ECF-HANFORD-22-0005
Revision 0

Predictive Contaminant Transport Simulation with the P2R Model for the Composite Analysis Inventory Sensitivity Case

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

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

P.O. Box 1464
Richland, Washington 99352

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Revision 0

Predictive Contaminant Transport Simulation with the P2R Model for the Composite Analysis Inventory Sensitivity Case

Document Type: ECF Program/Project: Composite Analysis

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APPROVED
By Lynn M Ayers at 10:39 am, Mar 22, 2022

Release Approval Date

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ENVIRONMENTAL CALCULATION COVER PAGE

SECTION 1 - Completed by the Responsible Manager

Project:
Composite Analysis

RELEASE / ISSUE

Date: 01/18/2022

Calculation Title and Description:
Predictive Contaminant Transport Simulation with the P2R Model for the Composite Analysis Inventory Sensitivity Case

DATE:
Mar 22, 2022
HANFORD RELEASE

Qualifications Summary

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Degree, Major, Institution, Year: BA, Earth/Planetary Sciences, Washington University, 1986

Professional Licenses:

Brief Narrative of Experience: Stephanie Tomusiak has well over a decade of expertise in geology, hydrology focused on analytical and numerical modeling, groundwater flow and transport modeling and inorganic chemistry to a wide-array of hydrogeological investigations, industries and environments. She has applied analytical models, and both finite-difference and finite-element numerical modeling techniques to dewatering systems and environmental impacts in the mining industry; simulated the fate and transport of various contaminants; predicted surface water-groundwater impacts from ongoing or proposed mining operations; and conducted water resource and aquifer characterizations. She has performed capture zone analyses and evaluated remediation systems for effectiveness. Her field experience ranges from conducting soil-gas surveys and oversight of remediation studies, to designing, conducting and evaluating field aquifer tests and fracture mapping. She has routinely run, automated and calibrated MODFLOW models, written model pre- and post-processor FORTRAN programs and evaluated and interpreted MODFLOW model results. She has significant experience in database management, data analysis and visualization using ArcGIS, automating workflows with Python scripts and has taken on projects querying large databases using PostgreSQL.

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ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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Professional Licenses:

Brief Narrative of Experience: Trevor Budge's experience encompasses characterizing and modeling hydrologic and hydrogeologic systems in support of a wide range of water resources, environmental, and waste isolation projects. His work has included analyzing and optimizing remediation well configuration and operation, investigating long-term remediation costs, characterizing complex geological settings with the use of geophysical and remote sensing data, designing slurry walls and hydraulic barrier walls near sensitive water bodies, emergency planning-based modeling of catastrophic dam failures and large storm events, and developing geographic information system tools to efficiently process data and modeling results. These tasks have been completed using a wide range of numerical, analytical, and geostatistical tools. His knowledge of computer hardware and software, including GIS and programming languages, allows him to solve problems that arise specific to each project that cannot be resolved using standard out-of-the-box software and hardware. Trevor has completed projects for organizations ranging from small municipalities and local water authorities to state and federal government agencies, and he has authored and developed software applications used by the US Environmental Protection Agency and the US Department of Defense.

SECTION 2 - Completed by Preparer

Calculation Number: ECF-HANFORD-22-0005 | Revision Number: 0

Revision History

Revision No.	Description	Date	Affected Pages
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SECTION 3 - Completed by the Responsible Manager

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Does document contain controlled-use information? ( ) Yes (●) No

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ENVIRONMENTAL CALCULATION COVER PAGE (Continued)

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SECTION 5 - Applicable if Calculation is a Risk Assessment or Uses an Environmental Model

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Safety Software Approved:
Integration Lead:

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Print First and Last Name	*Signature / Date*

Calculation Approved:

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Contents

Attachments

Figures

Tables

Terms

CA	composite analysis
CPCCo	Central Plateau Cleanup Company
ECF	environmental calculation file
F&T	fate and transport
HISI	Hanford Information System Inventory
HLAN	Hanford Local Area Network
HSS	Hydrocarbon Spill Source
ICF	integrated computational framework
MODFLOW	MODular Groundwater FLOW code
MT3DMS	Modular Three-Dimensional Multiple Species transport code
P2R	Plateau to River
PA	performance assessment
PUREX	Plutonium Uranium Extraction
USGS	U.S. Geological Survey

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1 Purpose

The Plateau to River (P2R) Model is a groundwater flow and contaminant fate and transport (F&T) simulation model used to support remedial activities conducted by the Central Plateau Cleanup Company (CPCCo) at the Hanford Site in Washington State. Figure 1 illustrates the P2R Model extents, discretization, and boundary conditions. The P2R Model is utilized in the composite analysis (CA) for the Hanford Site as the computational engine for computing F&T predictions as described in CP-60406, *Hanford Site Composite Analysis Technical Approach Description: Groundwater*. The model simulates contaminants of concern within the saturated zone of the uppermost aquifer beneath the Central Plateau and downgradient to the Columbia River. CP-57037, *Model Package Report for the Plateau to River Model Version 8.3* documents the current version of the P2R Model including a description of the conceptual site model, model development and calibration, and limitations to the model application. Simulations conducted to support the dose calculations required by the CA are documented in ECF-HANFORD-19-0119, *Predictive Flow Simulation with the P2R Model for the Composite Analysis Base Case* and ECF-HANFORD-19-0120, *Contaminant Transport Simulation with the P2R Model for the Composite Analysis Base Case*.

The overall objective of the saturated zone modeling effort is to provide a basis for making informed remedial action decisions based on descriptions of current and expected future contaminant concentrations in groundwater at decision points within and downgradient of the Central Plateau of the Hanford Site. Specifically, the purpose of this environmental calculation file (ECF) is to describe an inventory sensitivity case of the CA base case. The inventory sensitivity case implements a change in the activity contribution from the vadose zone in the A Trenches Area model (for tritium (H-3) and iodine-129 (I-129)), BC Cribs and Trenches model (for I-129 and technetium-99 (Tc-99)), and the PUREX Area model (for H-3 and I-129). All other simulated inventories are identical to the CA base case. The simulation of F&T of contaminants reported in this case will support dose predictions as part of the Hanford Site CA.

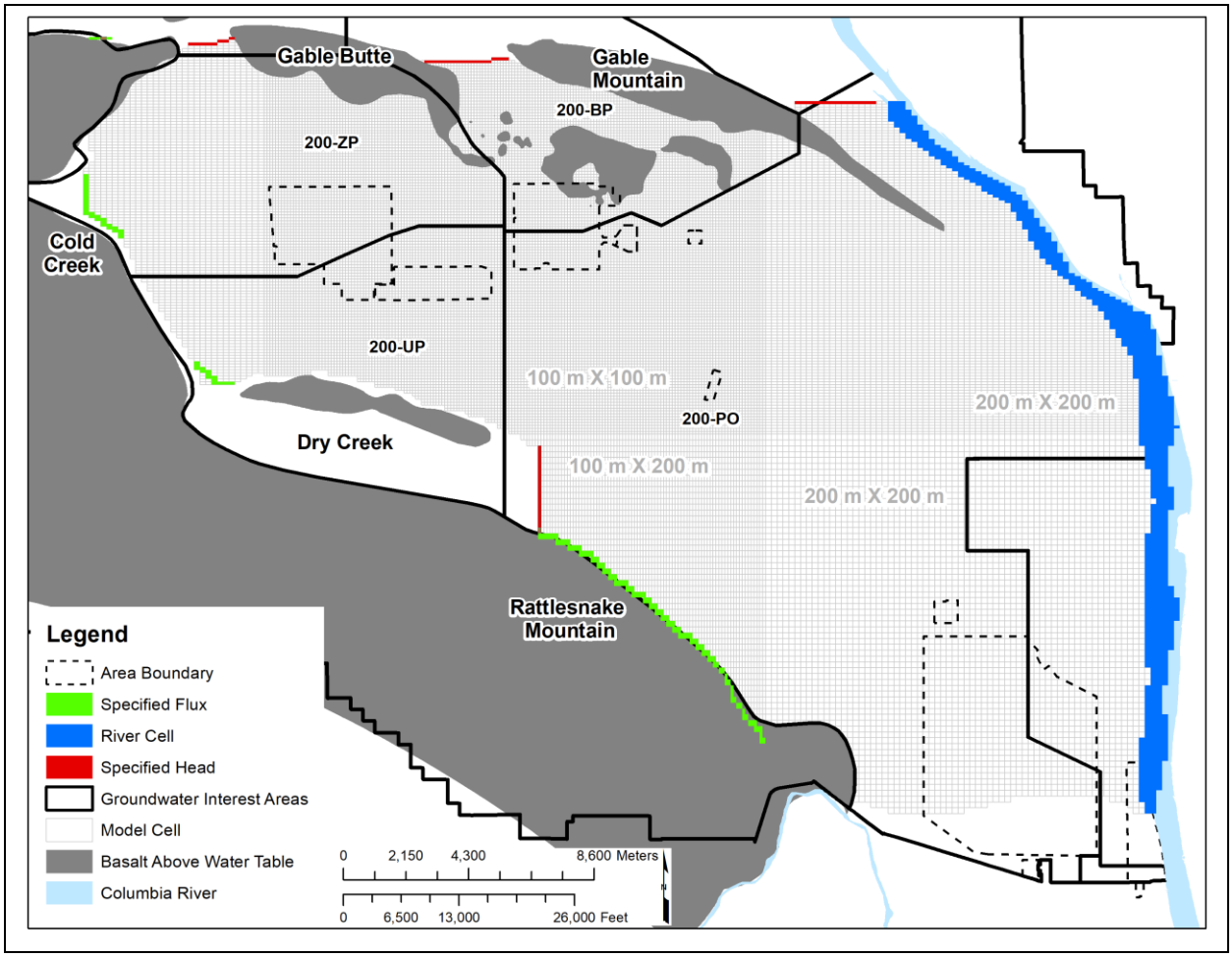

Figure 1. P2R Version 8.3 Model Extent, Discretization, and Boundary Conditions

2 Background

The development of the P2R Model is documented in CP-57037. Application of Version 8.3 of the P2R Model for the CA is documented in two separate environmental calculations (ECF-HANFORD-19-0119 and ECF-HANFORD-19-0120). The referenced report and environmental calculations provide the basis for the model development and specific application to the CA base case simulations. Simulations conducted for these calculations rely heavily on the input parameters, assumptions, limitations, and data discussed in the documents listed above. It is assumed that the reader is familiar with those documents as much of the information is not repeated in this calculation. Rather, this calculation will focus on those parameters and simulation outputs that differ from those utilized in the preceding reports and environmental calculations.

The difference between the CA base case and the inventory sensitivity case is the change in activity contributions from the vadose zone to the saturated zone for A Trenches Area, BC Cribs and Trenches, and Plutonium Uranium Extraction (PUREX) Area. Based on results presented in ECF-HANFORD-21-0140, *Composite Analysis: Recharge and Inventory Sensitivity Analyses for the A Trenches, BC Cribs and Trenches, and PUREX Area Vadose Zone Models*, the peak doses at the CA compliance boundary could be coming from the A Trenches Area Model (H-3 and I-129), BC Cribs and Trenches Model (I-129 and Tc-99), or the PUREX Area Model (H-3 and I-129). The activity contributions were developed by increasing the inventory in the named model to the 90th percentile inventory from Soil Inventory Model version 2 sources after 2018, compared to mean activity values used in the base case. Due to this change, more activity was transported to groundwater in the inventory sensitivity case. All other continuing sources of contaminants simulated as part of the base case remained the same for the dose calculation. Contamination sources from these three areas only effect the Tc-99, I-129, and H-3 concentrations. Thus, only simulations for Tc-99, I-129, and H-3 are simulated as part of this environmental calculation.

3 Methodology

The predictive F&T are simulated using the P2R Model developed using the acquired computer software: the U.S. Geological Survey (USGS) software MODular Groundwater FLOW code (MODFLOW) (USGS, 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-water Model – User Guide to Modularization Concepts and the Ground-Water Flow Process*) and the Modular Three-Dimensional Multiple Species transport code (MT3DMS) (Zheng and Wang, 1999, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide*) (see Section 5). The model simulates hydraulic head, groundwater fluxes, and contaminant F&T on a cell-by-cell basis within the model domain. The calculation of contaminant F&T in the saturated zone is completed by solving the governing equations of MT3DMS based on input parameters stored in the model input files that describe the nature of porous media in the subsurface. The results of vadose zone simulations are used to simulate the rates and locations of continuing sources of contaminants entering the saturated zone from the vadose zone. The steps for generating the F&T simulations to evaluate the inventory sensitivity case of the CA base case are as follows:

1. Simulate F&T using the CA base case simulation files with the exception of the continuing source term from the vadose zone.
    a. Link the simulated groundwater flow field documented in ECF-HANFORD-19-0119, to the MT3DMS simulation.
    b. Keep all F&T input parameters consistent with the base case simulations documented in ECF-HANFORD-19-0120.

c. Construct model inputs for continuing sources of contamination from the vadose zone (ECF-HANFORD-21-0140) for the inventory sensitivity case.

d. Execute simulations to obtain estimated concentrations that can be used to calculate the dose.

e. Create tables and figures that illustrate the predicted concentrations for comparison to results presented in ECF-HANFORD-19-0120.

4 Assumptions and Inputs

The input parameter selection for the base case flow and F&T simulations is discussed in ECF-HANFORD-19-0119 and ECF-HANFORD-19-0120, respectively. Alterations to input data files for the inventory sensitivity case include the continuing source of contaminants from the vadose zone to the saturated zone. These changes were the only required alterations for this environmental calculation. This section summarizes the source of model input parameters documented in other reports and the alteration of continuing source terms in the following sections.

4.1 Input Data Source

The input parameters used for the CA inventory sensitivity case are provided in Table 1. The input parameter set was derived from various sources and the readers are referred to these documents for further detail. All of the input parameters for the inventory sensitivity case flow and contaminant F&T simulations are kept the same as the CA base case model, except for the continuing source terms. More detailed descriptions of the model inputs and assumptions for the inventory sensitivity case flow and contaminant F&T simulations are given in Table 1.

Table 1. References for Input Parameters Used as Part of the Simulations Conducted for the Inventory Sensitivity Case to the CA Base Case

Input Type	Input Parameters	Description	Document
Flow Simulation Information			
Model Extents \aAnd Discretization	Active Model Domain	The domain and spatial discretization do not change from CA base case.	Section 4.2.1 in CP-57037
	Spatial Discretization		Sections 4.2.2 and 4.2.3 in CP-57037
	Temporal Discretization	No change between the CA base case and the inventory sensitivity case.	Section 4.2 in ECF-HANFORD-19-0120
Hydraulic Properties	Hydraulic Conductivity, Specific Storage, and Specific Yield	The hydraulic properties used in the inventory sensitivity case are the same as the CA base case.	Section 4.2 in CP-57037
	May-Junction Fault Hydraulic Characteristic	No changes were made to the hydraulic characteristic for the inventory sensitivity case.	Section 4.4.2 in CP-57037
Sources and Sinks	Injection/Extraction Rates	Rates match the assumptions presented as part of the CA base case.	Section 4.4 in ECF-HANFORD-19-0119
	Columbia River Stage and Bottom Elevation	River stage and bottom elevation match the inputs from the CA base case.	Section 4.4.3 in CP-57037 and Section 4.2.1 in ECF-HANFORD-19-0119

Input Type	Input Parameters	Description	Document
Boundary Conditions	Natural and Anthropogenic Recharge	The approach and parameter values used for defining recharge are the same as the CA base case.	Section 4.4.3 in CP-57037 and Section 4.2.3 in ECF-HANFORD-19-0119
	Specified Head Boundaries	Specified heads match the assumptions presented as part of the CA base case.	Section 4.2.2 in ECF-HANFORD-19-0119
F&T Simulation Information			
Initial Concentration	Initial State Variable for Contaminant Concentration	The same files used to define these parameters in the best estimate initial concentration of the base case were used for the inventory sensitivity case	Section 4.3.1 in ECF-HANFORD-19-0120
Aquifer Properties	Effective Porosity and Bulk Density		Section 4.3.2.1 in ECF-HANFORD-19-0120
Adsorption and Decay	Linear Adsorption and Radioactive Decay Constants		Section 4.3.2.2 in ECF-HANFORD-19-0120
Dispersion	Longitudinal, Transverse, and Vertical Dispersivity		Section 4.3.3 in ECF-HANFORD-19-0120
Continuing Sources of Contamination from the Vadose Zone	Contaminant Activity Flux Rates*	The total activity and timing of arrival of contaminants at the water table is the same in the base case, except for the change in the activity contribution from the vadose zone from the A Trenches Area model (for H-3 and I-129), BC Cribs and Trenches model (for I-129 and Tc-99), or the PUREX Area model (for H-3 and I-129). Changes made to the model layer assignments are described in Section 4.2 of this environmental calculation.	Section 4.3.4 in ECF-HANFORD-19-0120

*Portions of the inputs are changed for the application of this environmental calculation file and are discussed in Section 4.2 of this environmental calculation file.

Note: Complete reference citations are provided in Section 8 of this environmental calculation file.

CA = composite analysis
F&T = fate and transport
PUREX = Plutonium Uranium Extraction

4.2 Continuing Source of Contamination

The development of continuing source terms from the vadose zone to the saturated zone was carried out in the same manner as was completed for the CA base case (see Section 4.3.4 in ECF-HANFORD-19-0120). The HSSM Builder utility was used to transcribe vadose zone model results (a total of 26 models) into the Hydrocarbon Spill Source (HSS) packages for use with MT3DMS. The HSS inputs are documented as part of the integrated computational framework (ICF). Attachment A includes the ICF check-in form for

MT3DMS input HSS Packages under the title “HSSMCAREV1INV version 1.0”. The only alterations to the inventory sensitivity case HSS packages compared to the base case are as follows:

- The Tc-99 model used inventory sensitivity transfer rates (i.e., the transfer rates modified for the inventory sensitivity case) from the BC Cribs and Trenches model plus the compliance case (the base case) transfer rates from the other 25 models and performance assessment (PA) past leaks.
- The I-129 model used inventory sensitivity transfer rates from the A Trenches Area, BC Cribs and Trenches, and PUREX Area models plus the compliance case transfer rates from the other 23 models and the PA past leaks.
- The H-3 model used inventory sensitivity transfer rates from the A Trenches Area and PUREX Area models plus the compliance case transfer rates from the other 24 models and PA past leaks.

Figure 2, Figure 3, and Figure 4 show maps of the spatial distribution of total estimated activity of Tc-99, I-129, and H-3, respectively, that enters the saturated zone over the entirety of the 10,052-year simulation. Table 2 provides a comparison of the total simulated flux from the base case and the inventory sensitivity case.

