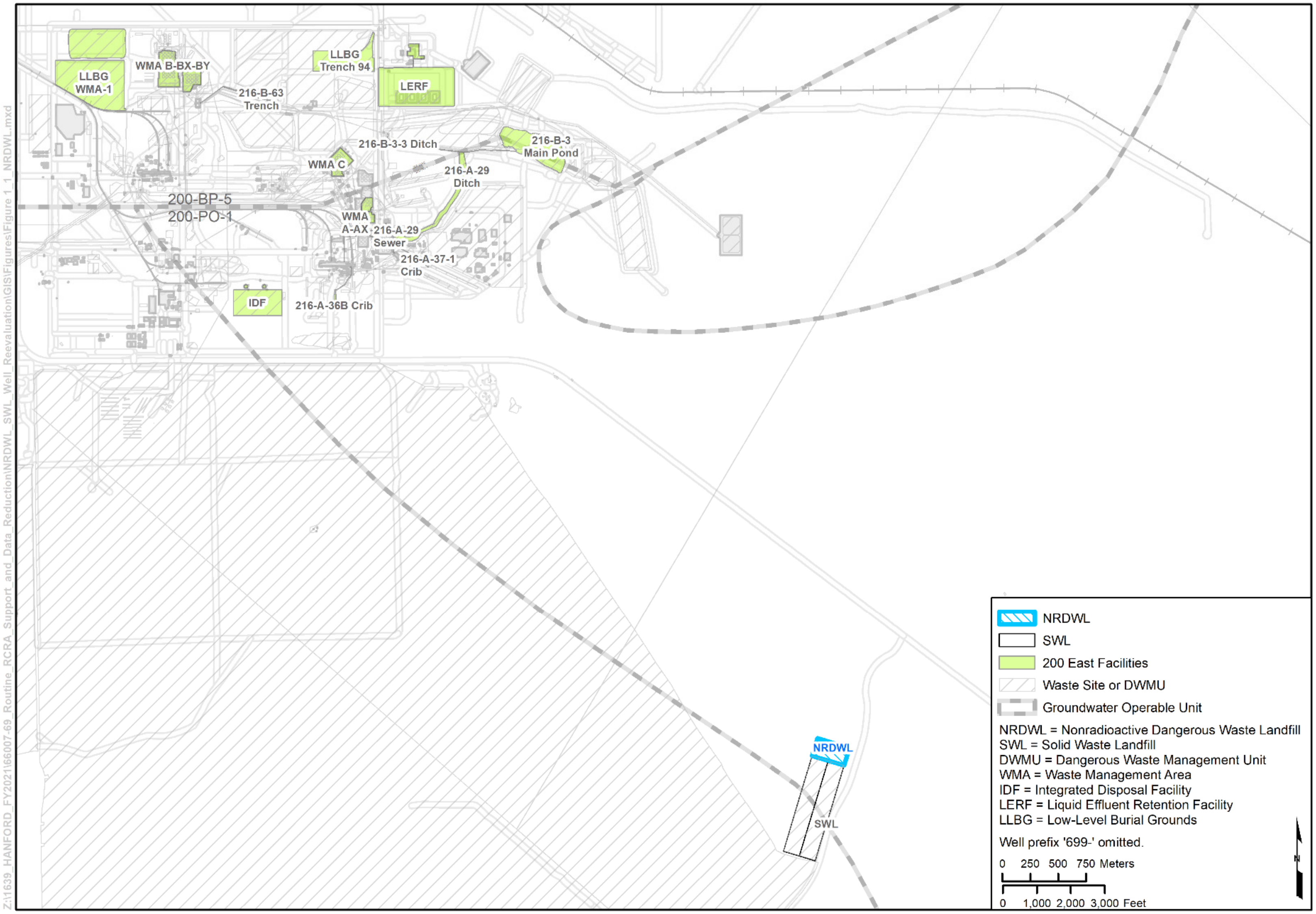


Figure 1. Locations of NRDWL and SWL

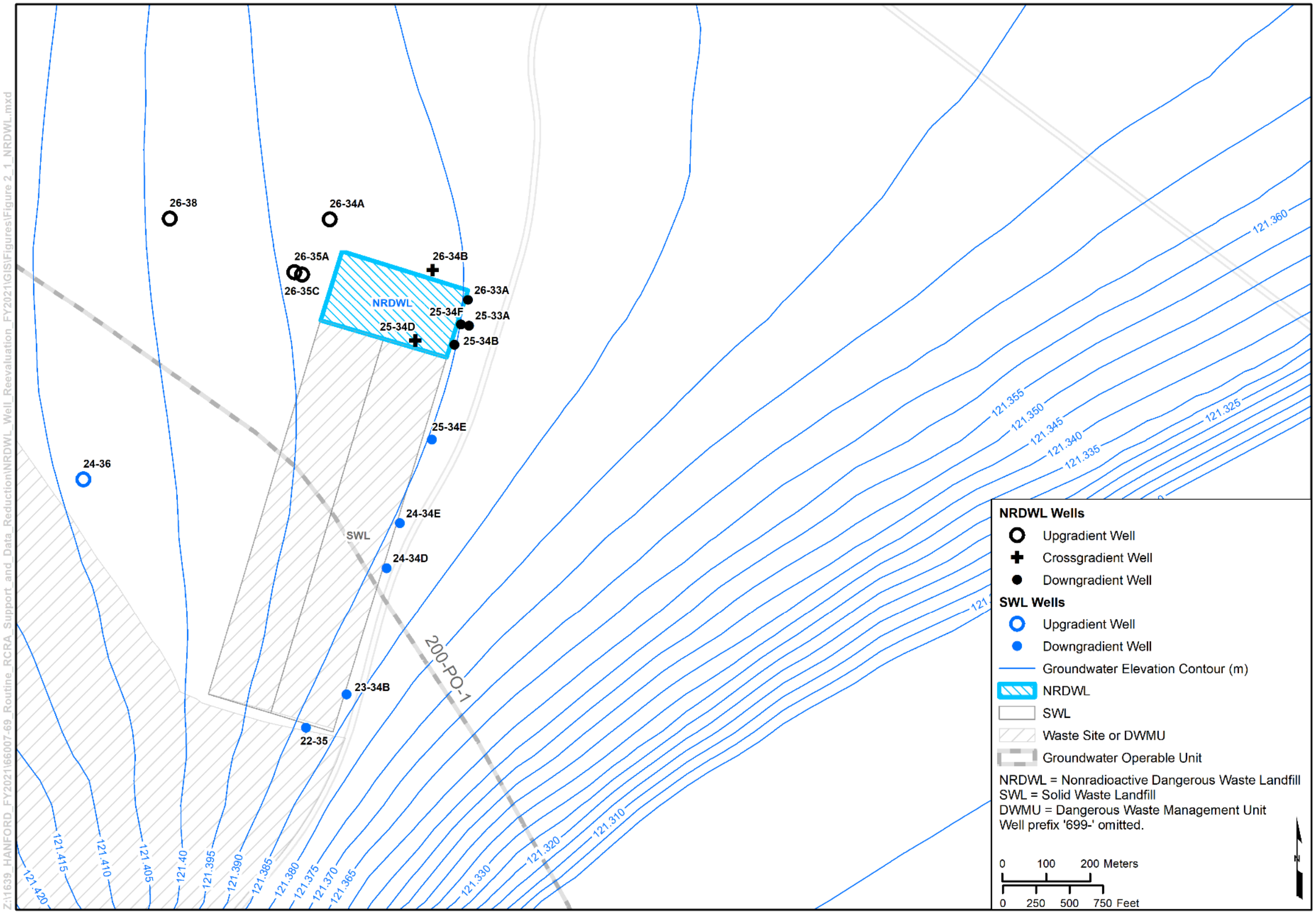


Figure 2. Final Status Monitoring Networks for NRDWL and SWL Superimposed on Water-Table Elevation Map

2.2 Water-Table Elevation Mapping

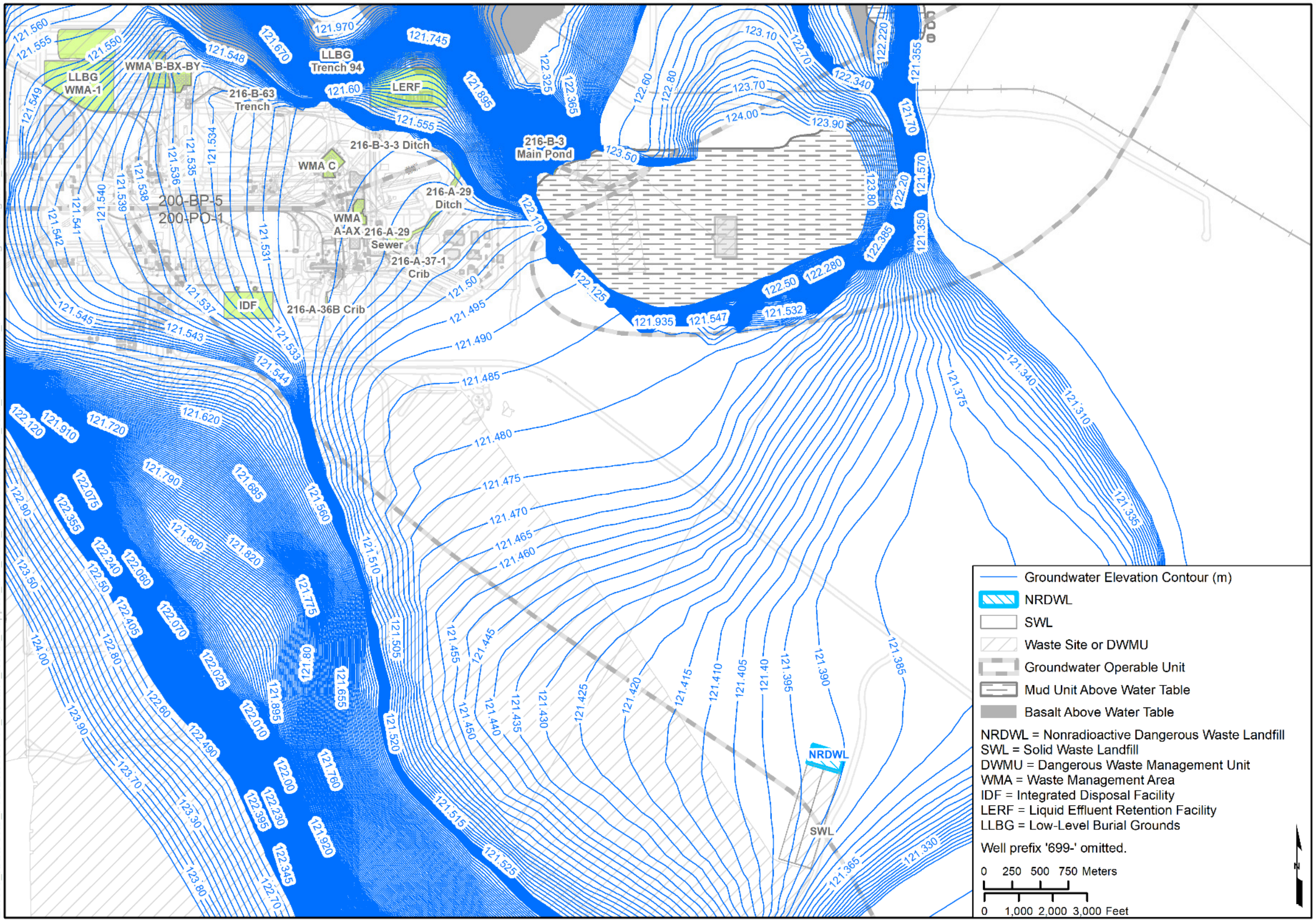
To support the assessment of the groundwater monitoring networks associated with NRDWL, the evaluation performed in this ECF was based on a piecewise, continuous (i.e., gridded) depiction of groundwater elevations and resulting hydraulic gradients encompassing the area surrounding NRDWL.

These calculations rely on a grid of groundwater elevations that was developed in ECF-HANFORD-21-0117, *Preparation of the March 2021 Hanford Site Water Table Map*. The method detailed in ECF-HANFORD-21-0117 combined a two-dimensional (2D) steady-state groundwater flow simulator developed using the MODFLOW-USG code (Panday et al., 2013, *MODFLOW-USG Version 1: An Unstructured Grid Version of MODFLOW for Simulating Groundwater Flow and Tightly Coupled Processes Using a Control Volume Finite-Difference Formulation*), with statistical methods to obtain a best estimate of groundwater flow patterns at the Hanford Site.

The parameters of the underlying groundwater flow simulator were determined through a regularized inverse interpolation technique referred to as the Tikhonov regularized inverse method (TRIM) (Tikhonov and Arsenin, 1977, *Solutions of Ill-Posed Problems*). TRIM is founded upon a formal mathematical method that seeks a tradeoff between the complexity of the method or parameterization used to interpret measured data versus the "fit" to the data that the chosen method or parameterization attains. TRIM implements a common application of Tikhonov regularization, by supplementing the measurement dataset (in this case, site-wide groundwater elevation measurements from January to March 2021) with other information derived from subject matter expert knowledge. This knowledge is cast as "prior information" representing an anticipated system condition (in this case an understanding of the distribution and variability of hydraulic conductivity). As described by Menke, 2018, *Geophysical Data Analysis: Discrete Inverse Theory,* the calibration process is a tradeoff between method or parameter complexity and data fit. The more complex the method or its parameterization, the more closely the outputs from that method or parameterization can be expected to fit the data. However, a better fit to the data does not guarantee a better estimator or predictor. Particularly in cases such as the 200 East Area, where there is a low signal-to-noise ratio in the data, "overfitting" can occur with parameters responding to the noise rather than the signal (Doherty, 2015, *Calibration and Uncertainty Analysis for Complex Environmental Models, PEST: Complete Theory and What it Means for Modelling the Real World*).

Without constraints that recognize the presence of a low signal-to-noise ratio, overfitting can attain a very good data fit by inferring high parameter or method complexity such as exaggerated heterogeneity in a homogeneous system. In contrast, underfitting can occur when the method or parameterization used is too simple because it does not reasonably approximate the underlying physics or reflect the dominant physical characteristics of the system. A result of underfitting is insufficient capability to reproduce measured data. In either case of overfitting or underfitting, the results often do not agree well with subject matter expert knowledge of the system or with other independent information.

Because the model is 2D and steady-state, only the parameters associated with horizontal hydraulic conductivity (HHK) and specified-flux boundary conditions representing the mountain-front recharge were calibrated against the groundwater elevation data. Figure 3 presents the result of water-table elevation mapping from ECF-HANFORD-21-0117 for the 200 East Area including NRDWL, and Figure 2 presents the area focused around NRDWL. This water-table elevation map is the basis for the calculations presented in this ECF. Particle-tracking calculations were performed at NRDWL based on the water-table elevation map to depict approximate directions of groundwater flow and potential contaminant migration in the vicinity of NRDWL.