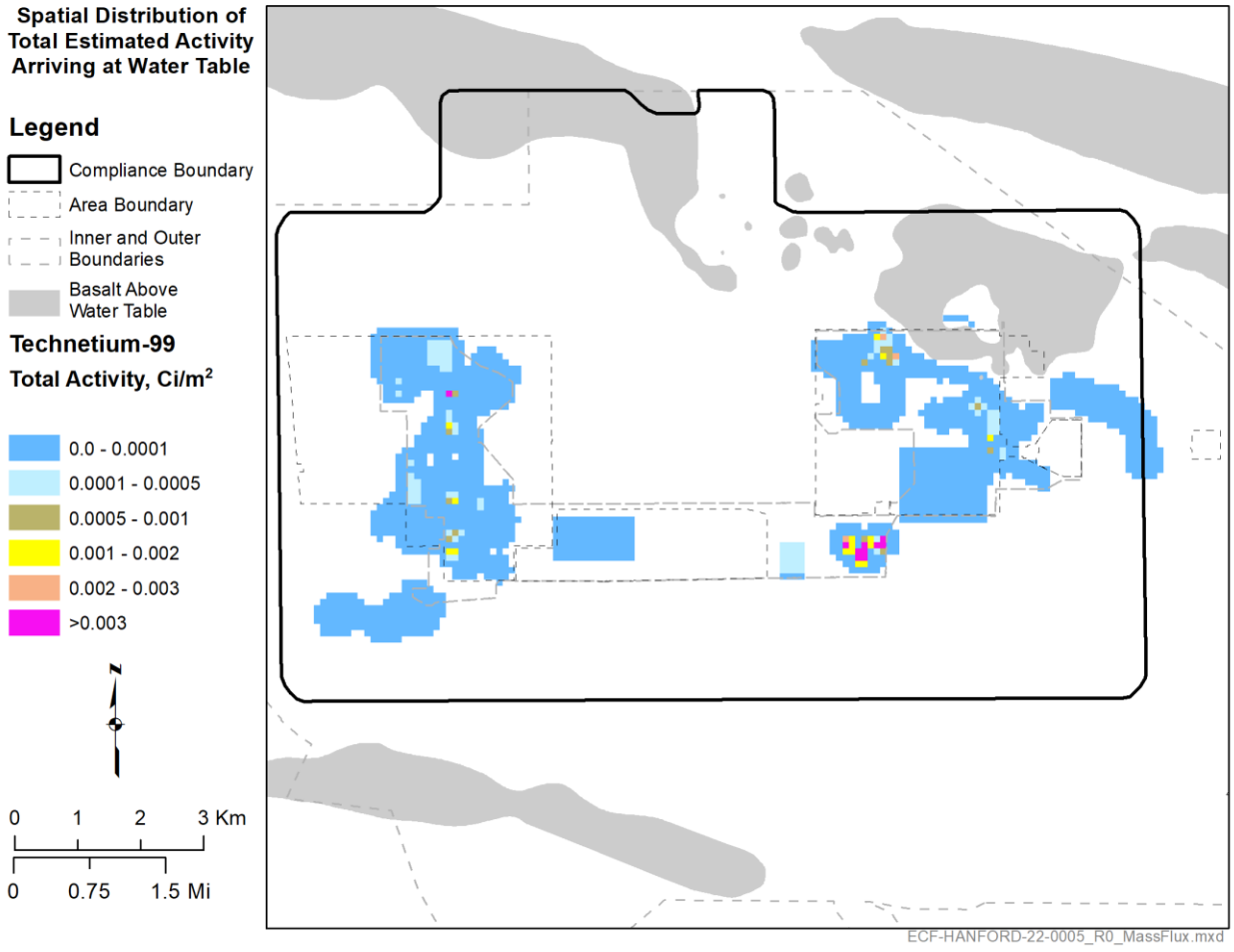

Figure 2. Spatial Distribution of Simulated Activity Entering the Saturated Zone from the Vadose Zone for Technetium-99 over the Entire Length of Simulation Temporal Discretization

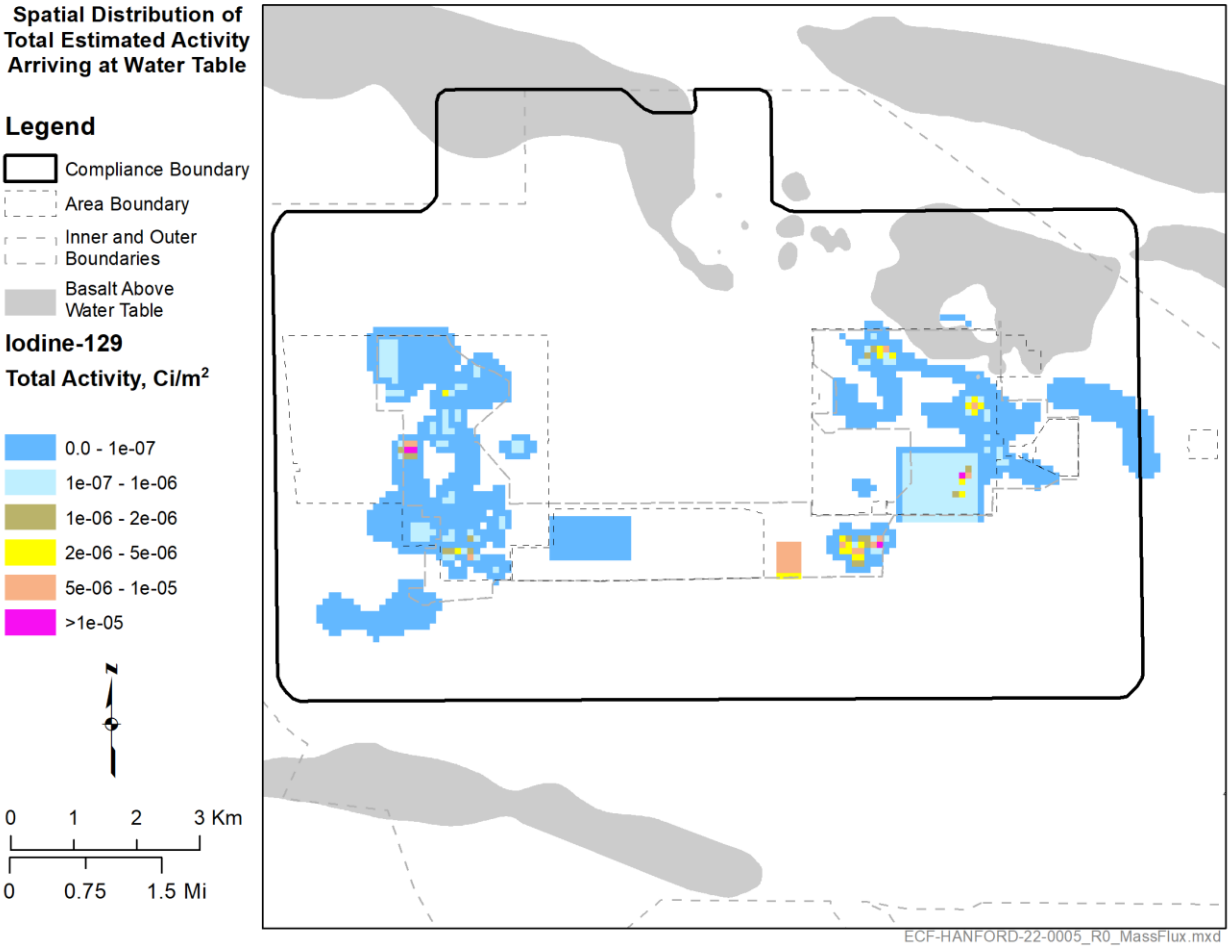

Figure 3. Spatial Distribution of Simulated Activity Entering the Saturated Zone from the Vadose Zone for Iodine-129 over the Entire Length of Simulation Temporal Discretization

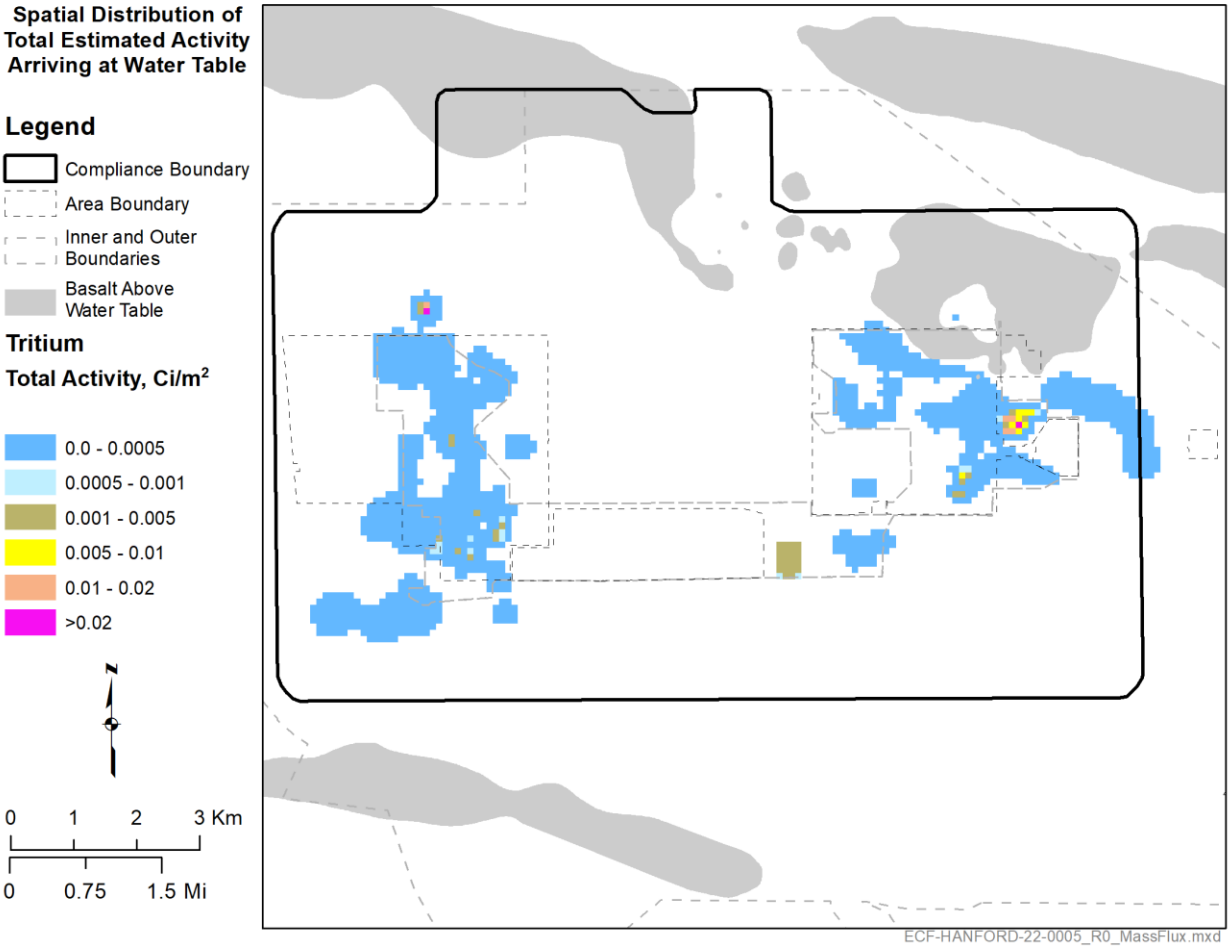

Figure 4. Spatial Distribution of Simulated Activity Entering the Saturated Zone from the Vadose Zone for Tritium over the Entire Length of Simulation Temporal Discretization

Table 2. Comparison of Total Simulated Activity Passing from the Vadose Zone to the Saturated Zone for Each Contaminant

	Total Activity (Ci)	
Contaminant	Base Case	Inventory Sensitivity Case
I-129	4.358E+00	4.665E+00
H-3	2.768E+03	3.115E+03
Tc-99	1.014E+03	1.194E+03

5 Software Applications

MODFLOW, MT3DMS, Microsoft® Excel®, ArcGIS[1]®, and R software programs were used for this ECF. MODFLOW and MT3DMS are Central Plateau Cleanup Company (CPCCo) approved software, managed and used in compliance with the policy regarding software. Excel, ArcGIS, and R are approved support software as established in CHPRC-00258, *MODFLOW and Related Codes Software Management Plan*.

MODFLOW and MT3DMS were executed on the GAIA cluster. The details regarding the cluster are presented below. Attachment B to this ECF is a copy of the *Software Installation and Checkout Form* for the MODFLOW and MT3DMS installation used for this ECF.

The GAIA F&T Modeling Platform, owned by CPCCo and operated by Mission Support Alliance, consists of ten Dell® PowerEdge® R740 Servers. Each with dual 28-core Intel® Xeon Platinum 8180M@2.5GHz, 768GB of RAM. The head node (DOE Property number WF32991) is running CentOS v.7.4.1708.

The results of CPCCo acceptance testing (CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report: CHPRC Build 8*) demonstrate that the MODFLOW-2000/MT3DMS software is acceptable for its intended use by the CPCCo. Installations of the software are operating correctly, as demonstrated by the GAIA F&T Modeling Platform.

5.1 Approved Software

For approved calculation software used in this ECF, the required descriptions are provided in the following sections.

5.1.1 Description

MODFLOW

- **Software Title:** MODFLOW
- **Software Version:** CHPRC Build 8 (executable “mf2k-mst-chprc08dpl.x”), double precision compilation
- **Hanford Information System Inventory (HISI) Identification Number:** 2517 (Safety Software, Level C)
- **Authorized Workstation type and property number**: Linux® Cluster**,** Hanford Local Area Network (HLAN) Property Tag (Front End Node) WD56054
- **Authorized User:** S. Tomusiak

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® Intel and Xeon are registered trademarks of the Intel Corporation, Santa Clara, California.

® Linux is a registered trademark of Linus Torvalds (individual), Boston, Massachusetts.

- **CHPRC Software Control Documents:**
  - CHPRC-00257, *MODFLOW and Related Codes Functional Requirements Document*
  - CHPRC-00258, *MODFLOW and Related Codes Software Management Plan*
  - CHPRC-00259, *MODFLOW and Related Codes Software Test Plan*
  - CHPRC-00260, *MODFLOW and Related Codes Requirements Traceability Matrix*
  - CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report*

MT3DMS

- **Software Title:** MT3DMS
- **Software Version:** CHPRC Build 0008 (executable name "mt3d-mst-chprc08dpl.x"), double precision compilation
- **HISI Identification Number:** 2518 (Safety Software Level C)
- **Authorized Workstation type and property number:** Linux Cluster, HLAN Property Tag (Front End Node) WD56054
- **Authorized User:** S. Tomusiak
- **CHPRC Software Control Documents:**
  - CHPRC-00257
  - CHPRC-00258
  - CHPRC-00259
  - CHPRC-00260
  - CHPRC-00261

5.1.2 Software Installation and Checkout

Copies of the *Software Installation and Checkout Forms* for the authorized users and authorized workstations for software used that requires this documentation are provided in Attachment B to this ECF.

5.1.3 Statement of Valid Software Application

The preparers of this ECF 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 tested and accepted by CPCCo. Because MODFLOW and MT3D are graded is Level C software, use of this software is required to be logged in the HISI. Accordingly, this ECF has been logged by the software owner in the HISI under Identification Number 2517 and 2518.

5.2 Support Software

The production of the HSS package used an approved utility calculation software in compliance with CHPRC-04032, *Composite Analysis/Cumulative Impact Evaluation (CA/CIE) Utility Codes Integrated Software Management Plan*. The utility code, "HSSM Builder" (a.k.a. build_hssm.py), was tested and qualified for use in compliance with the requirements specified in CHPRC-04032 and as documented in the consolidated tool package attachment for the tool. Other support software including Excel, ArcGIS, and R were used in figure making, adjusting file formats, and other support functions in creating this report. These support software were used in accordance with CHPRC-00258.

6 Calculation

The CA inventory sensitivity case simulations include simulations for three radionuclides: I-129, Tc-99, and H-3. This section describes the organization and execution of the simulation sets, and includes figures and tables that describe the results obtained.

6.1 Simulation Organization

Three F&T simulations for I-129, Tc-99, and H-3 were conducted for the CA inventory sensitivity case. All other concentrations that will be used for the dose calculation will be taken from the base case results documented in ECF-HANFORD-19-0120. Simulated initial concentration for the three radionuclides in the sensitivity simulations represent the best estimate initial concentration.

6.2 Assessing Plume Migration for Existing Plumes

The simulation outputs from each of the simulations mentioned previously were processed to create a set of figures that illustrate the F&T of the simulated contaminants. The figures created include plan view contour maps and summary charts for the maximum concentration for various regions of the model. The following sections describe the features of the figure layout to aid in figure interpretation. A full set of figures for all the simulations conducted for this ECF are included in Attachment C.

6.2.1 Plan View Contours

Figure 5 shows plan view contour plots for the Tc-99 plume after 52 years of simulation. Several aspects of the figure help identify the simulation scenarios. There is a title in the upper right-hand corner that describes the total number of years that have been simulated. The simulation time (0, 52, 152, 552, 1052, 2052, 4052, and 10,052 years) are provided for each contaminant and simulation in Attachment C. The simulation provides an estimate of concentration at each of the seven layers in the model domain. The plan view contour plots only display the maximum concentration from any layer in the model. Thus, the plan view contours provide a conservatively high estimate of the concentration within the aquifer by illustrating the maximum value of all seven layers.

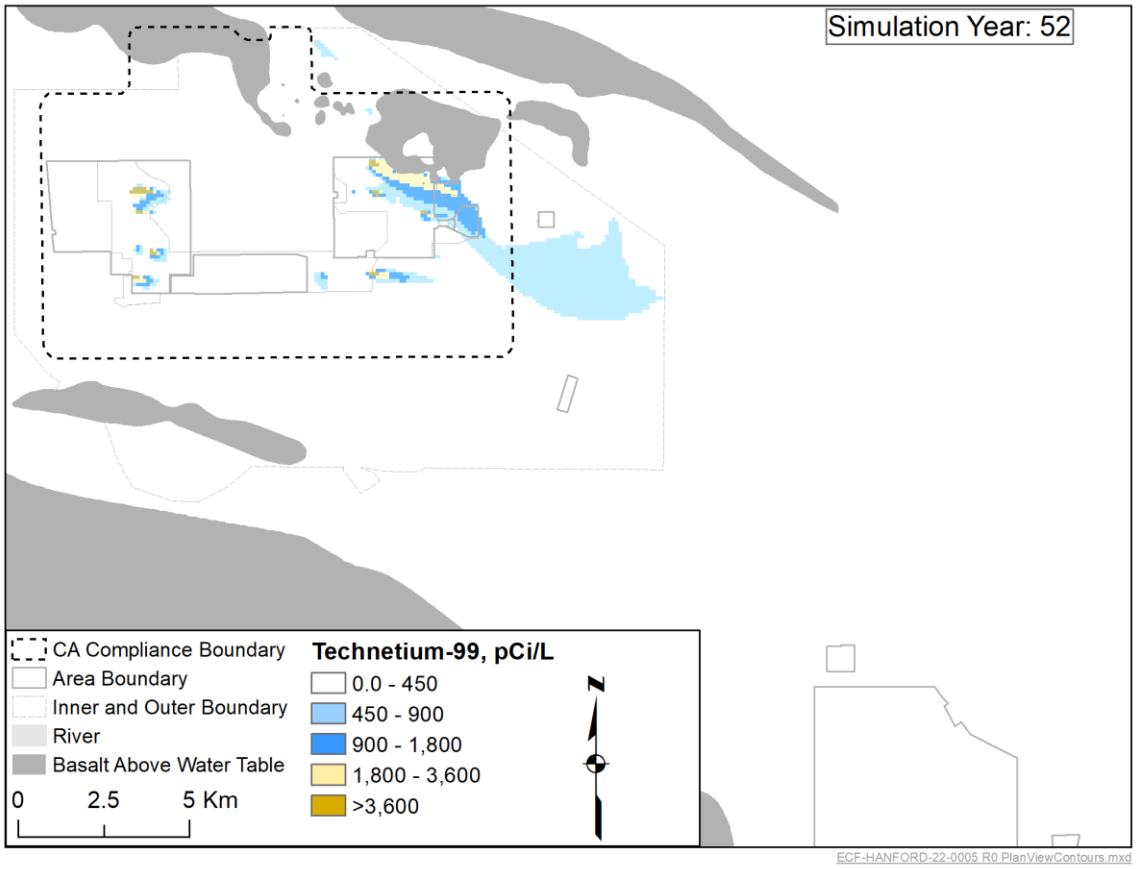

Figure 5. Plan View Contours of the Tc-99 Plume at Simulation Time 52 Years Based on Best Estimate Concentration Initial Conditions

6.2.2 Peak Concentration Summary

The extent of the P2R Model version 8.3 domain was subdivided into three zones as a means of presenting plume behavior with respect to the CA Compliance Area of the Hanford Central Plateau (Figure 6). These three zones were designated signifying the areas within the CA Compliance Boundary (Within_Compliance_Boundary), at the CA Compliance Boundary (At_Compliance_Boundary), and the remaining modeled extent of the Hanford Site (Beyond_Compliance_Boundary). Peak concentration (pCi/L) time series plots for both 1,000 and 10,000 year time series were generated for each simulation conducted as part of this calculation for each of the three zonation extents. Peak concentration is defined as the maximum concentration within a zone for a given point in time. Figure 7 and Figure 8 provide an example of the 1,000 and 10,000 years (respectively) time series plot for Tc-99 peak concentration values for all three zones. The remaining two radionuclide figures are presented in Attachment C of this ECF.