Groundwater Elevation Contours Source: ECF-HANFORD-21-0117, *Preparation of the March 2021 Hanford Site Water Table Map*.

Figure 3. Water-Table Elevation Map for NRDWL and SWL

3 Calculation Methods

Calculations were completed to re-evaluate the final status groundwater monitoring networks at NRDWL. The objective of the calculations was to determine whether interpreted groundwater flow conditions in CY 2021 continue to support the suitability of the locations of the final status groundwater monitoring wells that were originally proposed.

This chapter describes the calculation methods used to support this ECF. The groundwater elevation map used for the evaluation developed using the sitewide TRIM was provided in Chapter 2. The groundwater elevation map was used in particle-tracking calculations. The required data and the method for each calculation for CY 2021 are described in this chapter.

3.1 Particle Tracking and Relative Detectability

The sitewide groundwater elevation map depicts general patterns of hydraulic gradients and groundwater flow. The water-table elevation map also helps identify potential directions of contaminant migration if a release from a facility reaches the water table. Particle tracking provides a method of visualizing these directions and integrating the gradients to depict potential paths of migration and enables a more thorough assessment of the suitability of monitoring well locations.

After the groundwater elevation grid was created using TRIM, the grid was used as the base for particle tracking. Particle tracking was performed using mod-PATH3DU, considering advective and dispersive transport mechanisms (Muffels et al., 2018, *User's Guide for mod-PATH3DU, A Groundwater Path and Travel-Time Simulator*). The use of the particle-tracking method assumes migration of a conservative (i.e., nonreactive) dissolved contaminant. Calculated particle pathlines provide a way to visualize how a hypothetical release from NRDWL reaching the water table would move and spread under conditions representative of CY 2021. Particle-tracking calculations are used in this ECF to produce maps of particle pathlines and relative detectability for evaluation of the location of the final status monitoring wells.

3.1.1 Particle Tracking

Particle tracking considering both advection and dispersion was performed on the groundwater elevation grid generated using the sitewide TRIM for the first quarter of CY 2021 to calculate the movement of a one-time release of a large number of particles representing an instantaneous release reaching the water table.

Twenty particles were released from each release location, resulting in 20 pathlines originating from each location, each of which depicts a potential path of a dissolved contaminant particle released at the water table beneath each facility. To represent potential variations in migration pathways that may result from dispersive processes, the random-walk particle-tracking option within mod-PATH3DU was used. With this option, particles are advected at the average groundwater velocity and dispersed randomly. The option implements a generalized stochastic differential solution that satisfies the Fokker-Planck equation (Muffels et al., 2018). The solution assumes constant porosity and isotropic dispersion values. The underlying theory of the random walk method and its implementation within mod-PATH3DU is discussed in greater detail in Muffels et al., 2018. The calculated particle pathlines provide a way to visualize how a hypothetical release to the water table from the facility would move and spread downgradient under flow conditions representative of CY 2021.

Calculated particle pathlines were further post-processed following the steps described in Chapter 6 to create maps of relative detectability for the purposes discussed below.

3.1.2 Relative Detectability

Counts of particles can be used to evaluate the relative efficacy of groundwater monitoring well locations. To show the relative migration potential of releases from NRDWL and SWL, the absolute particle counts were converted into a relative-particle detectability index. This index was created by counting the number of particles that pass through a predefined uniform particle-calculation grid and then dividing the particle count in each grid cell by the maximum number of unique particles that crossed a single grid cell.

3.2 Evaluation of Vertical Migration Potential

Dissolved constituents that are released within the vadose zone (i.e., above the water table) and migrate downward ultimately make their first impact to groundwater at the top of the aquifer (i.e., at the water table). Although the initial impact is at the water table, dissolved constituents that mix with moving groundwater over time have the potential to move vertically within the aquifer. When attempting to monitor and detect potential releases that have arrived at the water table, the possibility that constituents may migrate beneath the bottom of the screen interval of monitoring wells must be considered.

An analysis of the potential for the vertical migration of dissolved constituents is presented in ECF-200PO1-18-0010, *Groundwater Flow and Migration Calculations to Support the Assessment of the NRDWL Groundwater Monitoring Network*. The analysis used an analytical calculation, the American Petroleum Institute plume-diving calculation (Nichols and Roth, 2006, *Downward Solute Plume Migration: Assessment, Significance, and Implications for Characterization and Monitoring of "Diving Plumes"*) to estimate the likely rate of vertical migration of dissolved constituents downward under the influence of recharge at the water table. The calculations concluded that the plume depth fell within the intervals between the top of the water table and the bottom of the well screens for the final monitoring wells of NRDWL that were screened across the water table, indicating that the well depths were appropriate for detecting releases. The aquifer and hydrogeological conditions assumed in ECF-200PO1-18-0010 have not changed, so changes in the results of those calculations are not expected at this time. Therefore, these calculations have not been repeated herein but will be repeated if conditions change in the future.

4 Assumptions and Inputs

This chapter outlines the assumptions and inputs that underlie the calculations presented in this ECF.

4.1 Assumptions and Limitations

Assumptions and limitations used for the particle tracking are discussed in this section.

Particle tracking is calculated based on the mapped groundwater elevations computed using TRIM. As a result, the assumptions and limitations described in ECF-HANFORD-21-0117 that underlie the preparation of the maps are implicit in any subsequent particle-tracking calculations.

As described in ECF-HANFORD-21-0117, the accuracy of the contours is influenced by several factors, including the accuracy of the measured or recorded groundwater elevations; the number, distribution, and location of monitoring wells; and the relationship between the vertical open interval(s) of the monitoring wells and those of any extraction and injection wells. These potential sources of error mean that the water-table elevation maps are considered reasonable approximations that provide useful inference in the interpretation of likely directions and rates of groundwater movement (Section 4.1 of ECF-HANFORD-21-0117).

The simplified 2D groundwater flow model that underlies TRIM is not a substitute for existing three-dimensional groundwater flow and contaminant transport models at the Hanford Site, such as the Central Plateau Groundwater Model and the Plateau to River Groundwater Model. There are many simplifications in the underlying groundwater flow simulator including the use of a single layer representing only water-table conditions; the regularization objective sought in TRIM of homogeneity without specific regard for the values or physical meaning of the resulting parameters; and the simplified representation of the lateral boundaries of the area of interest. Because of these simplifications and limitations, the MODFLOW-USG simulator underlying TRIM should not be used as an alternative to the existing three-dimensional groundwater flow and contaminant transport models (Section 3.3 of ECF-HANFORD-21-0117).

Dispersivity in the two principal horizontal directions (i.e., longitudinal and transverse) is generally perceived to be dependent on the observation scale (Gelhar et al., 1992, "A Critical Review of Data on Field-Scale Dispersion in Aquifers").

Dispersivity values used in calculations were considered to be on the lower end of the range of values considered typical of field-scale sites. These lower-end values are appropriate for the calculations presented in this ECF primarily because the hydraulic gradient from wastewater disposal, which is the dominant historical mechanism leading to contamination spread at the Central Plateau, has diminished over time. Although the historical Central Plateau groundwater plumes are on the order of hundreds of meters in length or width, the distance and scale relevant to specifying dispersion lengths for this ECF are the distances from potential release locations to downgradient monitoring wells, which are substantially less than the scale of the historical plumes.

The assumption of a lower-end value for longitudinal dispersivity has two implications for evaluating the efficacy of a monitoring network for detecting a release: (1) lower-end values result in relatively narrower plumes than using higher-end values, and (2) the lower values result in relatively higher detectability for monitoring wells that are located directly on the path of a release. Given the objective of verifying the suitability of the spatial distribution of final network monitoring wells, emphasis was placed on implementing this conservative approach that does not overestimate the likely extent of groundwater impacts resulting from a hypothetical release.

The time required for any release from NRDWL or SWL to migrate downward within the vadose zone is not addressed in these calculations. The calculations assumed the particle-release time to be the time when contamination from hypothetical releases reaches the water table under the groundwater flow conditions representative of the particle-release year (in this ECF, for CY 2021). Therefore, the release time is not the year of the release from the facility. Also, for the purposes of this ECF, it is assumed that the water-table elevation surface generated by TRIM is steady-state over the time the particles are tracked. All particles were tracked for a length of time that allowed for the majority of the particles to migrate beyond monitoring wells at NRDWL and SWL.

4.2 Input Data

This section summarizes the general input requirements for the calculations described in this ECF.

4.2.1 Transport Parameters for Particle Tracking

The particle-tracking calculations described herein require the following aquifer transport parameters to be defined: HHK, effective porosity, and longitudinal and transverse dispersivities.

The HHK and effective porosity were assumed constant throughout the entire region. The primary purpose of the calculations presented in this ECF is to estimate the pathways of potential contaminant migration in order to assess the spatial distribution of each facility-specific monitoring well network. Because the particles released from each facility are tracked until they migrate beyond the corresponding monitoring well networks, the HHK and effective porosity in this case only serve as a combined scaling factor on the timing of migration beyond these monitoring wells. The values themselves do not affect pathline directions, which is exclusively a function of the gradients across the underlying groundwater elevation grid used for tracking. Thus, specifying a constant HHK and effective porosity has no bearing on the overarching goal of this ECF, which is to evaluate whether each of the final monitoring well networks span the potential pathways of contaminants downgradient of each facility.

It is widely recognized that the dispersion parameters are scale-dependent in solute transport process in saturated porous media. Based on the field scale specified in this analysis, 2D dispersivity values are assumed as the dispersion processes in the saturated zone are considered only in the horizontal direction. The horizontal longitudinal and transverse dispersivities are specified as 3.5 m (11.5 ft) and 0.7 m (2.3 ft), respectively. These values are adopted from Version 8.3 of the Plateau to River groundwater model (CP-57037, *Model Package Report: Central Plateau Groundwater Model, Version 8.3*) and are on the lower end of values identified as typical of field-scale sites by Gelhar et al., 1992; and Xu and Eckstein, 1995, "Use of Weighted Least-Squares Method in Evaluation of the Relationship Between Dispersivity and Field Scale," among others.

The following range of values for longitudinal dispersion are based on a typical migration distance from the potential source to the monitoring network of about 200 m (656 ft) and the recommendations of Gelhar et al., 1992; and Xu and Eckstein, 1995, as incorporated in the U.S. Environmental Protection Agency's online calculator (EPA, 2016, *Estimated Longitudinal Dispersivity*):

- 0.37 m (1.2 ft) (lower limit) (Gelhar et al., 1992)
- 1100 m (3,609 ft) (upper limit) (Gelhar et al., 1992)
- 6.21 m (20.4 ft) (Xu and Eckstein, 1995)
- 20 m (66 ft) (1/10th of migration distance; rule of thumb)

4.2.2 Particle Starting Locations

The starting locations for the particle-tracking calculations represent the plausible release sites from which a potential release would impact the underlying water table. The particle-starting locations within NRDWL were specified to be equally spaced by approximately 7 m (22 ft) between release points, along each of the six trenches that contain dangerous waste (Figure 4). A total of 22 release points were specified for each of the six trenches in NRDWL.

Twenty particles were released from each particle-release location to provide sufficient density of particles in space and time as required for the calculations. The particles were tracked forward using random seed values to mimic the random walk component of the dispersion process.
Thus, 2,640 (2,640 = 6 [trenches] by 22 [release locations] by 20 [releases]) particles were tracked.

The release locations for SWL are shown in Figure 5. A total of 37 release points were specified along the centerline of SWL.

4.2.3 Uniform Calculational Grid

Contour maps of relative detectability are generated by counting the number of particles that pass through a predefined uniform calculational grid. The grid that was used to develop the relative detectability maps is defined by 10 m by 10 m (33 ft by 33 ft) cells and is oriented to be parallel to the predominant groundwater flow direction at NRDWL and SWL.

The calculation grid used to conduct relative detectability calculations for each facility and the corresponding contour (or color-scaled) maps are presented in the facility-specific sections in Chapter 7.