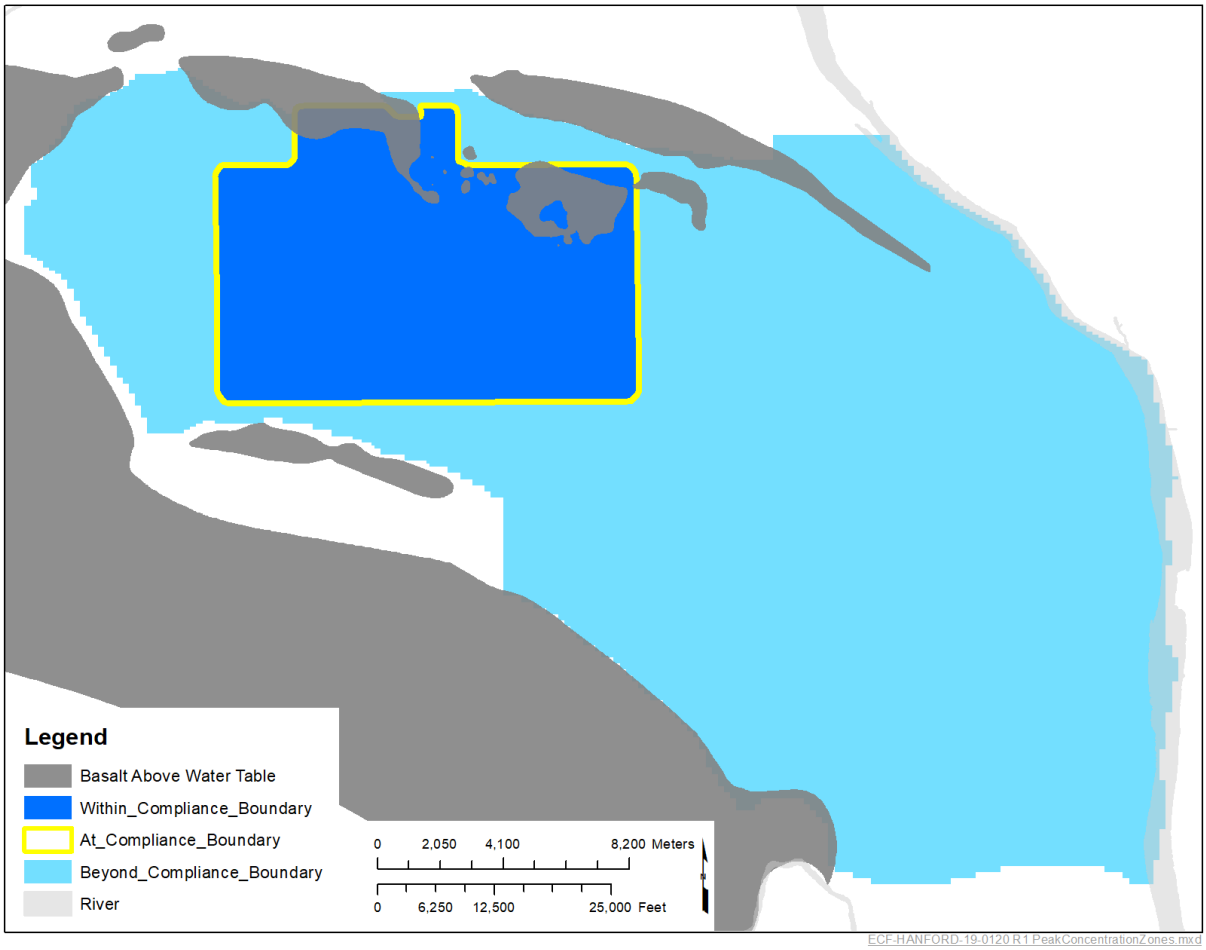

Figure 6. P2R Version 8.3 Peak Concentration Summary Zonation Extents

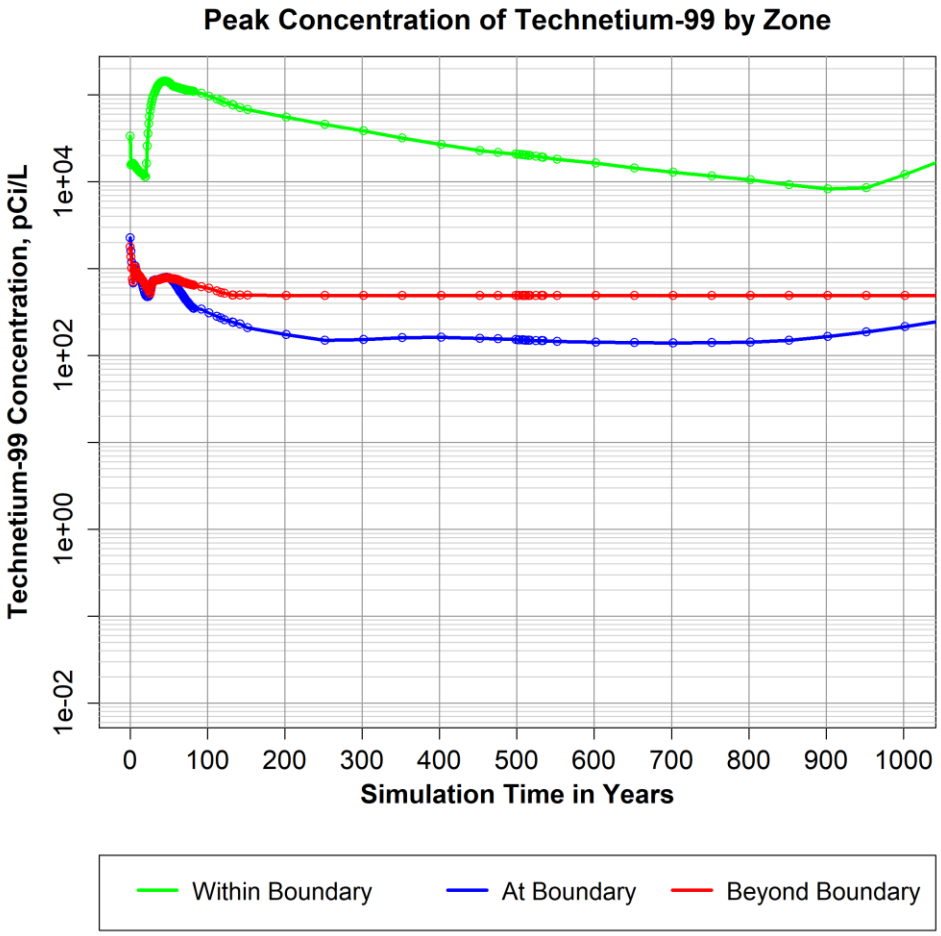

Figure 7. Peak Concentration of Technetium-99 from the Start of Simulation Until the End of the Compliance Period Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

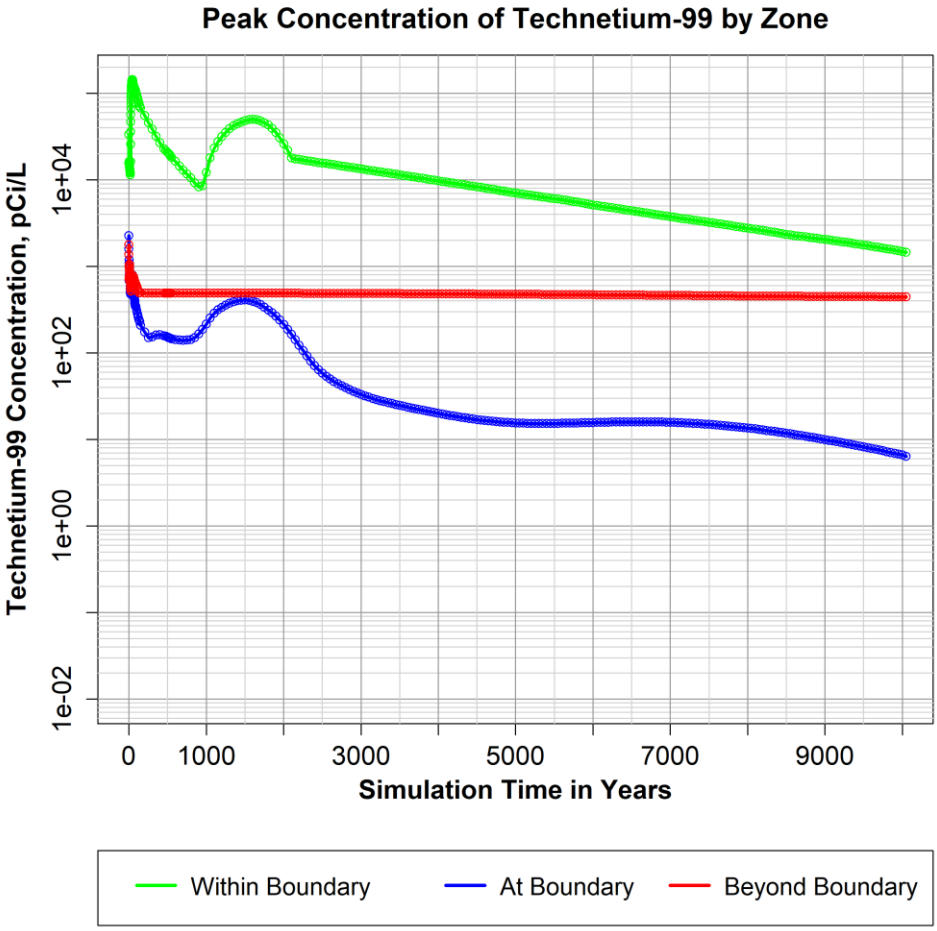

Figure 8. Peak Concentration of Technetium-99 from the Start of Simulation to the End of the Simulation Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

7 Results/Conclusions

Table 3 summarizes the simulation results including peak concentration and the time they occurred for each of the five zones for the inventory sensitivity case model results.

Table 3. Summary of Peak Concentration Values Estimated for Zones Within the P2R Model Boundary Domain

	Within_Boundary		At_Boundary		Beyond_Boundary	
Contaminant	Time (YR)	Concentration (pCi/L)	Time (year)	Concentration (pCi/L)	Time (year)	Concentration (pCi/L)
I-129	10052	1.11E+03	9	3.86E+00	0	7.36E+00
Tc-99	45	1.44E+05	0	2.27E+03	0	1.78E+03
Tritium	19	3.90E+06	5	4.98E+04	0	4.46E+05

Note: The Plateau-to-River Model boundary domain is shown in Figure 6.

8 References

CHPRC-00257, 2010, *MODFLOW and Related Codes Functional Requirements Document*, Rev. 1, CH2M HILL Plateau Remediation Company, Richland, Washington.

CHPRC-00258, 2015, *MODFLOW and Related Codes Software Management Plan*, Rev. 4, CH2M HILL Plateau Remediation Company, Richland, Washington.

CHPRC-00259, 2014, *MODFLOW and Related Codes Software Test Plan*, Rev. 3, CH2M HILL Plateau Remediation Company, Richland, Washington.

CHPRC-00260, 2015, *MODFLOW and Related Codes Requirements Traceability Matrix*, Rev. 8, CH2M HILL Plateau Remediation Company, Richland, Washington.

CHPRC-00261, 2015, *MODFLOW and Related Codes Acceptance Test Report, CHPRC Build 8*, Rev. 8, CH2M HILL Plateau Remediation Company, Richland, Washington.

CHPRC-04032, 2020, *Composite Analysis/Cumulative Impact Evaluation (CA/CIE) Utility Codes Integrated Software Management Plan,* Rev. 0, CH2M HILL Plateau Remediation Company, Richland, Washington.

CP-57037, 2020, *Model Package Report for the Plateau to River Model Version 8.3,* Rev. 2, CH2M HILL Plateau Remediation Company, Richland, Washington. Available at: https://www.osti.gov/servlets/purl/1601635.

CP-60406, 2017, *Hanford Site Composite Analysis Technical Approach Description: Groundwater*, Rev. 0, CH2M HILL Plateau Remediation Company, Richland, Washington.

ECF-HANFORD-19-0119, *Predictive Flow Simulation with the P2R Model for the Composite Analysis Base Case*, Rev. 1 pending, Central Plateau Cleanup Company, Richland, Washington.

ECF-HANFORD-19-0120, *Contaminant Transport Simulation with the P2R Model for the Composite Analysis Base Case*, Rev. 1 pending, Central Plateau Cleanup Company, Richland, Washington.

ECF-HANFORD-21-0140, *Composite Analysis: Recharge and Inventory Sensitivity Analyses for the A Trenches, BC Cribs and Trenches, and PUREX Area Vadose Zone Models*, Rev. 0 pending, Central Plateau Cleanup Company, Richland, Washington.

USGS, 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-water Model – User Guide to Modularization Concepts and the Ground-Water Flow Process*, USGS Open File Report 00-92, U.S. Geological Survey, Denver, Colorado. Available at: http://water.usgs.gov/nrp/gwsoftware/modflow2000/ofr00-92.pdf.

Zheng, C. and P.P. Wang, 1999, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide*, Contract Report SERDP-99-1, U.S.\ Army Engineer Research and Development Center, U.S. Army Corps of Engineers, Vicksburg, Mississippi. Available at: Available at: http://www.dtic.mil/cgi-bin/GetTRDoc?Location=U2&doc=GetTRDoc.pdf&AD=ADA373474.

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Attachment A

HSS Package ICF Check-in Form

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ICF Submittal Data Form

Title: HSSM package inputs for MT3D (CA) REV 1 Sensitivity Case Inv			**Date: 1/19/2022**
1. Data Name (for ICF database) *(to be filled in by QA Officer)*		**Work Product Name: HSSMCAREV1INV**	
2. Data Version Number:	**v1.0**		
This numbering system will be used in the ICF database to distinguish between previous revisions, particularly in the case of provisional data that is being tracked with various renditions/versions of the same provisional data.			
3. Data Citation | Revision Number	**No.: N/A**		**Rev.: 0**
Where possible, all data should be tied to a final number that corresponds with its final QA/QC'd designation. If the data is documented (or will be documented) with an ECF, then that ECF and revision number should be captured here.			
3. QA/QC Flag (*What is the QA/QC status of the product?*)	**Not-Checked:** ☐	**Checked: X**	**Problem/Post-Check:** ☐
4. Disk Location of Data (*Where is this information stored?*)			
[redacted]**\HSSMCAREV1INV\v1.0**			
5. Description of Data (*What is the general description of the data?*)			
Hydrocarbon Spill Screening Model (HSSM) packages for the Composite Analysis (CA) REV 1 Sensitivity case Inventory. These packages are inputs to MT3D generated from the Vadose Zone data (VZ2SRI/SRI2SZ and PAPL2SZ). This is a limited data set meant to be used with the original CA Rev 1 data set, replacing 2-3 models in the h-3, i-129, tc-99 radionuclides. *For Tc-99, use the Recharge Sensitivity transfer rates from BC Cribs and Trenches (ICF ID CAVZ2SRIINV v1.0), plus the Compliance Case transfer rates from the other 25 models (ICF ID VZSRIREV1 v1.1) and PAPL (PAPL2SZ v1.1).* *For I-129, use the Recharge Sensitivity transfer rates from the A Trenches Area, BC Cribs and Trenches, and PUREX Area models (ICF ID CAVZ2SRIINV v1.0), plus the Compliance Case transfer rates from the other 23 models (ICF ID VZSRIREV1 v1.1) and PAPL (PAPL2SZ v1.1).* *For H-3, use the Recharge Sensitivity transfer rates from the A Trenches Area and PUREX Area models (ICF ID CAVZ2SRIINV v1.0), plus the Compliance Case transfer rates from the other 24 models (ICF ID VZSRIREV1 v1.1) and PAPL (PAPL2SZ v1.1).*			
6. Corresponding Project			
Composite Analysis			
7. Parent Data *(Listing of pertinent parent data; if existing blockchain reference exists in the ICF, use this key and capture a snapshot from the ICF database)*			
SRICAREV1 (v1.0), SRICAREV1INV (v1.0), P2RHDS (v2.0), P2RCAL (v8.3a), PAPL2SZ (v1.1)			
8. ICF Location *(to be filled in by QA Officer):*			
[redacted]**\HSSMCAREV1INV\v1.0**			
Data Provider: Eugene O'Neil Powers Position: Software Engineer	Eugene O. Powers Digitally signed by Eugene O. Powers DN: cn=Eugene O. Powers, o=Intera, ou, email=npowers@intera.com, c=US Date: 2022.01.25 11:07:28 -08'00' *Signature* *Date*		
Data Reviewer: Hai Pham Position: Groundwater Modeler	Hai Pham Digitally signed by Hai Pham Date: 2022.01.25 13:45:21 -06'00' *Signature* *Date*		

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Attachment B

Software Installation and Checkout Forms for Approved Software Installations

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B1 Software Installation and Checkout Forms for Approved Software Installations

This attachment provides the requisite software installation and checkout forms for application of the U.S. Geological Survey software MODular Groundwater FLOW code (USGS, 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-water Model – User Guide to Modularization Concepts and the Ground-Water Flow Process*) to simulate flow and the Modular Three-Dimensional Multiple Species transport code (Zheng and Wang, 1999, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide*) to simulate contaminant transport.

B2 References

USGS, 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-water Model – User Guide to Modularization Concepts and the Ground-Water Flow Process*, USGS Open File Report 00-92, U.S. Geological Survey, Denver, Colorado. Available at: http://water.usgs.gov/nrp/gwsoftware/modflow2000/ofr00-92.pdf.

Zheng, C. and P.P. Wang, 1999, *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide*, Contract Report SERDP-99-1, U.S.\ Army Engineer Research and Development Center, U.S. Army Corps of Engineers, Vicksburg, Mississippi. Available at: Available at: http://www.dtic.mil/cgi-bin/GetTRDoc?Location=U2&doc=GetTRDoc.pdf&AD=ADA373474.

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM

Software Owner Instructions:
Complete Fields 1-13, then run test cases in Field 14. Compare test case results listed in Field 15 to corresponding Test Report outputs. If results are the same, sign and date Field 19. If not, resolve differences and repeat above steps.

Software Subject Matter Expert Instructions:
Assign test personnel. Approve the installation of the code by signing and dating Field 21, then maintain form as part of the software support documentation.

GENERAL INFORMATION:

1 Software Name: MODFLOW & Related Codes Software Version No.: Bld 8

EXECUTABLE INFORMATION:

2. Executable Name (include path):

The following executable files in directory: [redacted]/bin on head node and each compute node (compute-0-0 through compute-0-10, inclusive)

MD5 Signature (unique ID)	Executable File Name	Code
8b0b28c5e102e63df95de542d83d013b	mf2k-chprc08spl.x	MODFLOW-2000 single precision
2fade33e27978063a9a70ff8605e4c0c	mf2k-chprc08dpl.x	MODFLOW-2000 double precision
d879defafdc5ad25be51a484d73ea65d	mf2k-mst-chprc08spl.x	MODFLOW-2000-MST single precis.
80d670658425653bf5bcbb97ad2a2730	mf2k-mst-chprc08dpl.x	MODFLOW-2000-MST double precis.
8b0b28c5e102e63df95de542d83d013b	mf2k-chprc08spl.x	MT3DMS single precision
2fade33e27978063a9a70ff8605e4c0c	mf2k-chprc08dpl.x	MT3DMS double precision
2d0a8a4c480318763b6aaaa0f880348a	mt3d-mst-chprc08spl.x	MT3DMS-MST single precision
1e468c4409ac913843ce783aabed819c	mt3d-mst-chprc08dpl.x	MT3DMS-MST double precision

3. Executable Size (bytes): MD5 signatures above uniquely identify each executable file

COMPILATION INFORMATION:

4. Hardware System (i.e., property number or ID):

INTERA Austin Linux(R) Cluster

5. Operating System (include version number):

Linux head.cluster 2.6.32-358.11.1.el6.centos.plus.x86_64 #1 SMP Wed Jun 12 19:12:17 UTC 2013 x86 64 x86 64 x86 64 GNU/Linux

INSTALLATION AND CHECKOUT INFORMATION:

6. Hardware System (i.e , property number or ID):

Caia Subsurface Transport Modeling Linux Platform

7. Operating System (include version number):

Linux gaia1.rl.gov 3.10.0-1160.25.1.el7.x86_64 #1 SMP Wed Apr 28 21:49:45 UTC 2021 x86_64 x86 64 x86 64 GNU/Linux

8. Open Problem Report? (●) No ( ) Yes PR/CR No.

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]/test/modflow/build-8-a on head node and each compute node

10. Procedure(s):

CHPRC-00259 Rev. 3, MODFLOW and Related Codes Software Test Plan

11. Libraries

N/A (static linking)

Page 1 of 2 A-6005-149 (REV 0)

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: MODFLOW & Related Codes Software Version No.: Bld 8

12. Input Files:

Per CHPRC-00259 Rev. 3

13. Output Files:

Found in test subdirectories

14. Test Cases:

MF-ITC-1 (both standard and MST versions of MODFLOW); run both single & double precision
MT-ITC-1 run for single and double precision, multiple solvers

15. Test Case Results:

All PASS, All Tests, on all nodes of Gaia. Test log attached.