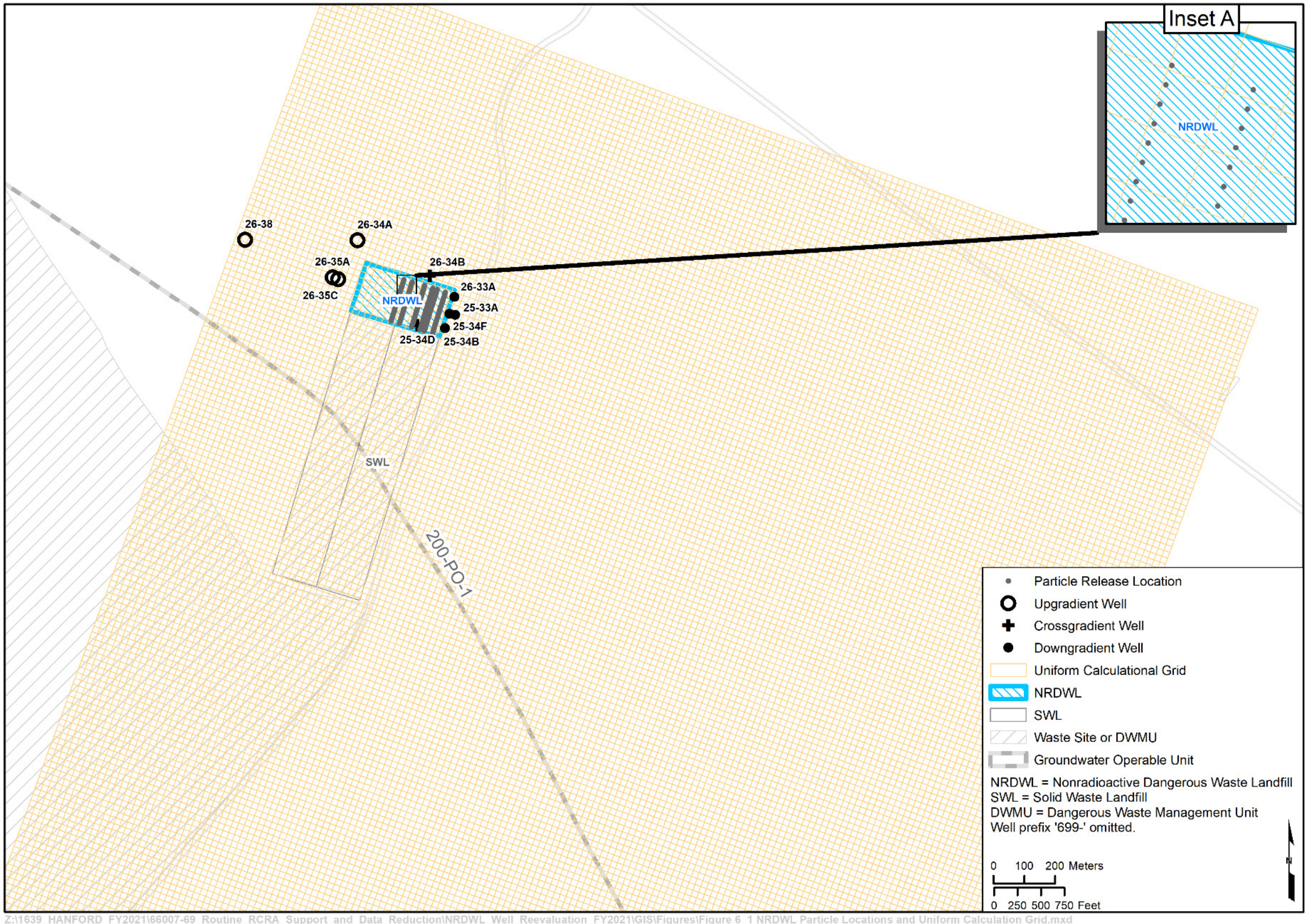
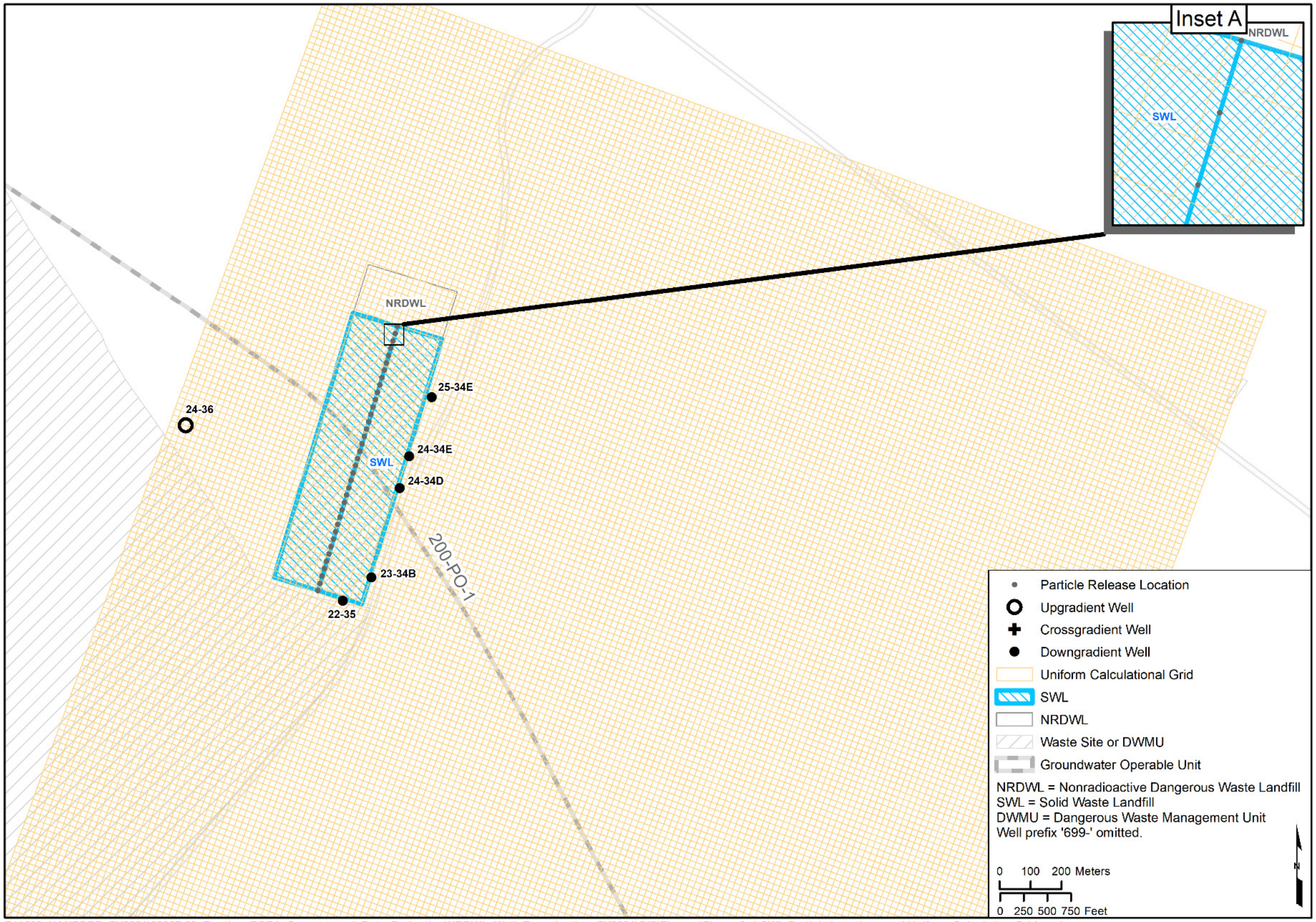


Figure 4. Release Locations and Calculational Grid for NRDWL



Z:\1639_HANFORD_FY2021\66007-69_Routine_RCRA_Support_and_Data_Reduction\NRDWL_Well_Reevaluation_FY2021\GIS\Figures\Figure 6_1 SWL Particle Locations and Uniform Calculation Grid.mxd

Figure 5. Release Locations and Calculational Grid for SWL

5 Software Applications

All software to perform the calculations presented in this ECF was used in accordance with Central Plateau Cleanup Company's (CPCCo's) controlled software management procedure, which implements DOE O 414.1D, *Quality Assurance*.

5.1 Approved Software

The software used to perform the calculations for this ECF was approved, managed, and used consistent with CPCCo's controlled software management procedure under the following software lifecycle documentation:

- CHPRC-00258, *MODFLOW and Related Codes Software Management Plan*
- CP-66783, *200 Area RCRA Utility Codes Integrated Software Test Management Plan*
- CP-66786, *mod-PATH3DU Integrated Software Management Plan*

The controlled software management procedures distinguish between safety software and support software based on whether the software calculates reportable results or provides run support, visualization, or similar functions.

5.2 Safety Software

This section describes approved safety software used for the calculations in this ECF:

- Software title: mod-PATH3DU
- Software version: 2.1.4
- Hanford Information Systems Inventory identification number: 5052 (safety software, graded Level C)
- Approved user: Mashrur Chowdhury
- Workstation type and property number (from which software is run): S.S. Papadopulos & Associates, Inc. workstation, FE616

5.3 Support Software

This section describes approved support software that were used for the calculations in this ECF.

The following programs are included in CHPRC-00258:

- ArcGIS®: Geographic information system (GIS) software to process maps and geographic information was used to (1) visualize extraction/injection wells, monitoring wells, and particle pathlines; and (2) map results (Mitchell, 1999, *The ESRI Guide to GIS Analysis, Volume 1: Geographic Patterns & Relationships*).
- Groundwater Vistas™: Provided graphical tools used for visualization and processing of input and output (Rumbaugh and Rumbaugh, 2017, *Groundwater Vistas Version 7*).

® ArcGIS is a registered trademark of the Environmental Systems Research Institute, Inc., Redlands, California.
™ Groundwater Vistas is a trademark of Environmental Simulations, Inc., Reinholds, Pennsylvania.

The following program is included in CP-66783:

- ArcMap 1639 Relative_Detectability_NRDWL.py: Python™ script to post-process particle-tracking pathline files.

The following program is included in CP-66786:

- Writep3doutput: mod-PATH3DU utility software to convert mod-PATH3DU binary output files to commonly used file types (i.e., American Standard Code for Information Interchange [ASCII], DBF table, and shapefile).

5.4 Software Installation and Checkout

Safety software installations are checked and tested in accordance with procedures specified in CP-66786. Executables are obtained from the CPCCo software owner, who maintains the configuration-managed copies in MKS Integrity® and ensures that installation tests identified in CP-66786 are performed and that successful installation is confirmed. Checkout forms are required and must be approved for installations used to perform model runs. Approved users for safety software are registered in the Hanford Information Systems Inventory.