16. Test Performed By: WE Nichols

17. Test Results: (●) Satisfactory, Accepted for Use ( ) Unsatisfactory

18. Disposition (include HISI update):

This is a retest of the installation following system outage of June 1 to June 15, 2021 to update the Operating System on all nodes and apply all pending vulnerability patches. No change to HISI entries. This constitutes operational testing per the SMP.

Prepared By:

19 Christopher Farrow	Chris Farrow	
Software Owner (Signature)	Print	Date

20. Test Personnel:

WILLIAM NICHOLS (Affiliate) Digitally signed by WILLIAM NICHOLS (Affiliate) Date: 2021.06.15 10:49:24 -07'00'	William Nichols	
Sign	Print	Date
Sign	Print	Date
Sign	Print	Date

Approved By:

21.	N/R (CHPRC-00258 Rev. 3)	
Software SME (Signature)	Print	Date

A-6005-149 (REV 0)

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Attachment C

Plan View Contour and Simulated Peak Concentration plots for the Inventory Sensitivity Case Simulations

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Figures

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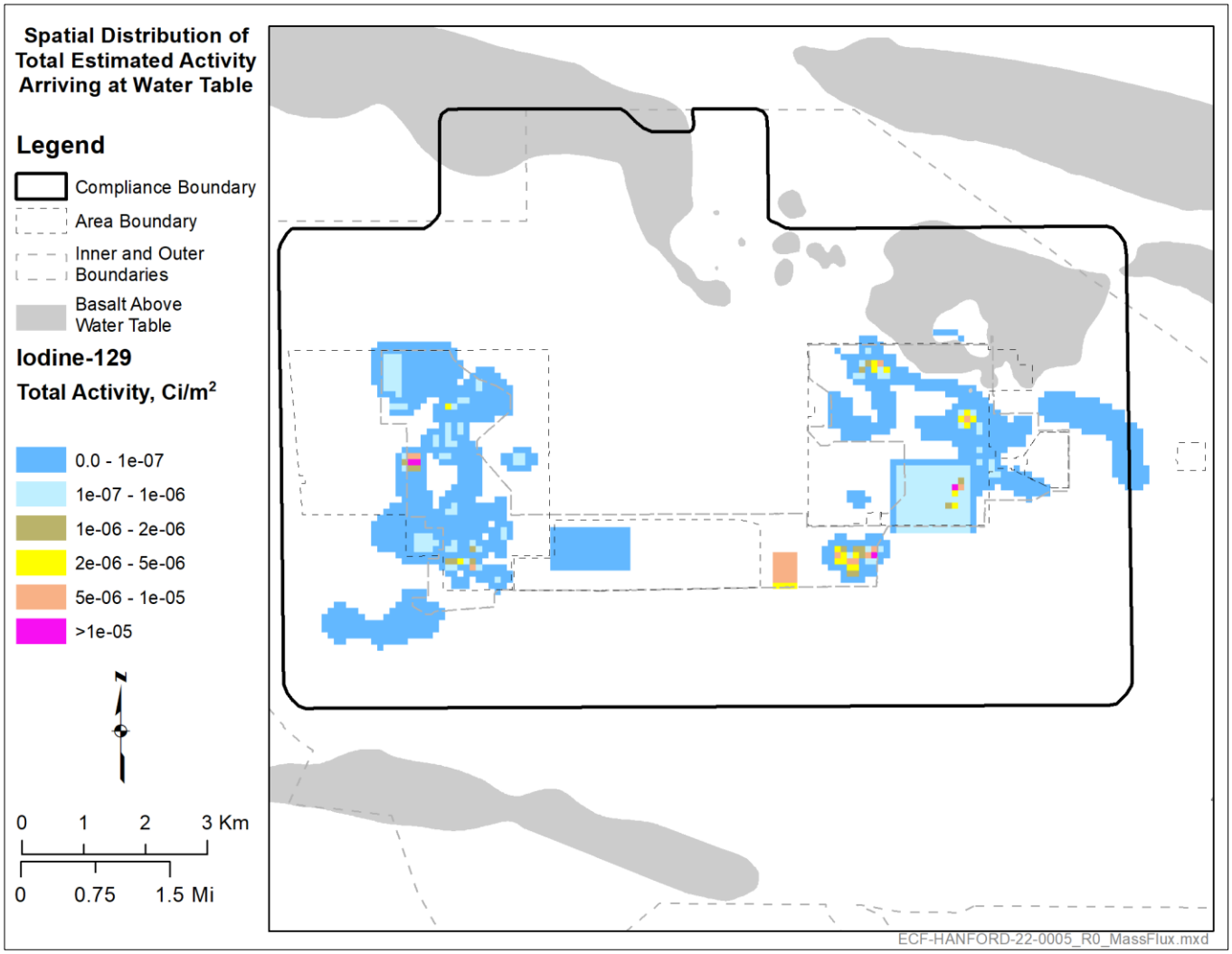

Figure C-1. Spatial Distribution of Iodine-129 that Enters the Saturated Zone from the Vadose Zone over the Entire Simulation Length

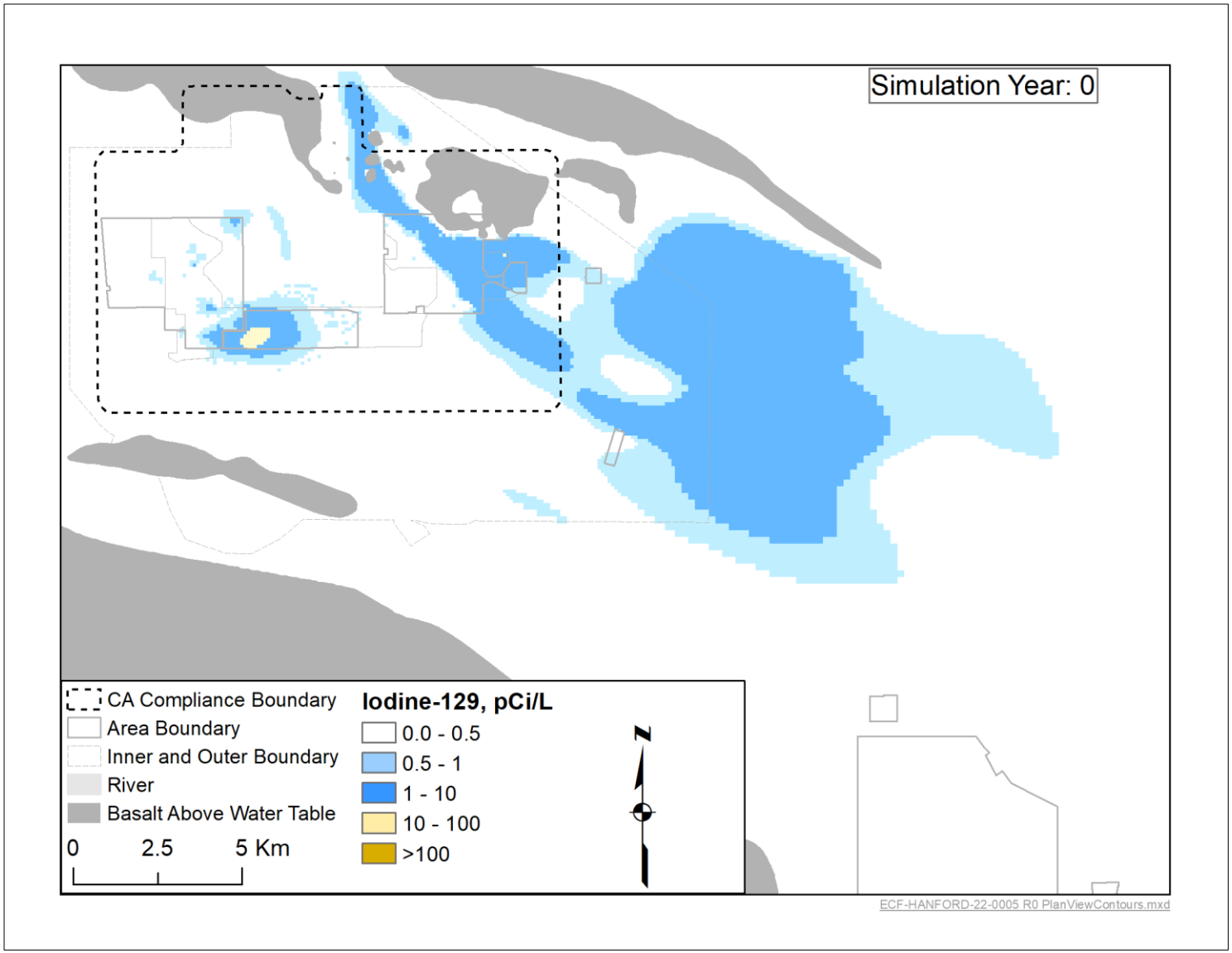

Figure C-2. Plan View Contours of Iodine-129 Concentration Simulated 0 Years (Calendar Year 2018) from the Start of Simulation Assuming the Best Estimate Initial Concentration

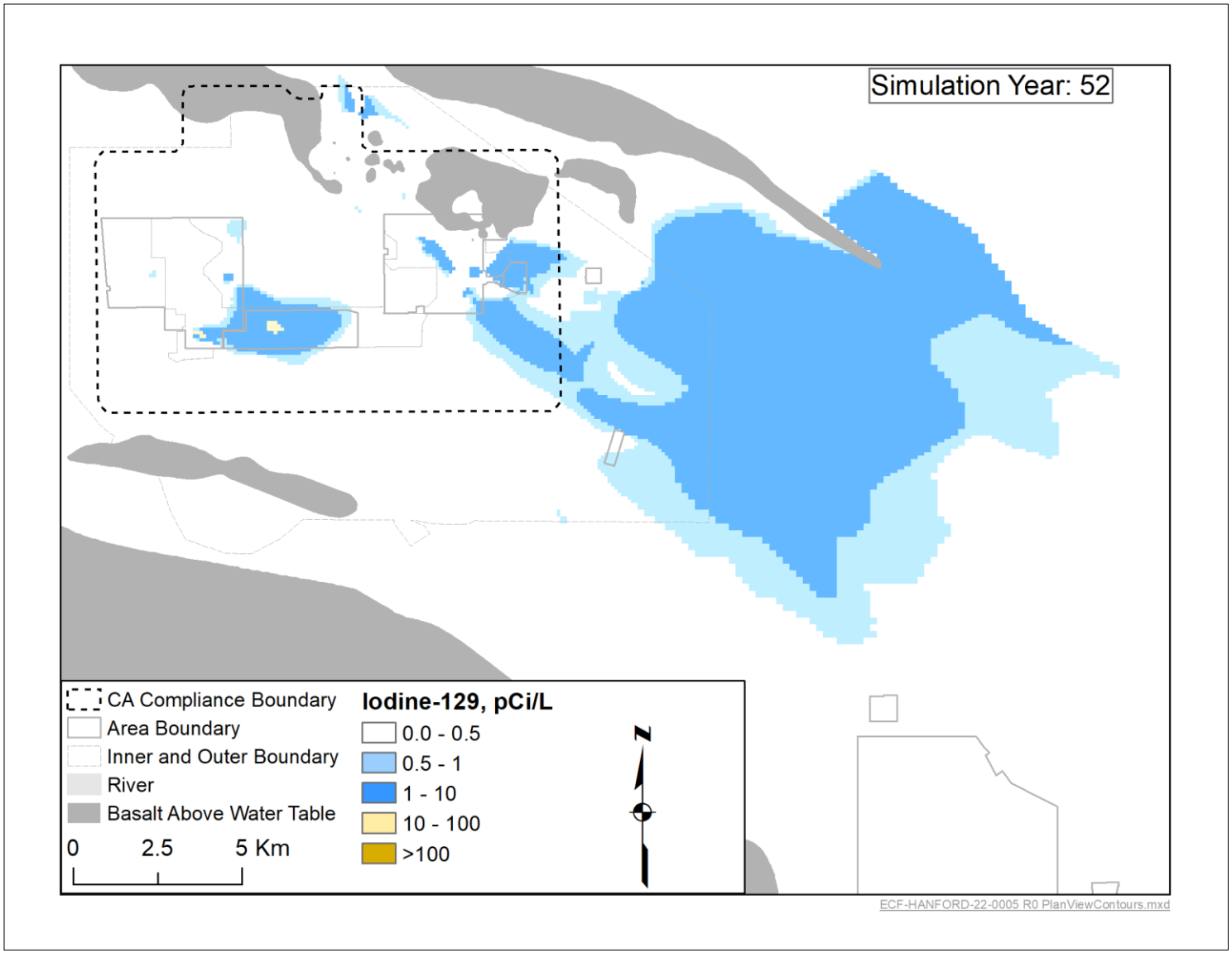

Figure C-3. Plan View Contours of Iodine-129 Concentration Simulated 52 Years (Calendar Year 2070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

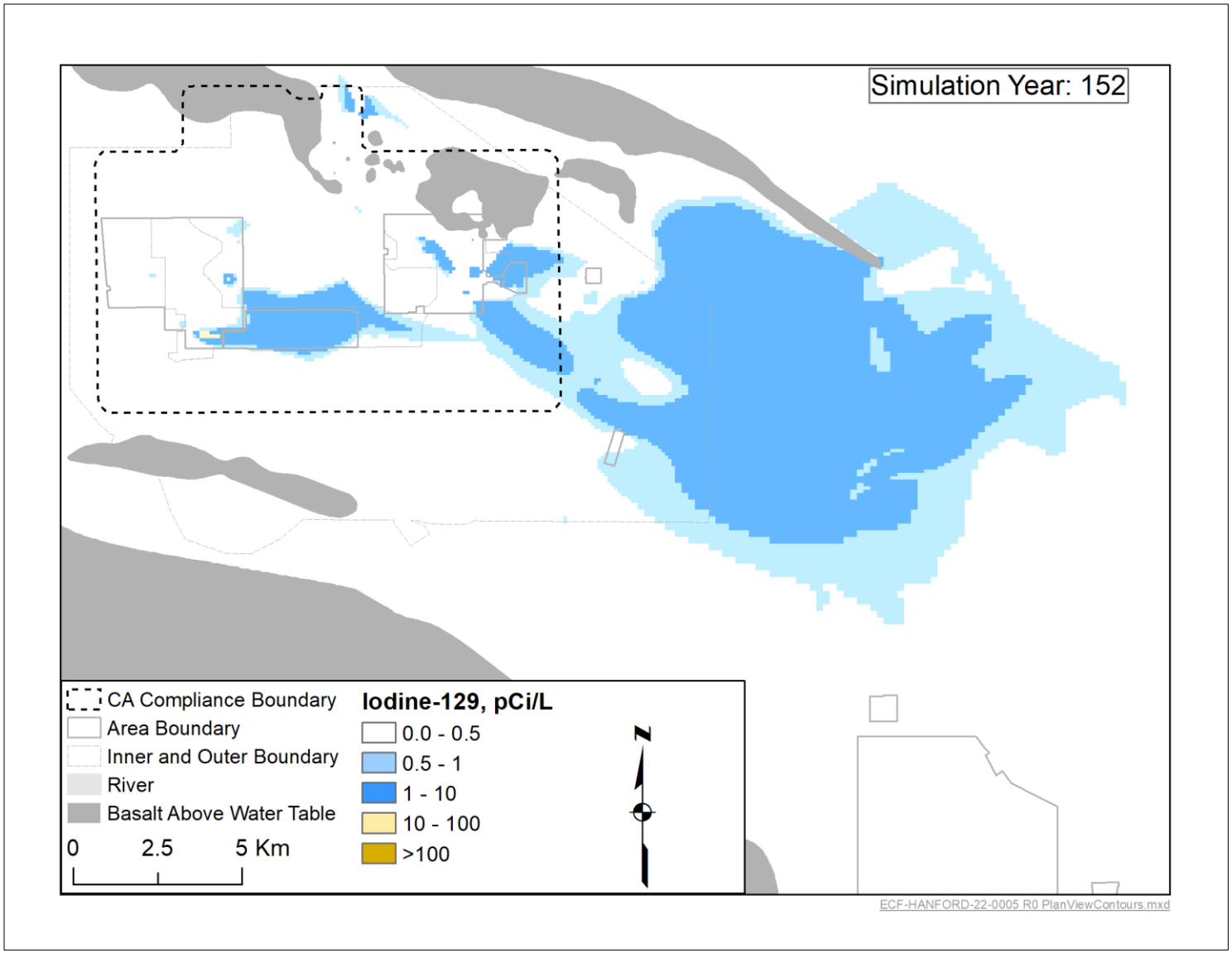

Figure C-4. Plan View Contours of Iodine-129 Concentration Simulated 152 Years (Calendar Year 2170) from the Start of Simulation Assuming the Best Estimate Initial Concentration

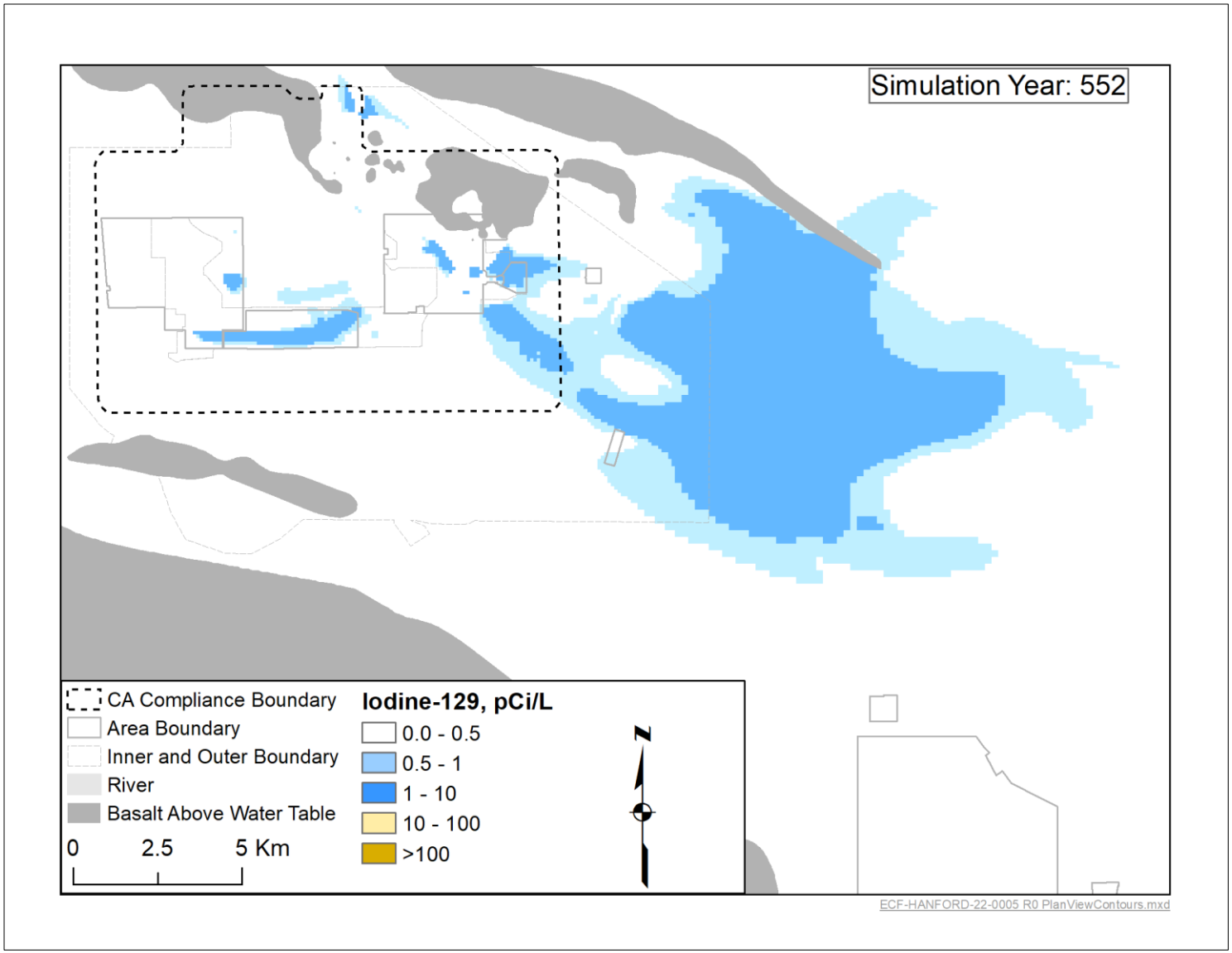

Figure C-5. Plan View Contours of Iodine-129 Concentration Simulated 552 Years (Calendar Year 2570) from the Start of Simulation Assuming the Best Estimate Initial Concentration

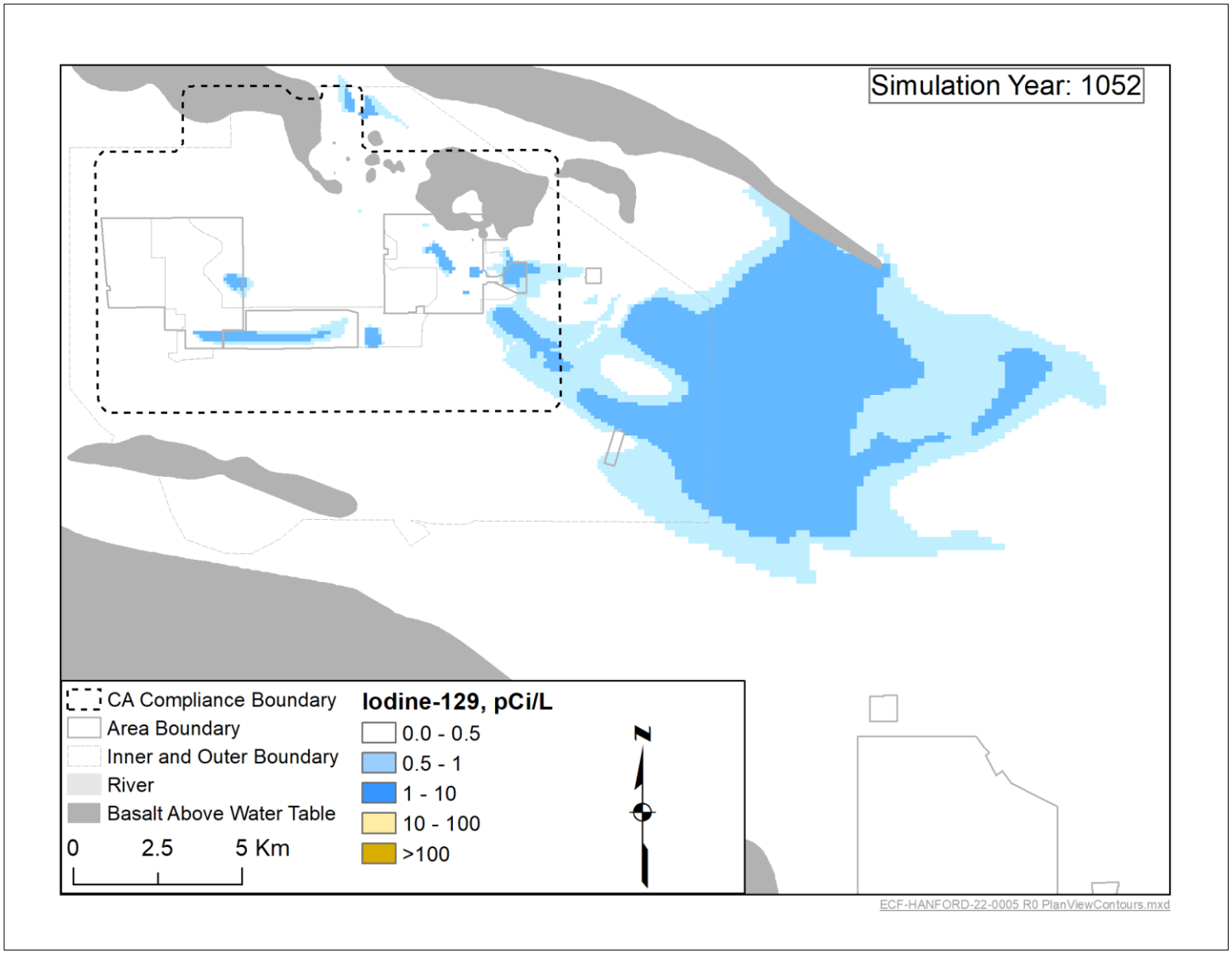

Figure C-6. Plan View Contours of Iodine-129 Concentration Simulated 1052 Years (Calendar Year 3070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

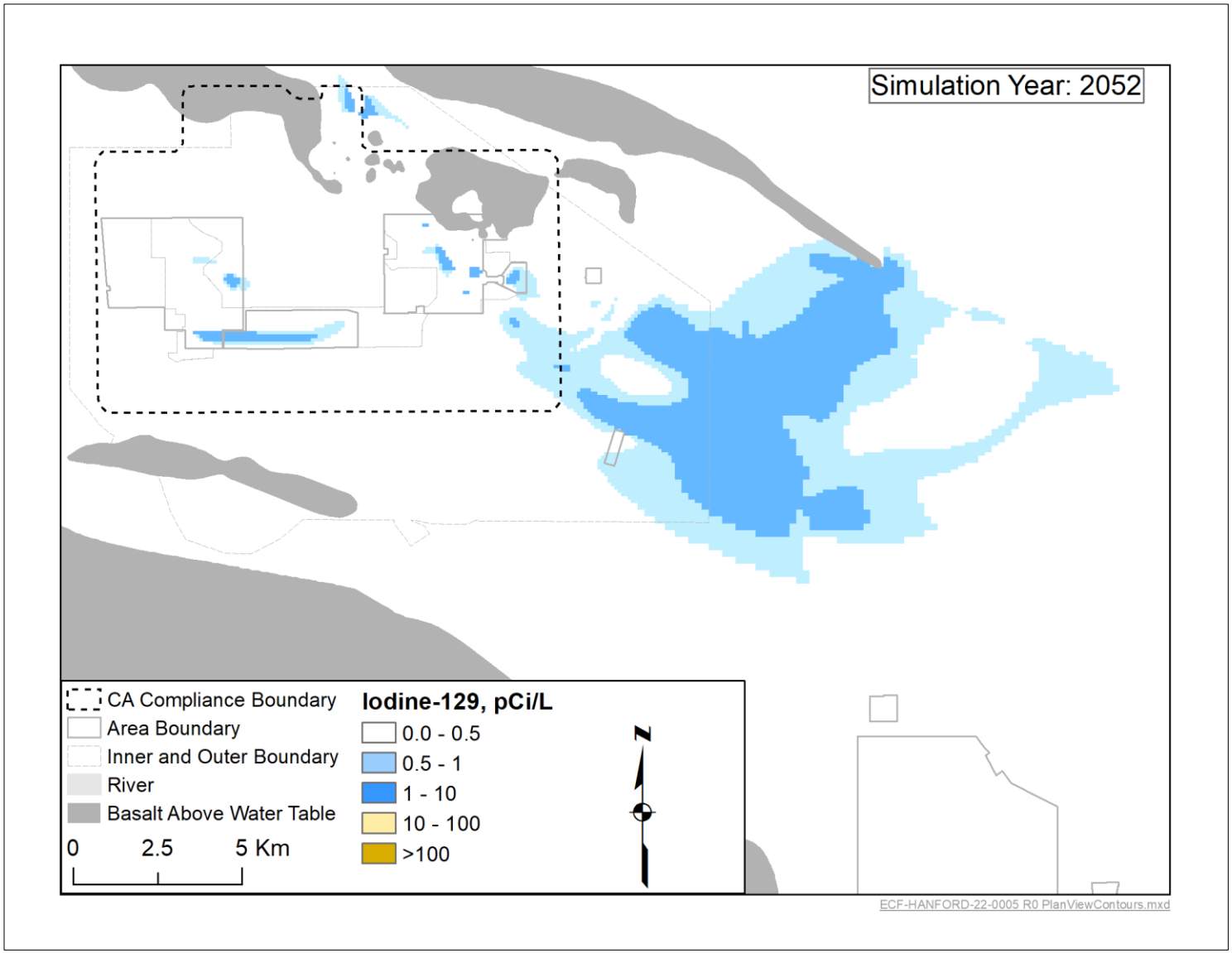

Figure C-7. Plan View Contours of Iodine-129 Concentration Simulated 2052 Years (Calendar Year 4070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

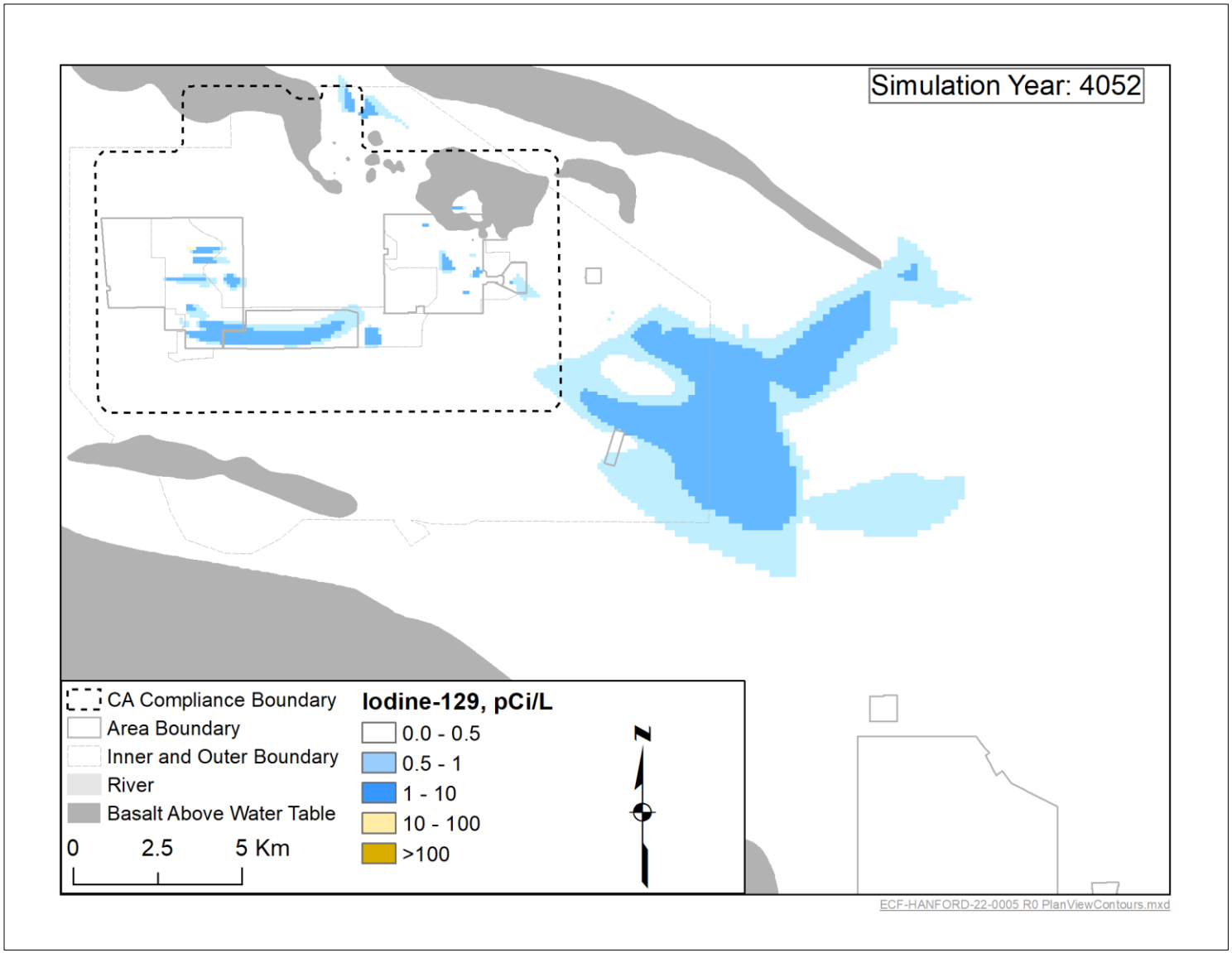

Figure C-8. Plan View Contours of Iodine-129 Concentration Simulated 4052 Years (Calendar Year 6070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

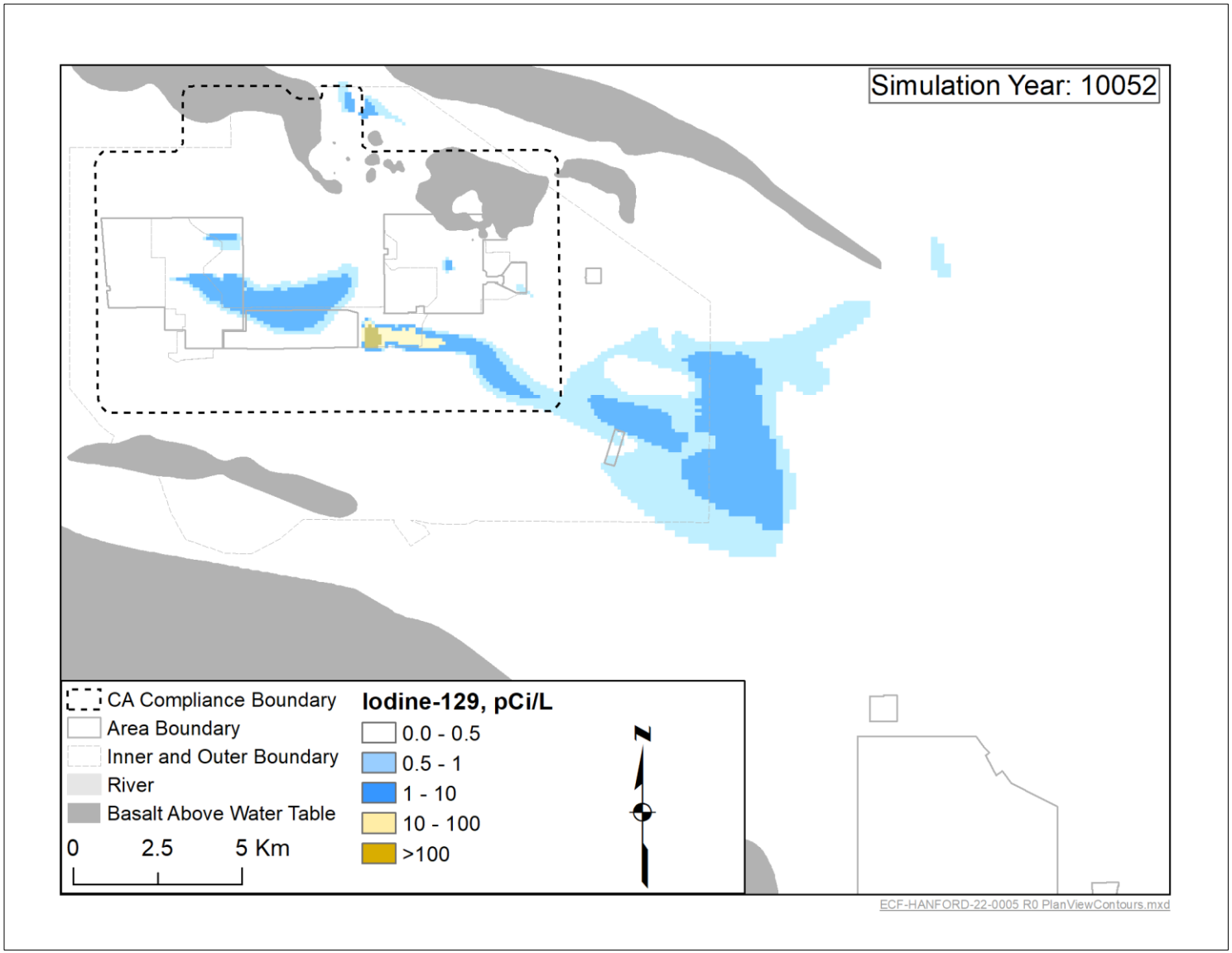

Figure C-9. Plan View Contours of Iodine-129 Concentration Simulated 10052 Years (Calendar Year 12070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

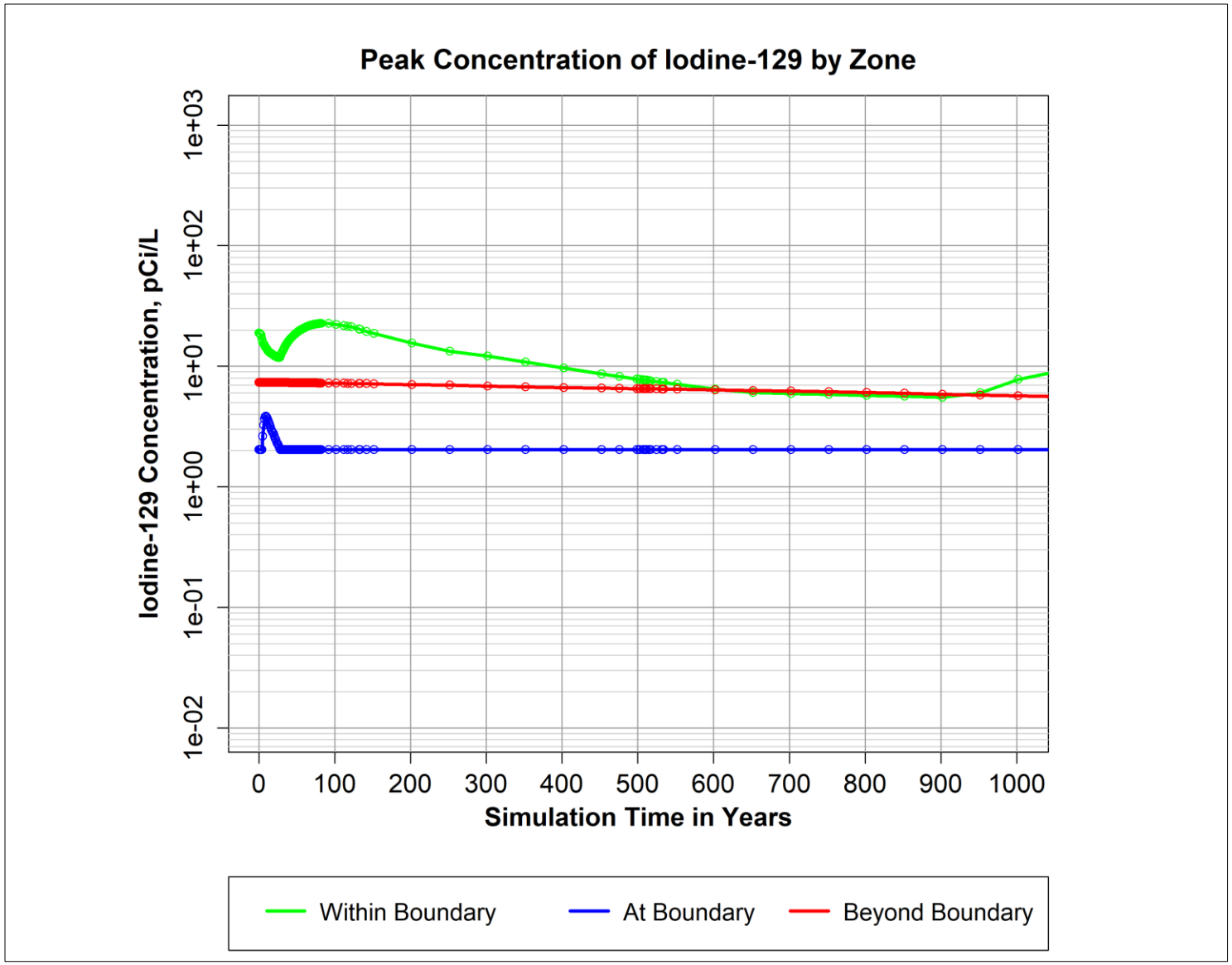

Figure C-10. Peak Concentration of Iodine-129 from the Start of Simulation Until the End of the Compliance Period Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