5.5 Statement of Valid Software Application

The preparers of this calculation attest that the software identified above, and used for the calculations described in this ECF, is appropriate for the application and used within the range of intended uses for which it was designated by CPCCo.

6 Calculations

This chapter describes the calculation procedures for developing the necessary input files, performing calculations, and post-processing the outputs to produce the results presented in this ECF.

6.1 Particle Tracking

For the particle-tracking calculations presented in this ECF, the primary input files required by the mod-PATH3DU include:

- Tracking grid (i.e., the surface on which particles will be tracked), provided as an ASCII grid
- Pumping well locations, which serve as termination points for particle pathlines
- Particle-starting locations, provided in the Environmental System Research Institute (ESRI) shapefile format

The groundwater elevation grid generated using TRIM as described in ECF-HANFORD-21-0117 was first imported into Groundwater Vistas graphical user interface and then exported as an ASCII file in the Surfer software regular grid format. This was used as the mod-PATH3DU input file representing the surface on which to track particles.

Particle-starting locations (release points) were generated in the ESRI shapefile format to be used as input to mod-PATH3DU.

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The following steps were then implemented:

1. A mod-PATH3DU particle-tracking input file that included the prescribed advection and dispersion parameters was generated to simulate both advection and dispersion.
2. To simulate dispersion in particle tracking, the random-walk particle-tracking option within mod-PATH3DU was used. As described in the software documentation (CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report, CHPRC Build 8*), this random-walk module reads and uses the same dispersion inputs as the Hanford Site version of the transport simulator MT3DMS (Modular Transport, Three-Dimensional, Multi-Species Model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems).
3. A maximum tracking time was specified for each facility that allowed the majority of the particles released to migrate beyond the locations of the monitoring wells.
4. Particles were released and tracked forward from each particle-starting location as follows:
   a. Twenty particles were released from each starting location to provide a lateral spread of particles moving by dispersion with random-walk capability along with advective processes.
   b. mod-PATH3DU was executed to perform the particle-tracking calculations and produced a binary pathline output file containing the particle trace for each tracked particle. Particles were tracked from each starting location using a different random seed value for the dispersion calculations.
5. A post-processing program (writep3doutput.exe) was executed to convert the mod-PATH3DU binary pathline output file into both an ArcGIS shapefile format and an ASCII text file format, both of which list particle locations and travel times.

The resulting particle tracks were superimposed upon figures that showed monitoring well locations to determine whether the monitoring locations lie in the migration pathway of the simulated releases from the facilities.

6.2 Relative Detectability

Relative detectabilities were calculated to create maps that illustrate potential impacts of releases downgradient of NRDWL and SWL. The following steps were used for the calculations:

1. An ArcGIS shapefile grid large enough to envelope all pathlines generated from particle-tracking analysis was defined. This subgrid was discretized into 10 m by 10 m (33 ft by 33 ft) cells.
2. The ArcGIS "Spatial Join" tool was used to intersect the pathlines with the subgrid and the count of unique pathlines intersecting each subgrid cell was then determined using a post-processing tool written in Python. The relative detectability within a subgrid cell for a given release scenario is calculated as follows:

$$RD = \frac{1}{MNP}\sum_{i1}^{n} P_i N_i \qquad \textbf{(Equation 1)}$$

where:

RD	=	relative detectability (ranging from zero to one)
MNP	=	maximum number of particles that traversed any subgrid cell in all scenarios
P_i	=	ascribed weight or probability of subscenario i
N_i	=	number of particles that traversed the calculation subgrid cell during sub-scenario i
n	=	total number of subscenarios within each simulated scenario.

Since only one scenario was being simulated, Equation 1 is rearranged into the following:

$$RD = \frac{N}{MNP}$$

3. This grid of relative detectability indices was converted to an ASCII grid format and imported into ArcGIS, after which bilinear interpolation was used to develop the relative detectability maps presented in Chapter 7.

The relative detectability maps illustrate two main features: (1) the relative likelihood of constituents impacting the water table migrating through different areas of the aquifer downgradient of NRDWL; and (2) the relative suitability of each existing or proposed monitoring well location for detecting releases from NRDWL and SWL (i.e., in comparison to other existing or proposed monitoring well locations).

The relative detectability calculations and maps do not provide an absolute quantitative metric against which an existing or proposed monitoring well location can be compared or measured (e.g., a relative detectability limit above which wells should be placed when new wells are proposed). There are many reasons for this limitation. First, there are many aspects of potential future releases that cannot be known with certainty (e.g., timing, volume, rate, mass, and precise location of the release). As a consequence, an absolute metric, which would depend on these and other unknowable quantities, cannot reasonably be determined. Second, the overarching goal for the final monitoring well network is to have a distribution of wells that spans the expected range of detectability for NRDWL and SWL, rather than locating wells preferentially in the highest detectability areas only.

During network evaluation, both areas of high relative detectability, as well as locations at the fringes of detectability, were identified as warranting monitoring due to uncertainties in flow and migration directions and the timing of any future releases. In this re-evaluation, the analysis emphasizes development of well networks that will continue to provide a collective coverage of the general area of detectability in acknowledgement of these goals and uncertainties.

7 Results

This chapter presents outputs from the calculations described in Chapter 6. Results of the calculations include the following:

- A map of calculated particle pathlines for NRDWL for the flow conditions determined for CY 2021 considering advective and dispersive migration. An equivalent map was produced for SWL.
- A map of relative detectability downgradient of NRDWL based on the flow conditions calculated for CY 2021. An equivalent map was produced for SWL.

The groundwater elevation contours shown in Figure 3 form the basis for the calculations performed in this ECF. The groundwater elevations near NRDWL for 2021 are shown in Figure 2, and the outputs of the particle tracking and relative detectability calculations are discussed in the following sections.

7.1 Particle Tracking

After an underlying piecewise continuous elevation grid was prepared using the sitewide TRIM, particle tracking was implemented considering both advection and dispersion transport mechanisms. The particle pathlines that were produced depict the patterns of spreading that might accompany contaminant migration near each facility for the flow conditions in 2021.

Figures 6 and 7 show the particle pathlines for the NRDWL and SWL facilities, respectively. All downgradient wells are within the solute transport pathways for both facilities.

7.2 Relative Detectability Map

To compare the relative density of the particles that pass by each monitoring well location, a relative detectability index was calculated at a subgrid level (described in Section 6.2), and a corresponding contour map was generated. Figure 8 shows areas of relatively higher and lower potential impact from a release at NRDWL that reaches the water table for conditions represented for CY 2021.

The goal of well placement is for well locations to span the range of detectable areas downgradient of NRDWL. The relative detectability map shows that all monitoring wells are in areas of detectability. Under the flow conditions for CY 2021, the final status well network continues to meet the well-placement goal.

Figure 9 is the relative detectability map for SWL. All the downgradient monitoring wells are within the range of detectable areas downgradient of SWL, indicating the SWL well network meets the goal of well placement.