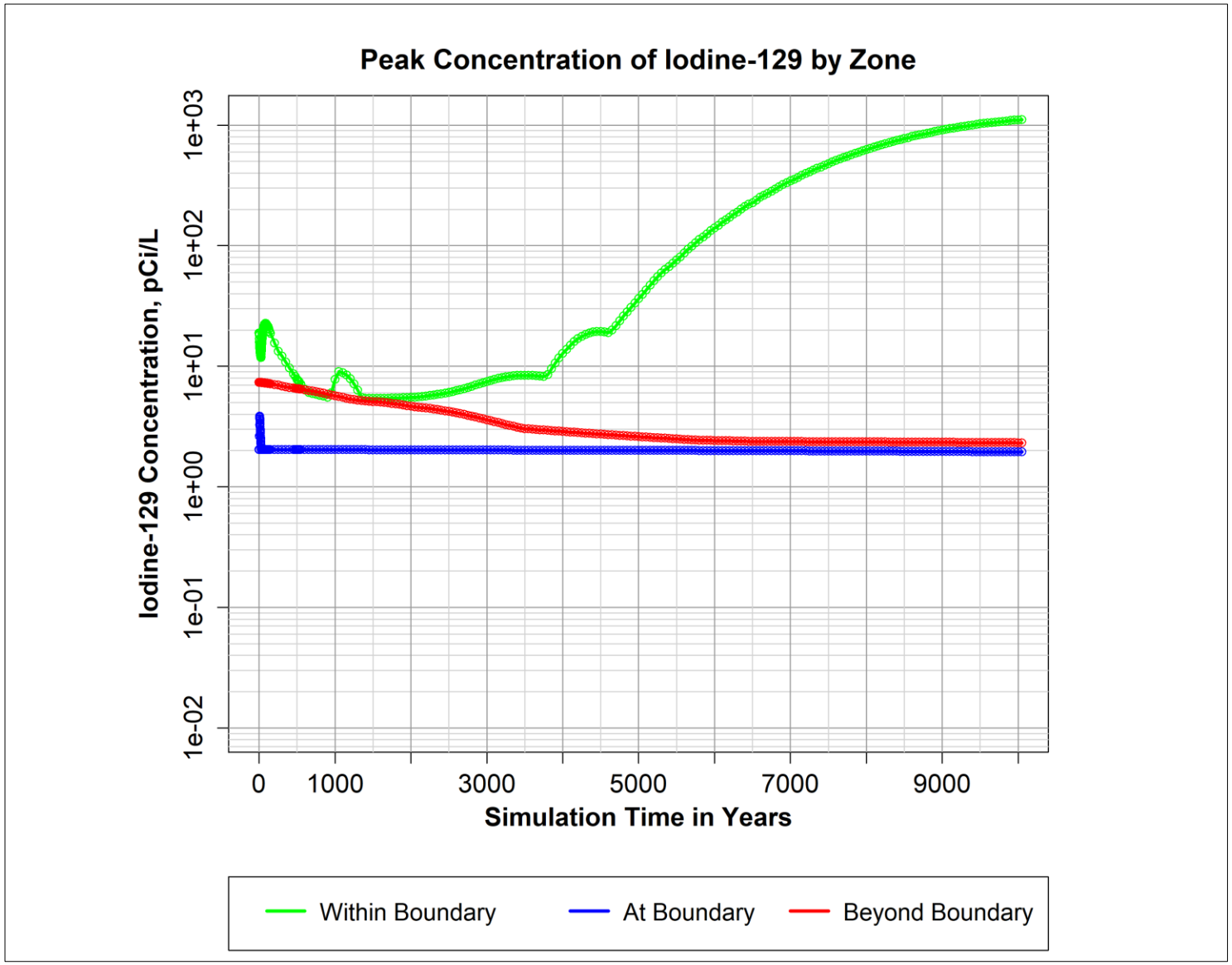

Figure C-11. Peak Concentration of Iodine-129 from the Start of Simulation to the end of the Simulation Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

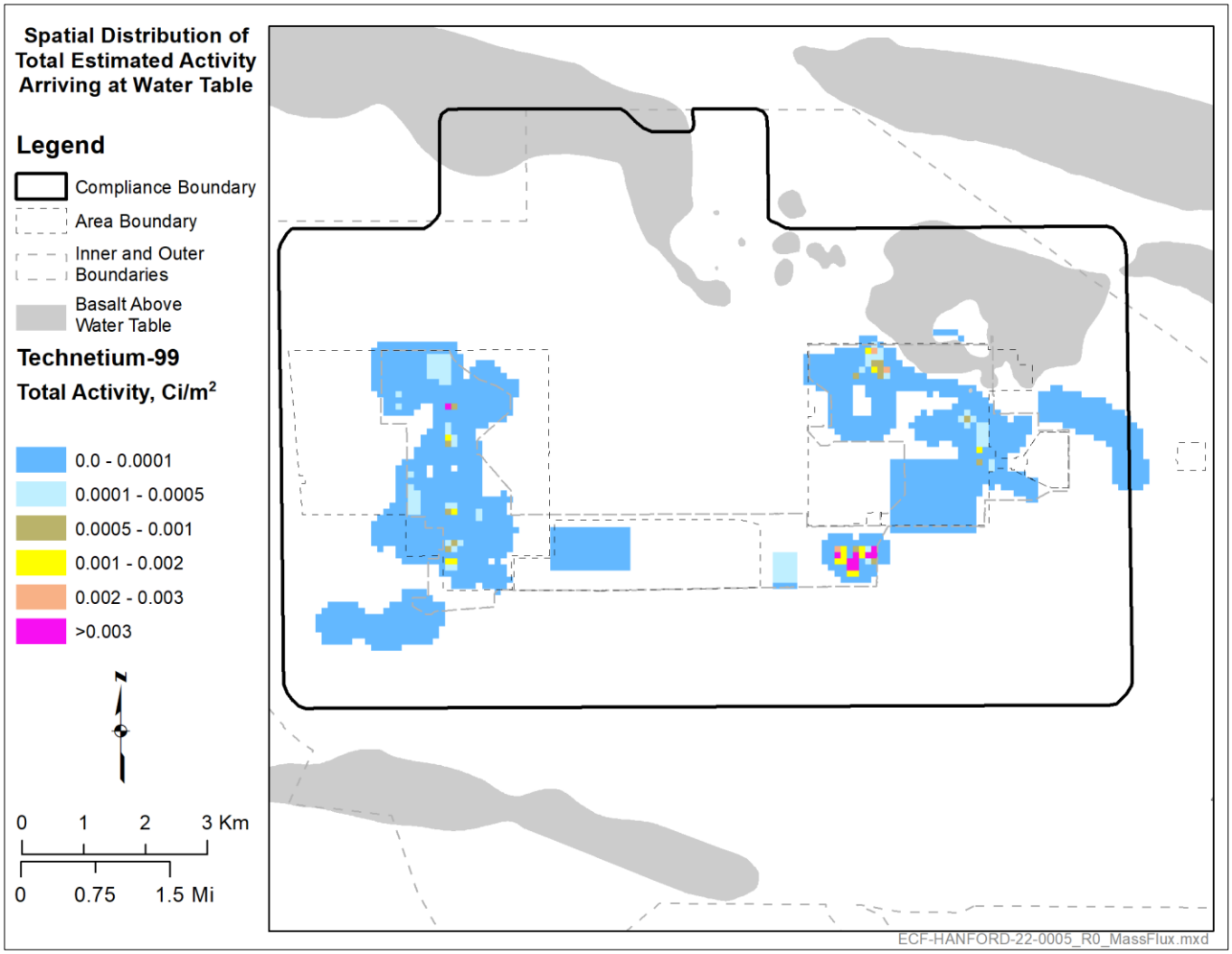

Figure C-12. Spatial Distribution of Technetium-99 that Enters the Saturated Zone from the Vadose Zone over the Entire Simulation Length

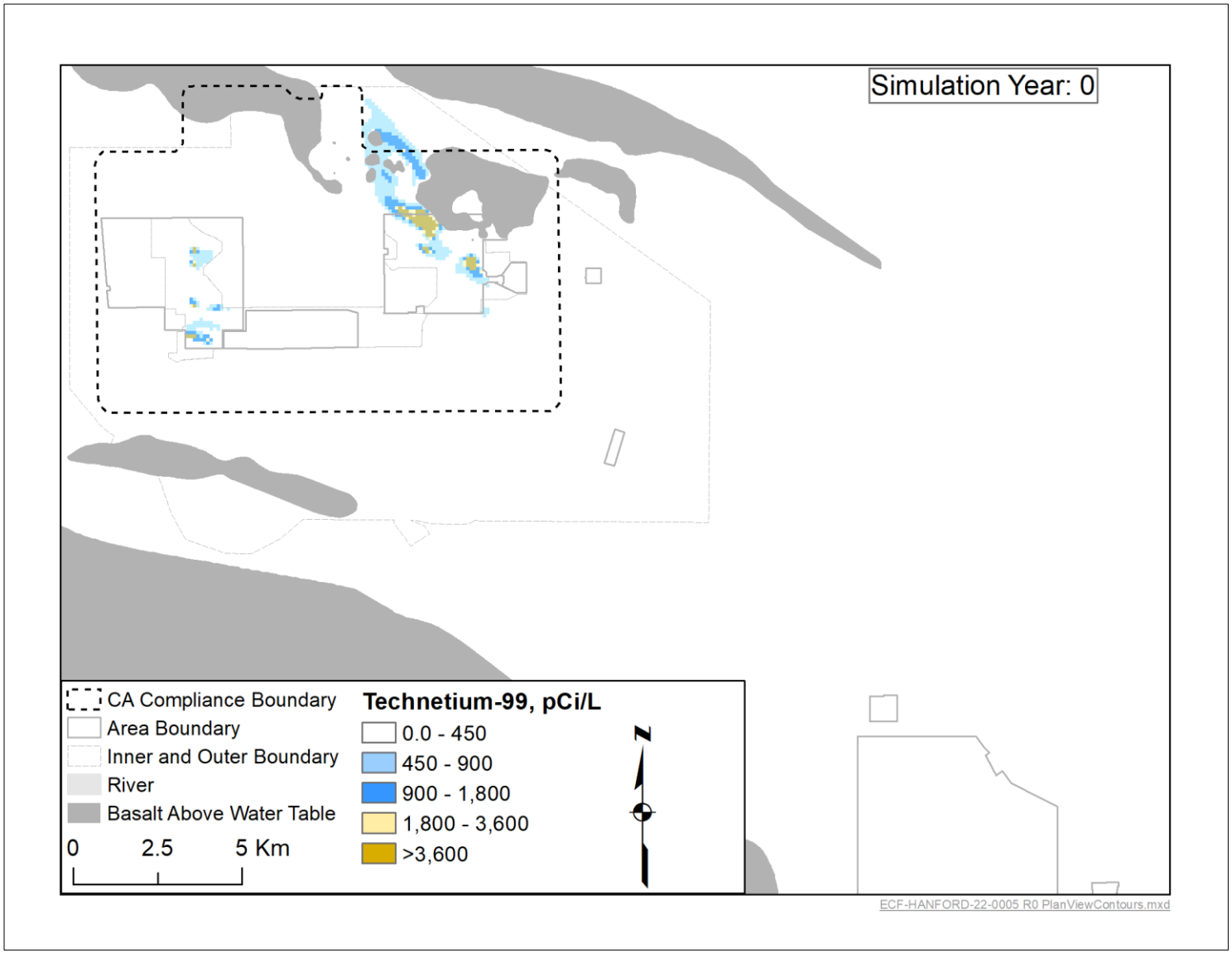

Figure C-13. Plan View Contours of Technetium-99 Concentration Simulated 0 Years (Calendar Year 2018) from the Start of Simulation Assuming the Best Estimate Initial Concentration

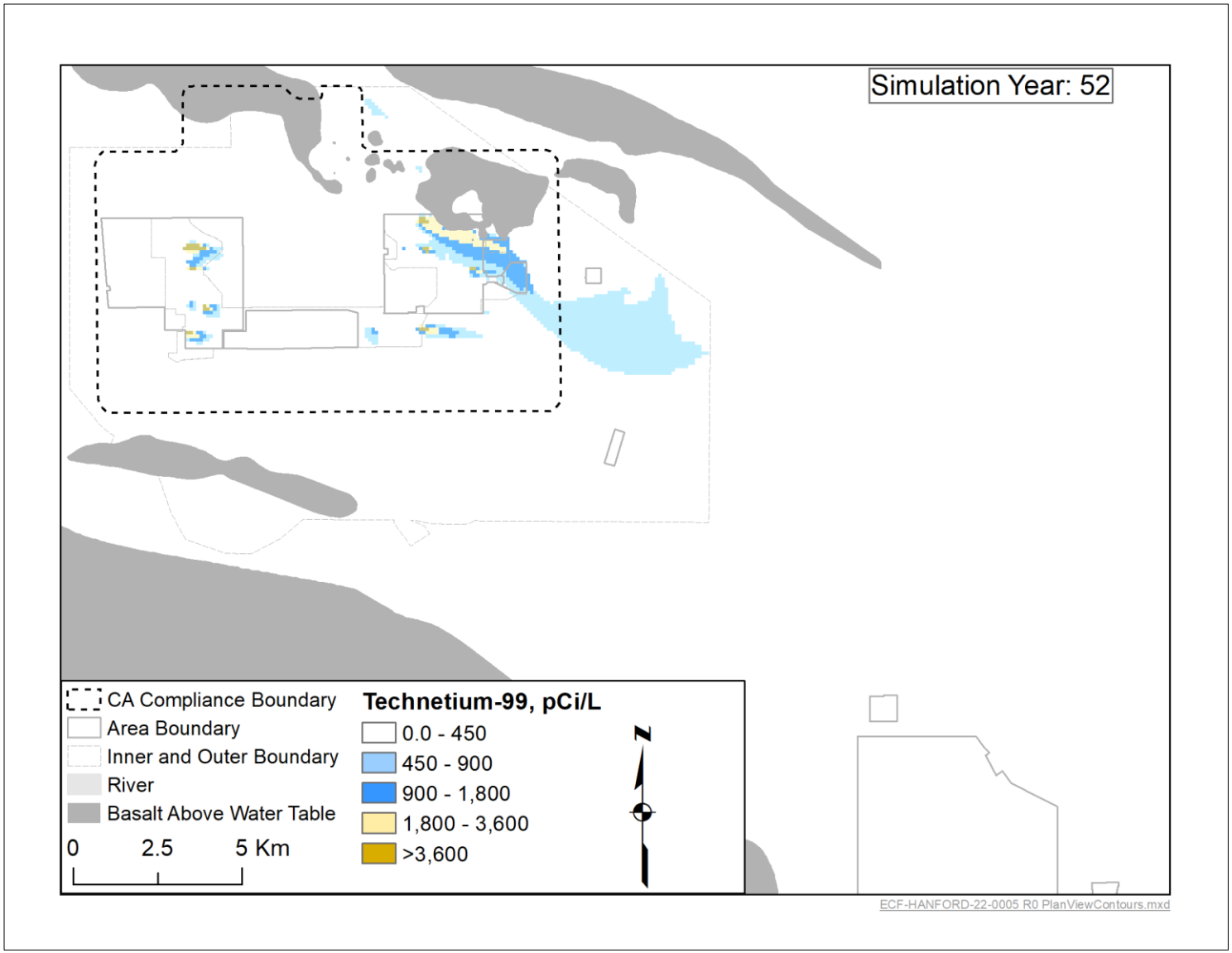

Figure C-14. Plan View Contours of Technetium-99 Concentration Simulated 52 Years (Calendar Year 2070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

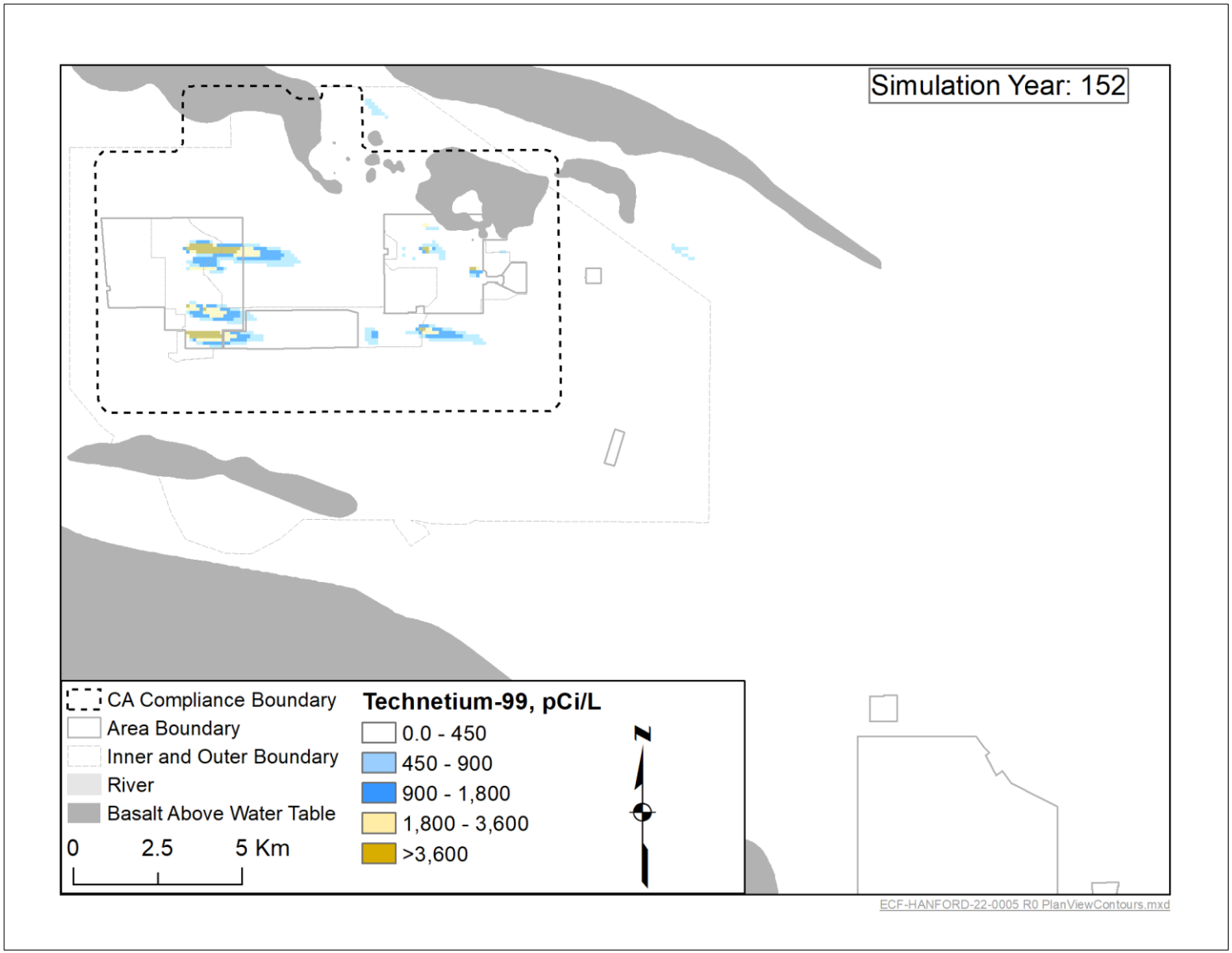

Figure C-15. Plan View Contours of Technetium-99 Concentration Simulated 152 Years (Calendar Year 2170) from the Start of Simulation Assuming the Best Estimate Initial Concentration