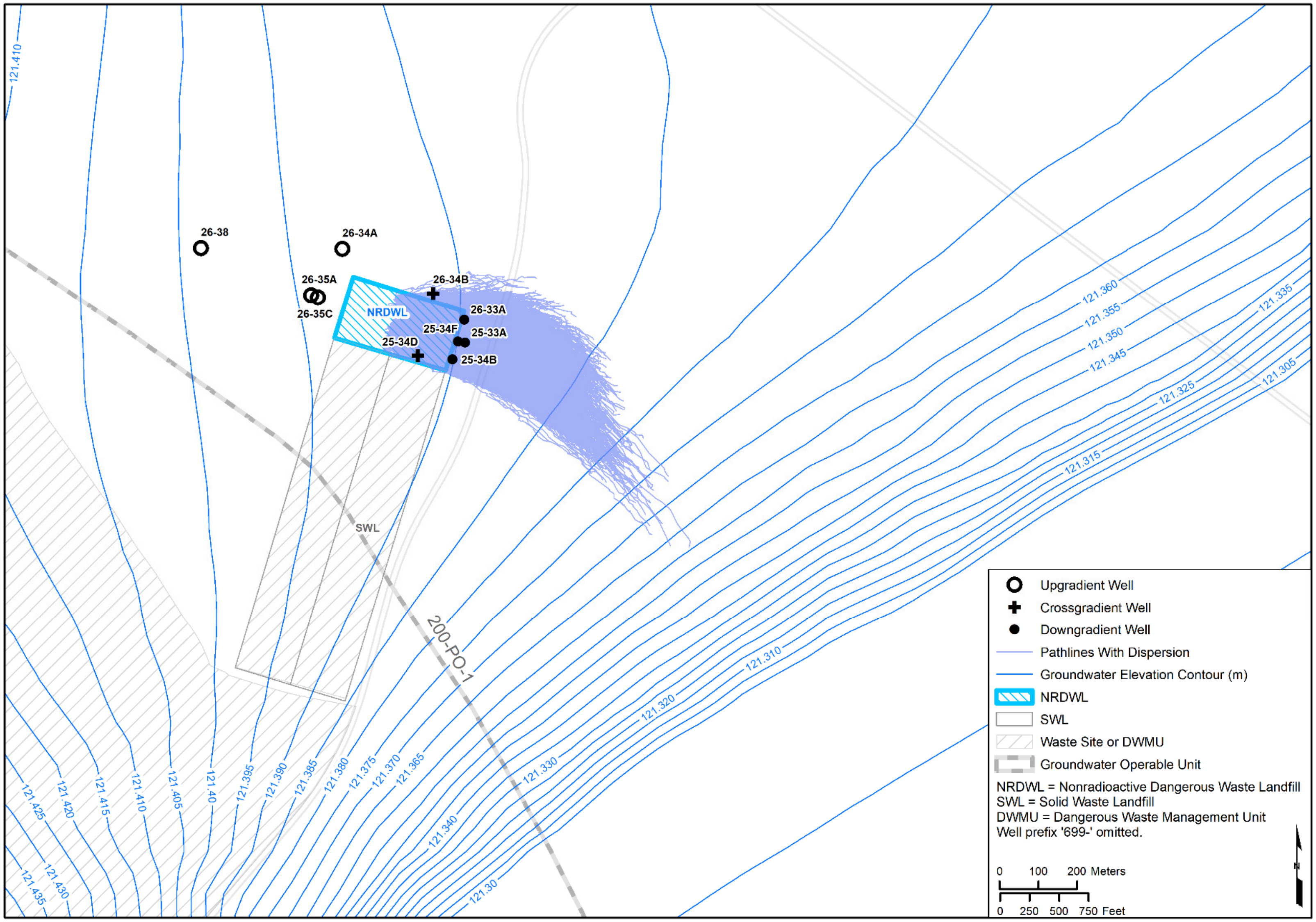

Figure 6. Groundwater Elevations and Particle Pathlines for NRDWL, 2021

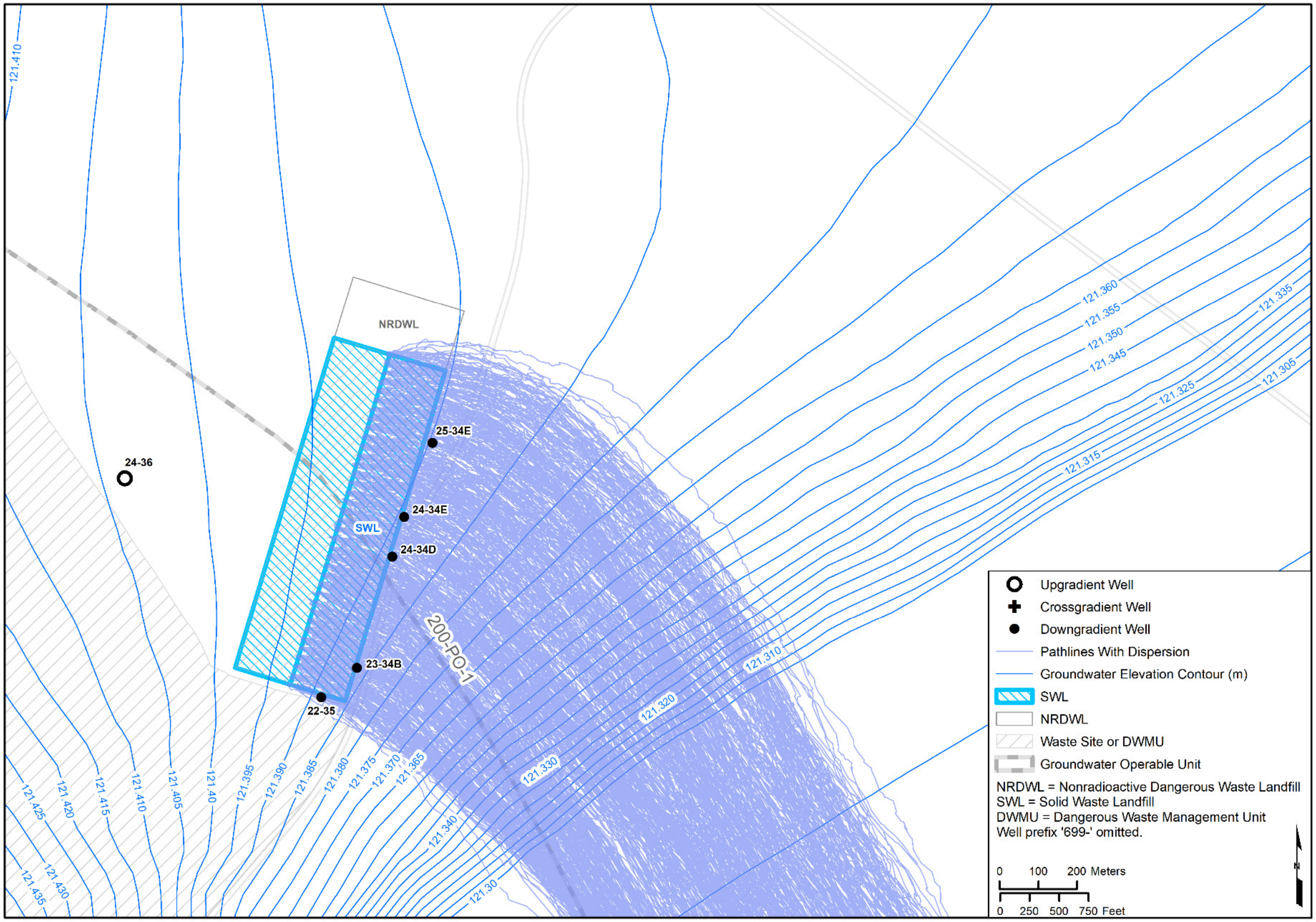

Figure 7. Groundwater Elevations and Particle Pathlines for SWL, 2021