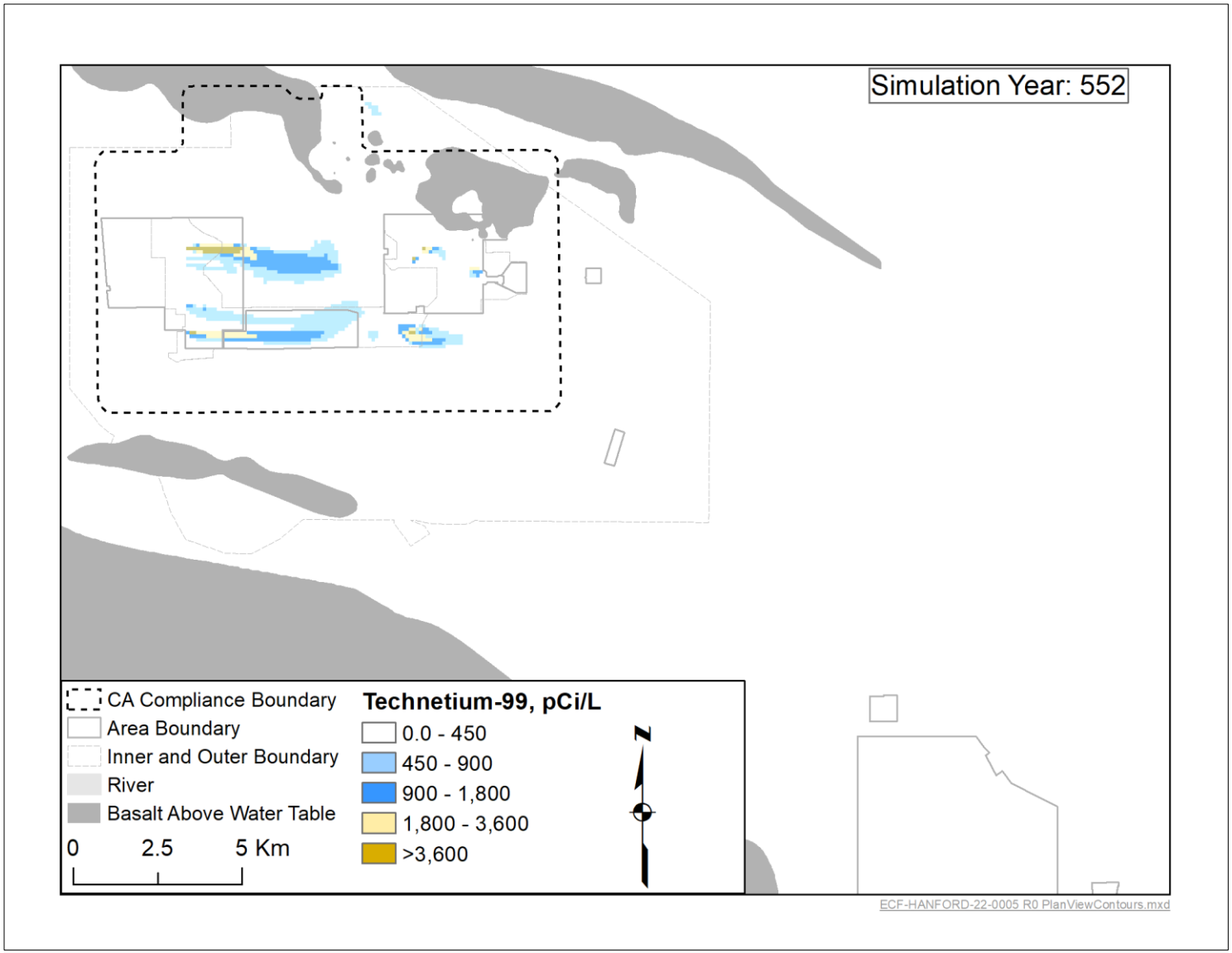

Figure C-16. Plan View Contours of Technetium-99 Concentration Simulated 552 Years (Calendar Year 2570) from the Start of Simulation Assuming the Best Estimate Initial Concentration

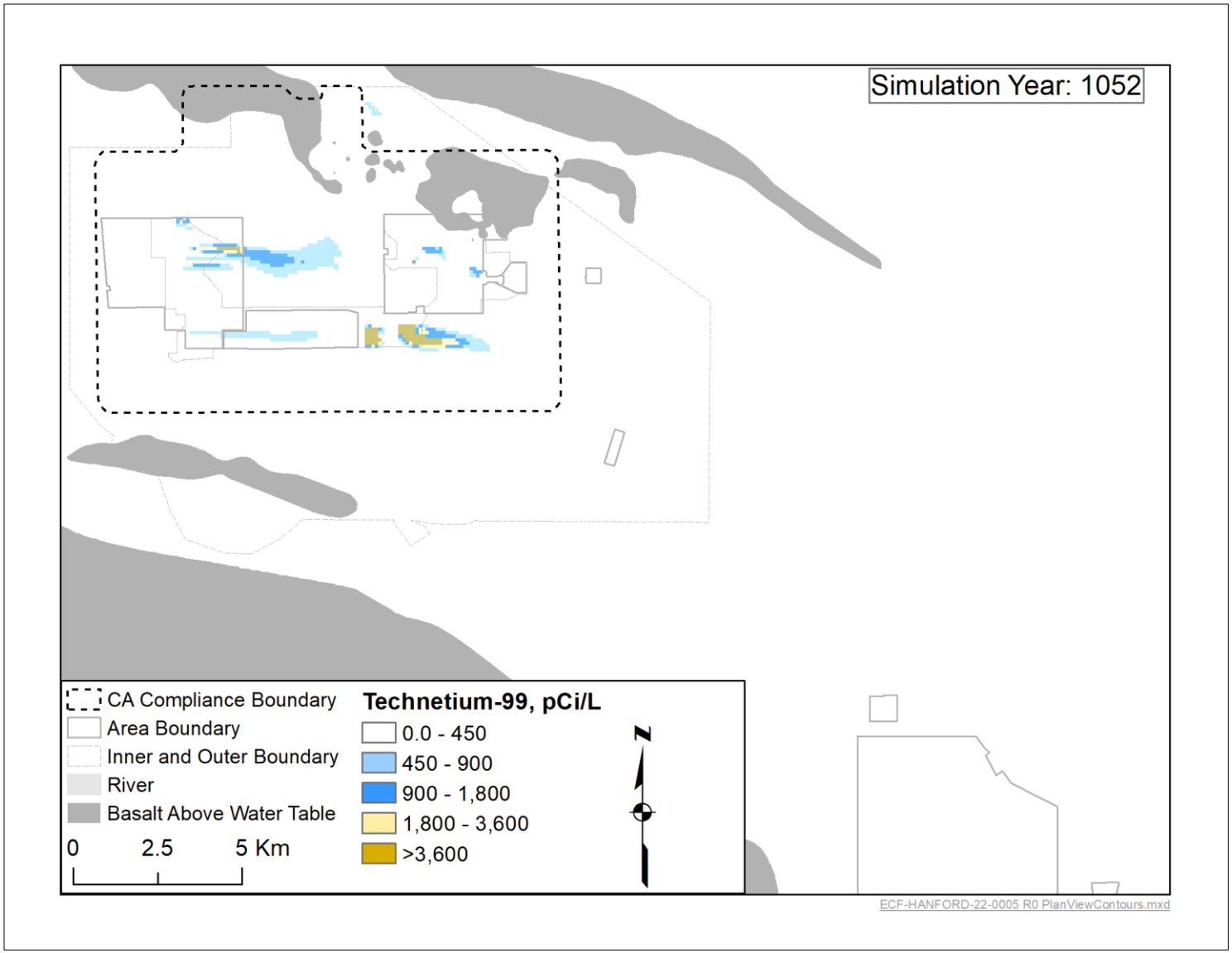

Figure C-17. Plan View Contours of Technetium-99 Concentration Simulated 1052 Years (Calendar Year 3070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

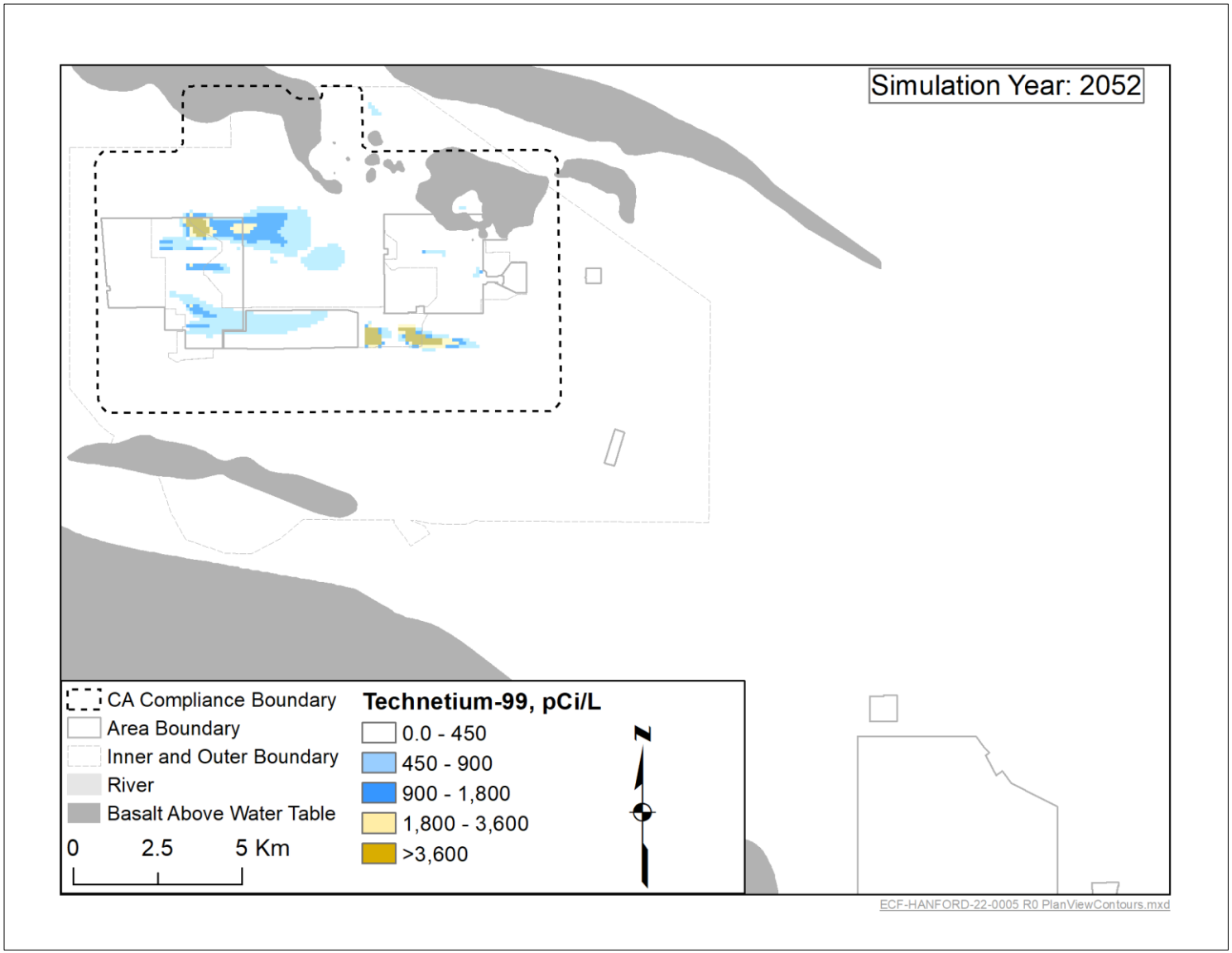

Figure C-18. Plan View Contours of Technetium-99 Concentration Simulated 2052 Years (Calendar Year 4070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

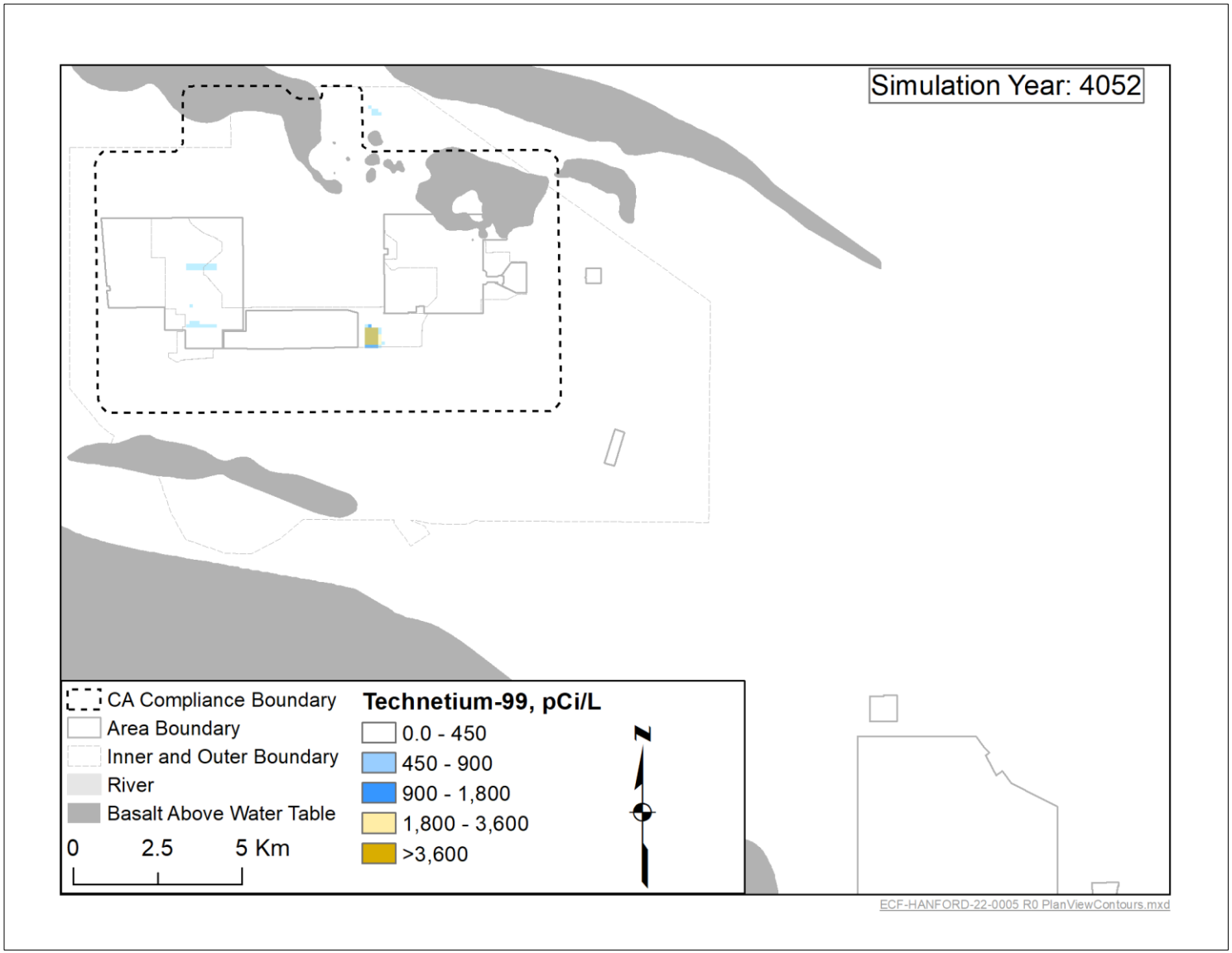

Figure C-19. Plan View Contours of Technetium-99 Concentration Simulated 4052 Years (Calendar Year 6070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

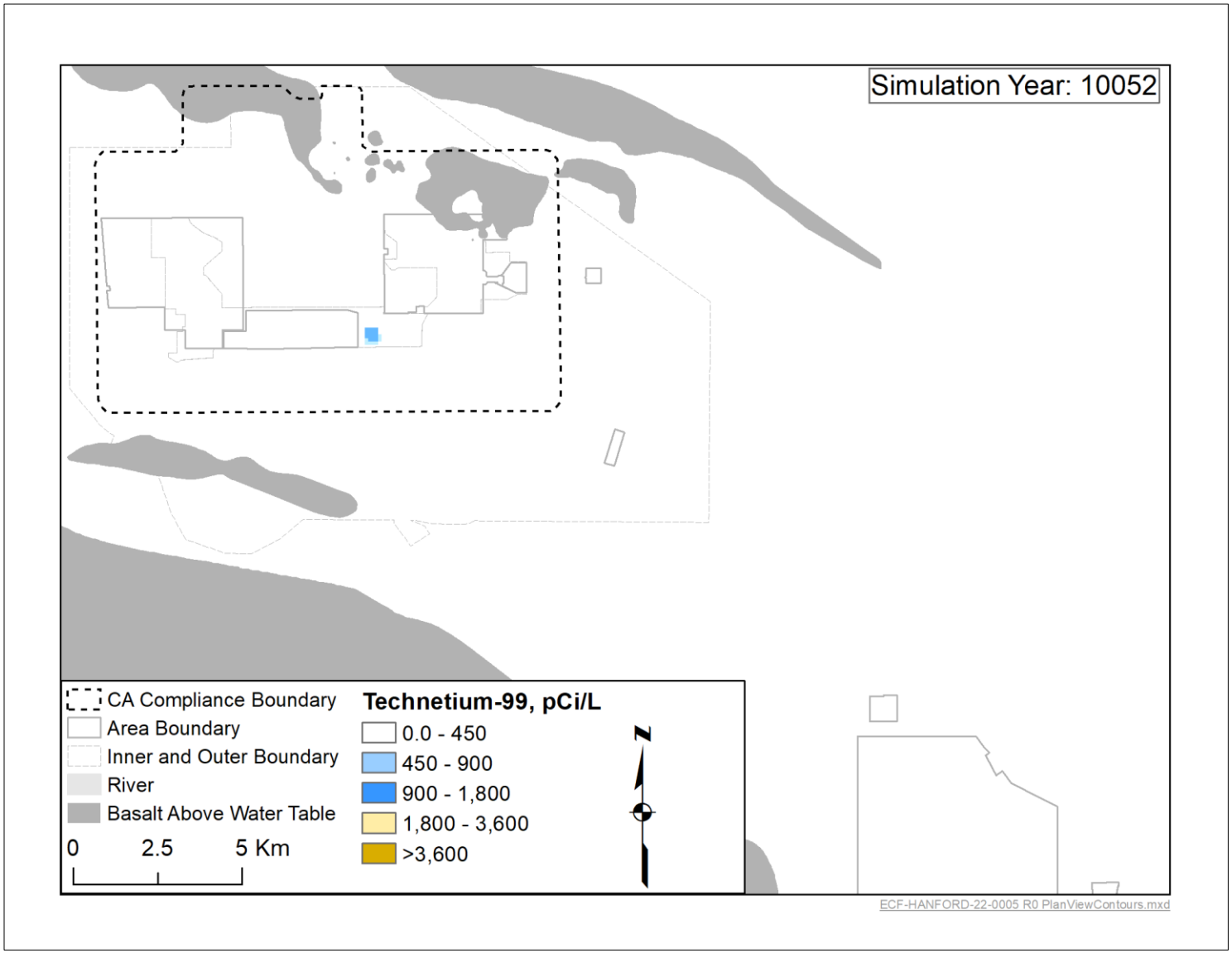

Figure C-20. Plan View Contours of Technetium-99 Concentration Simulated 10052 Years (Calendar Year 12070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

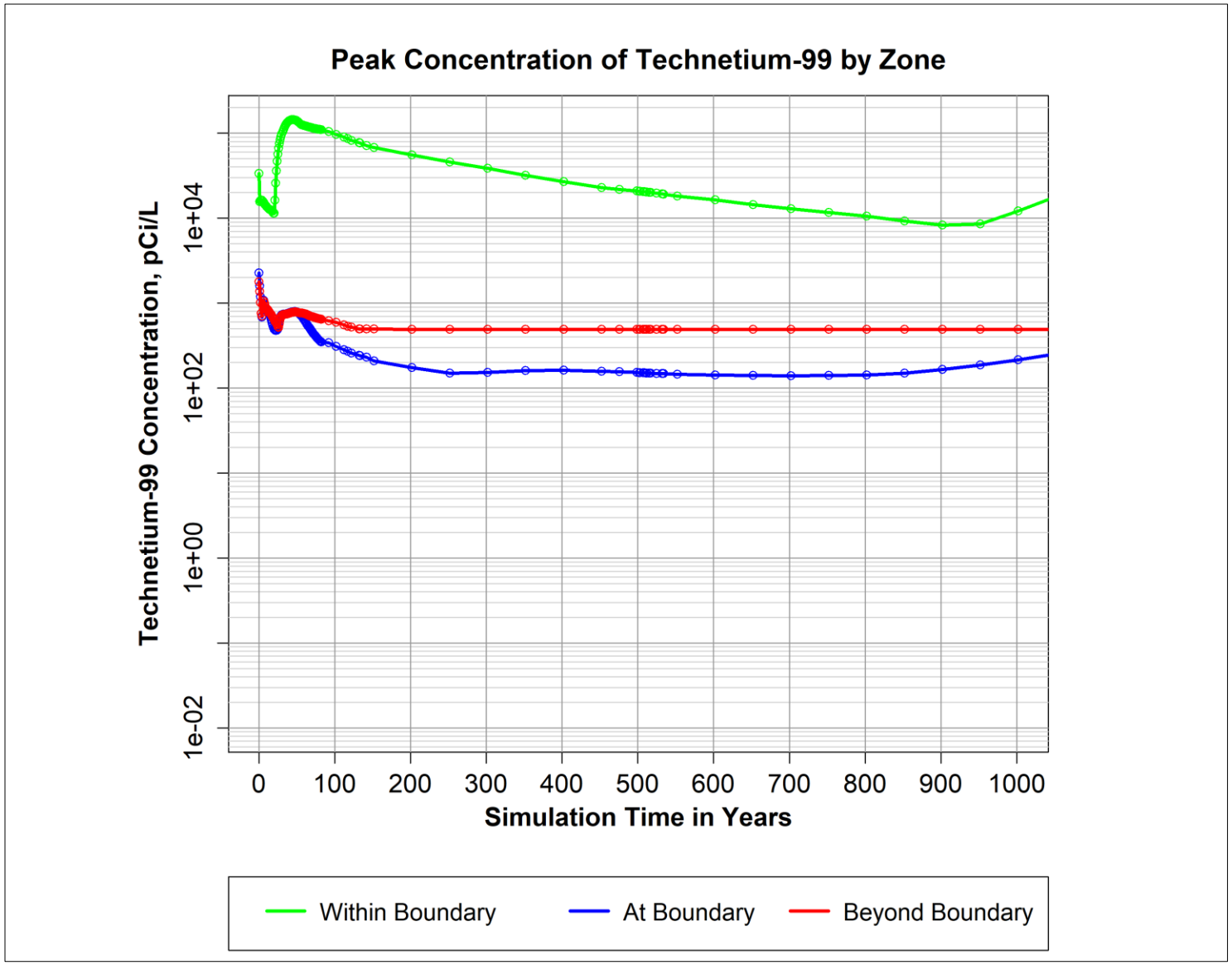

Figure C-21. Peak Concentration of Technetium-99 from the Start of Simulation Until the End of the Compliance Period Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