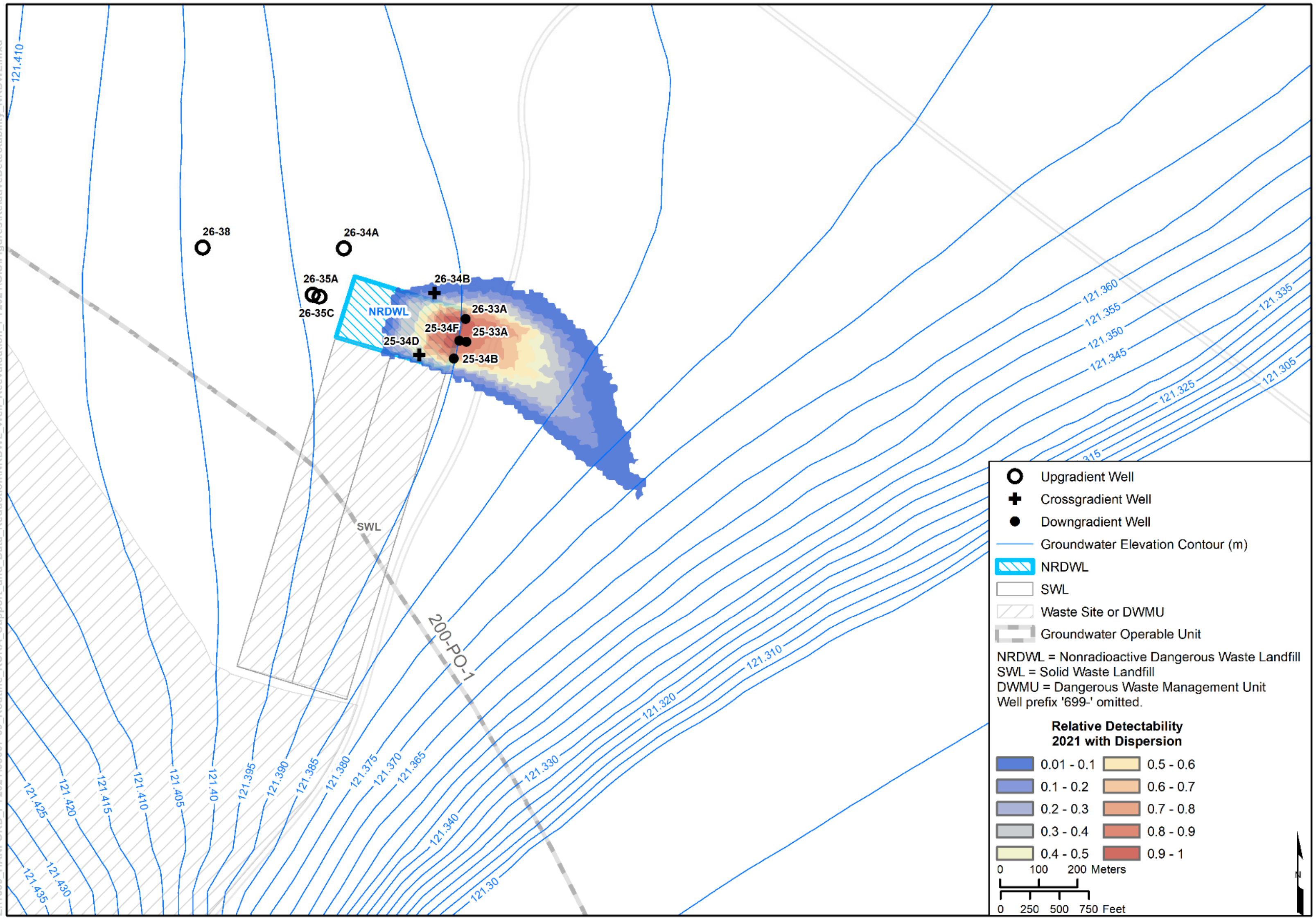

Figure 8. Relative Detectability Map for NRDWL, 2021

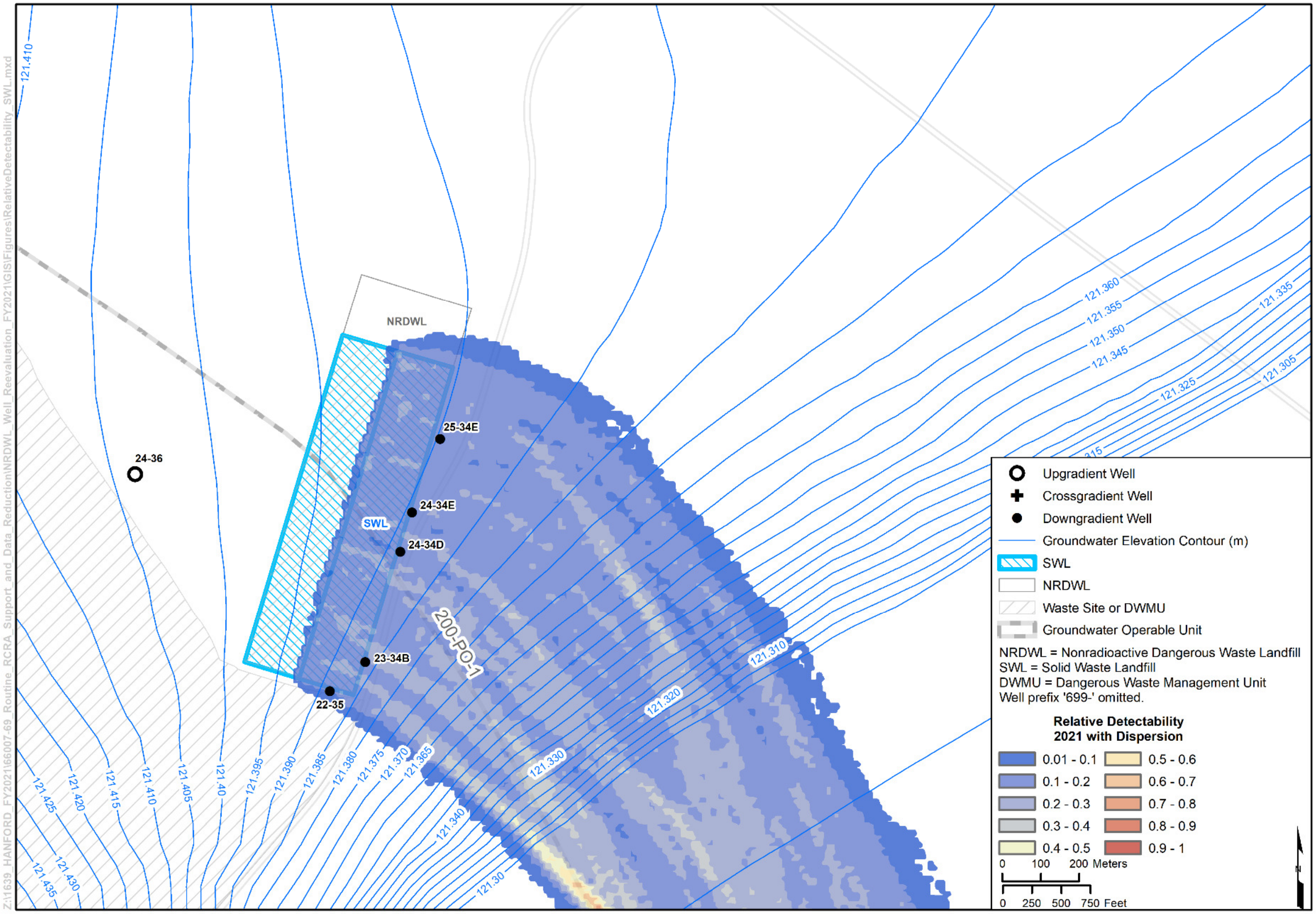

Figure 9. Relative Detectability Map for SWL, 2021

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