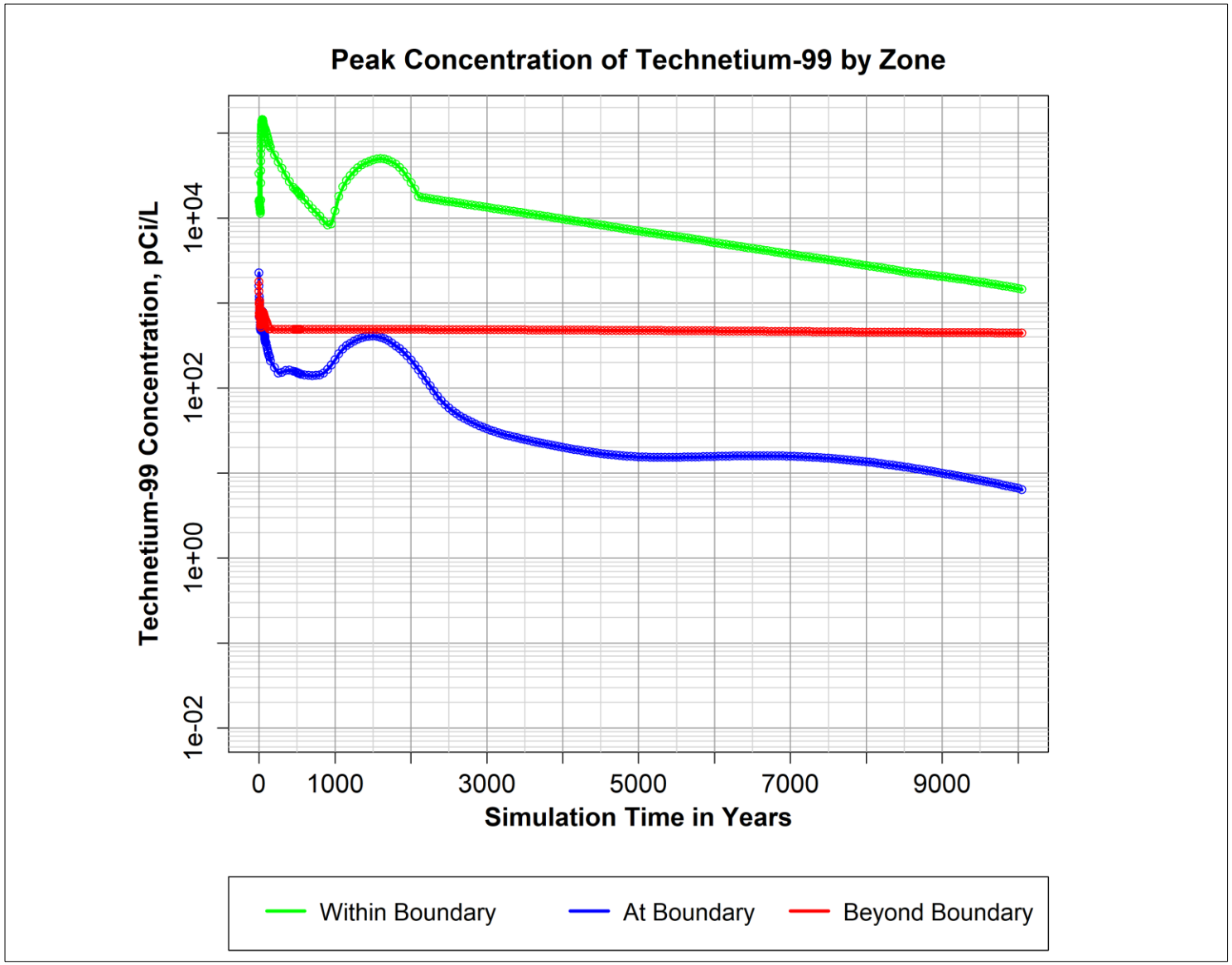

Figure C-22. Peak Concentration of Technetium-99 from the Start of Simulation to the end of the Simulation Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

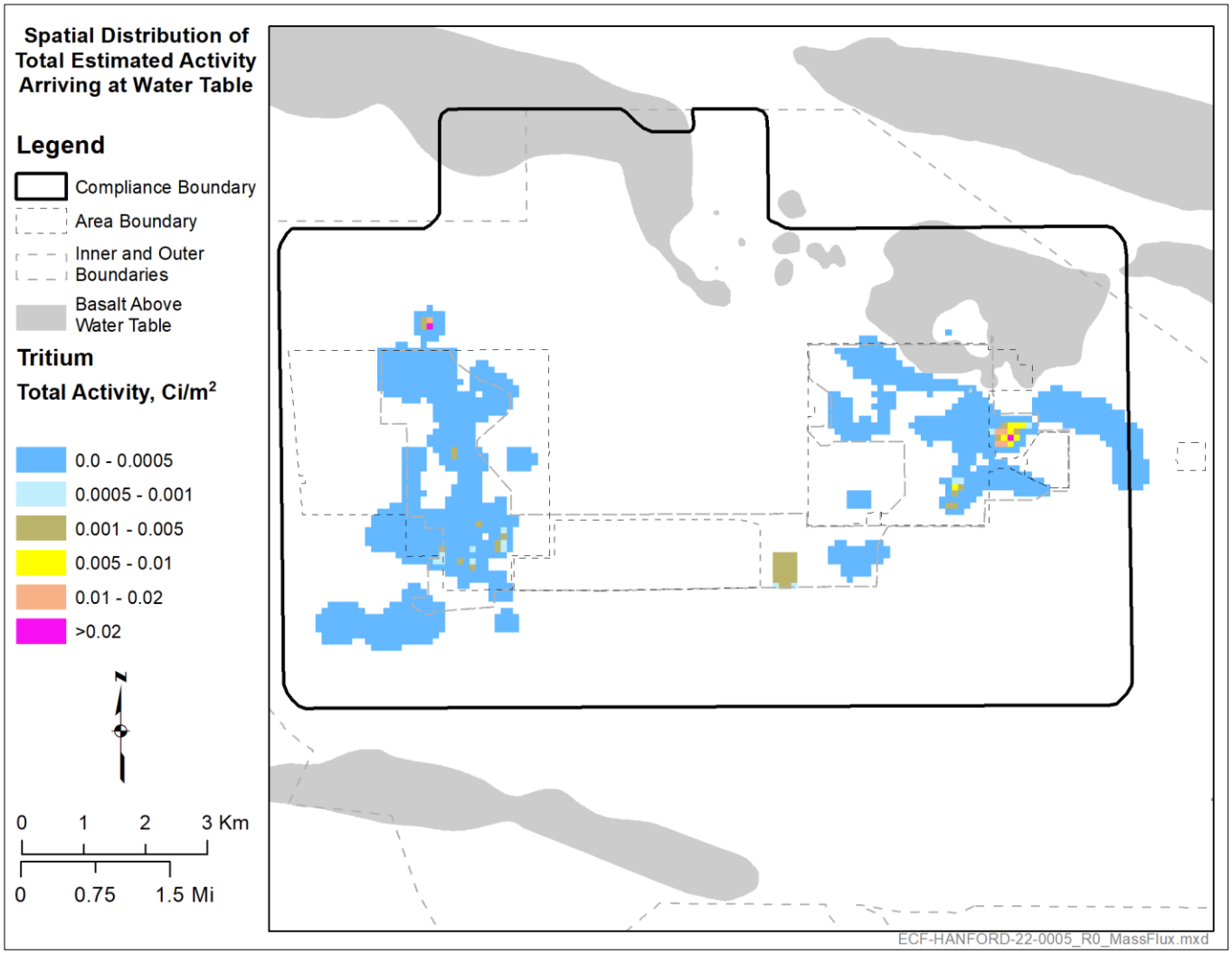

Figure C-23. Spatial Distribution of Tritium that Enters the Saturated Zone from the Vadose Zone over the Entire Simulation Length

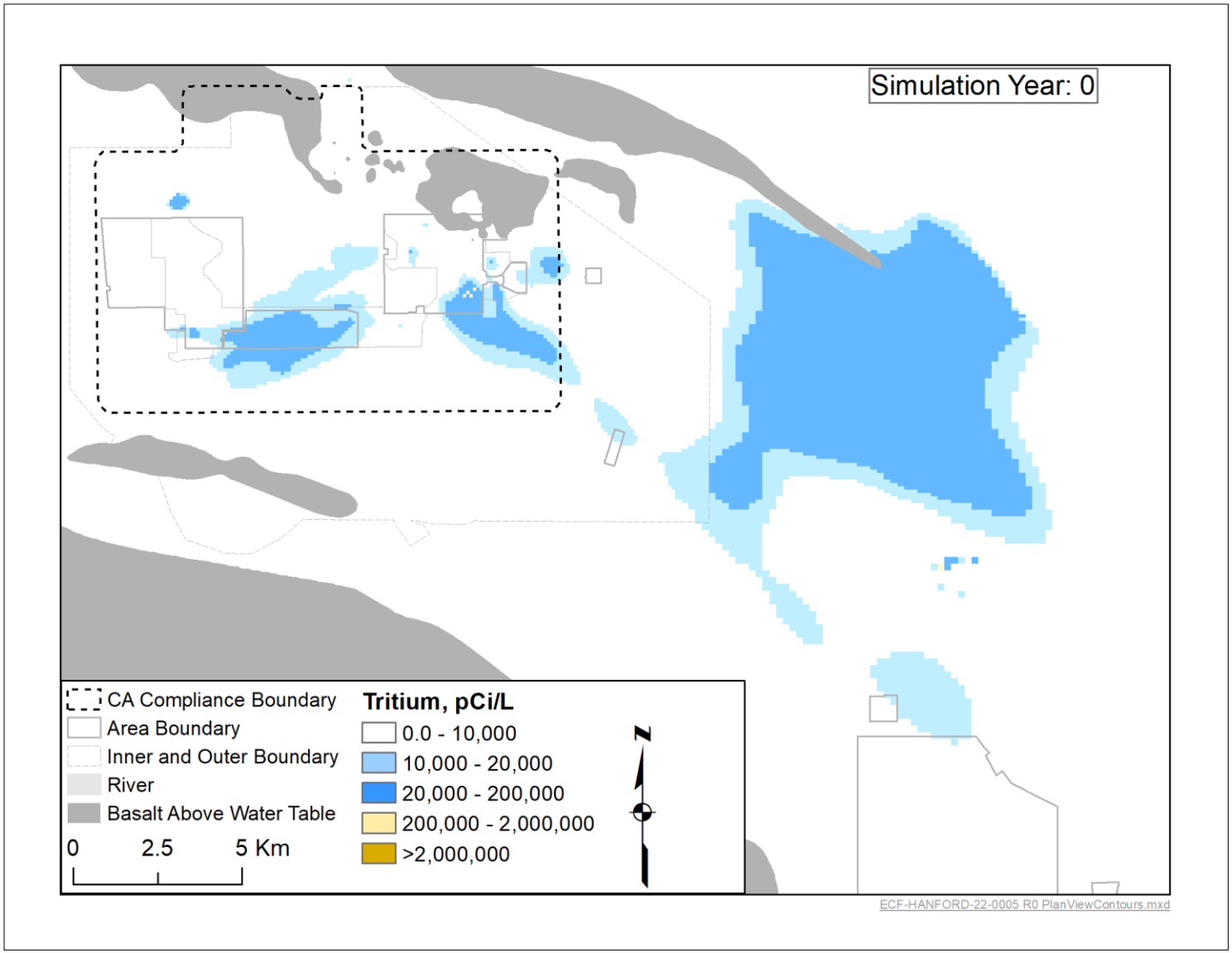

Figure C-24. Plan View Contours of Tritium Concentration Simulated 0 Years (Calendar Year 2018) from the Start of Simulation Assuming the Best Estimate Initial Concentration

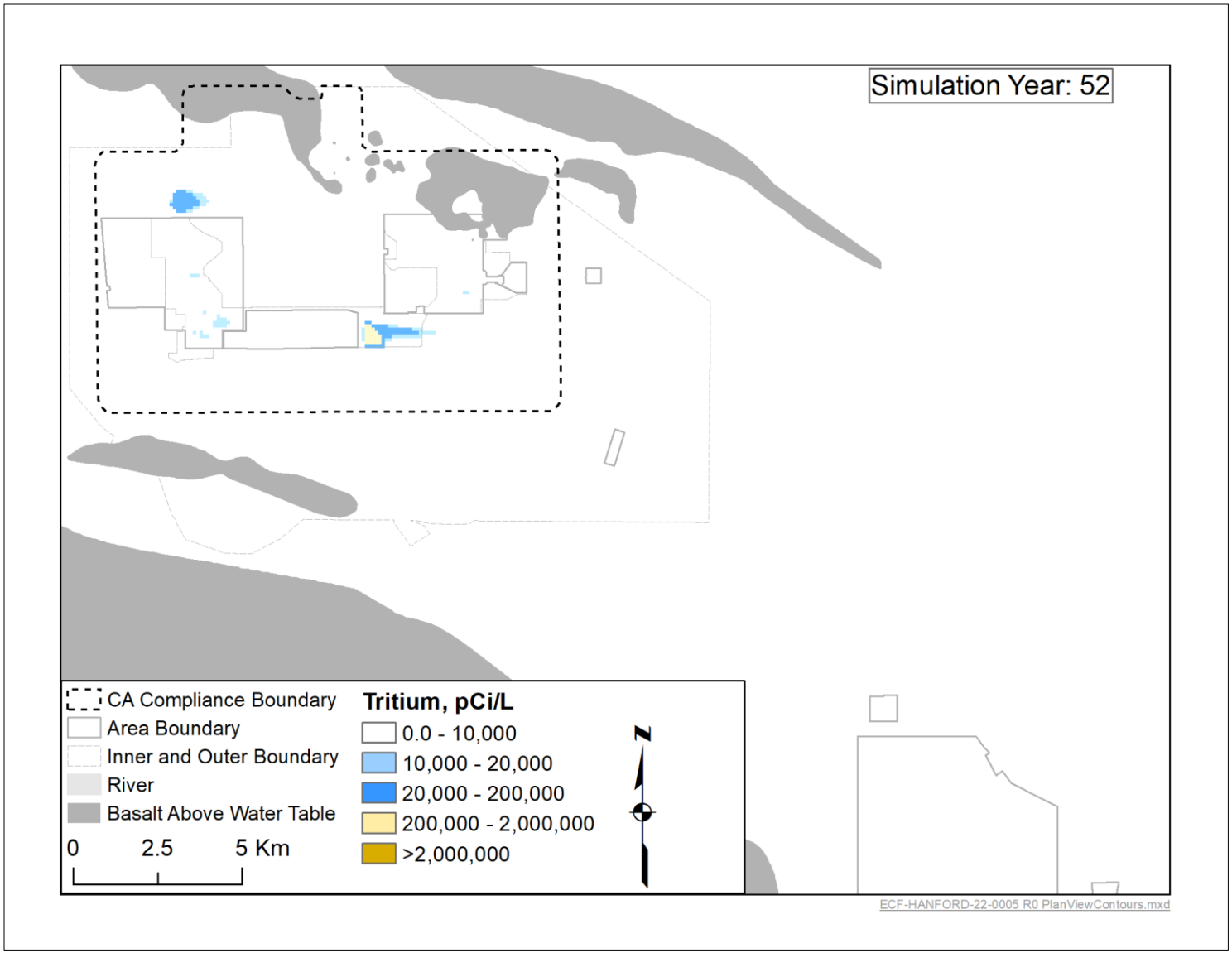

Figure C-25. Plan View Contours of Tritium Concentration Simulated 52 Years (Calendar Year 2070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

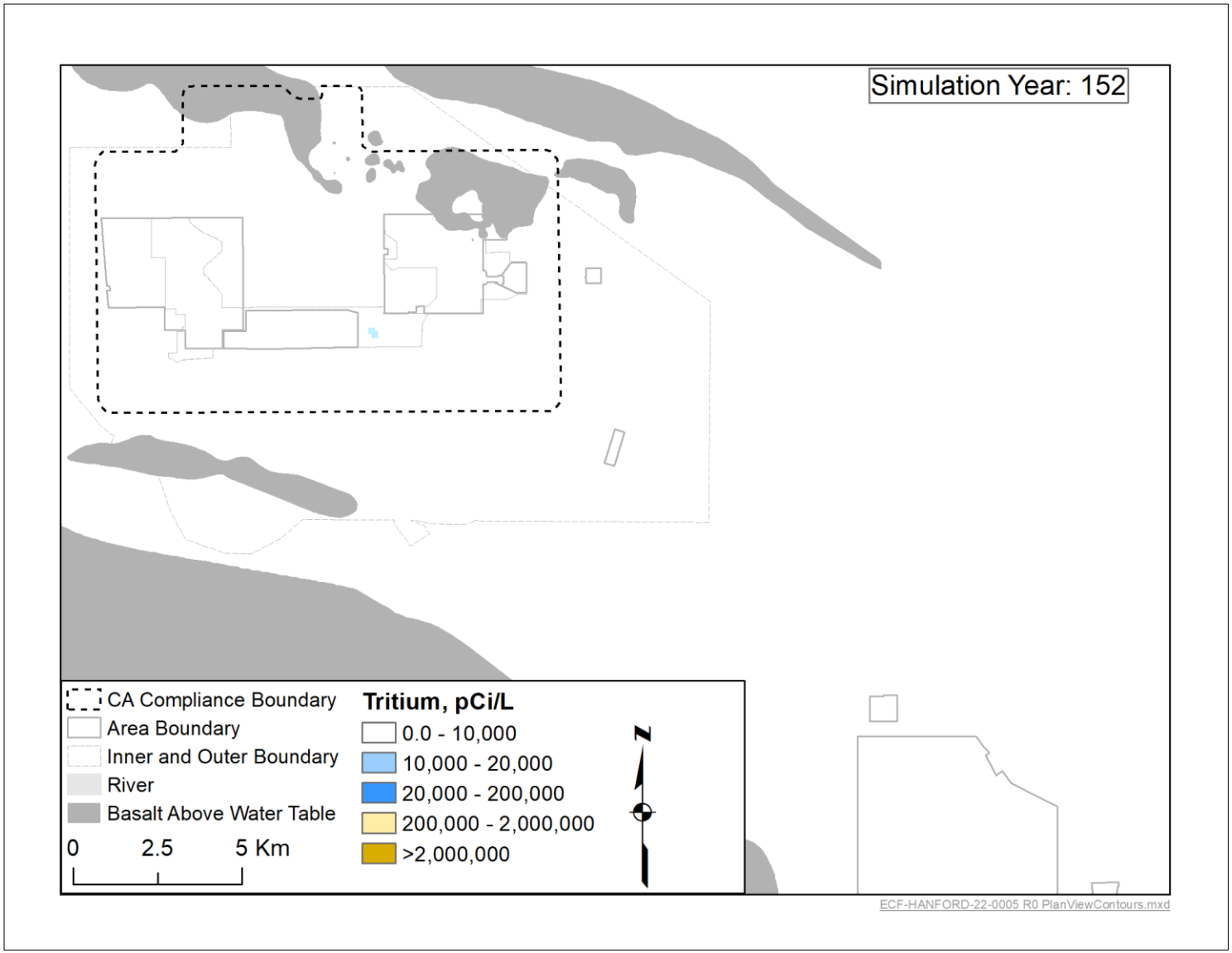

Figure C-26. Plan View Contours of Tritium Concentration Simulated 152 Years (Calendar Year 2170) from the Start of Simulation Assuming the Best Estimate Initial Concentration

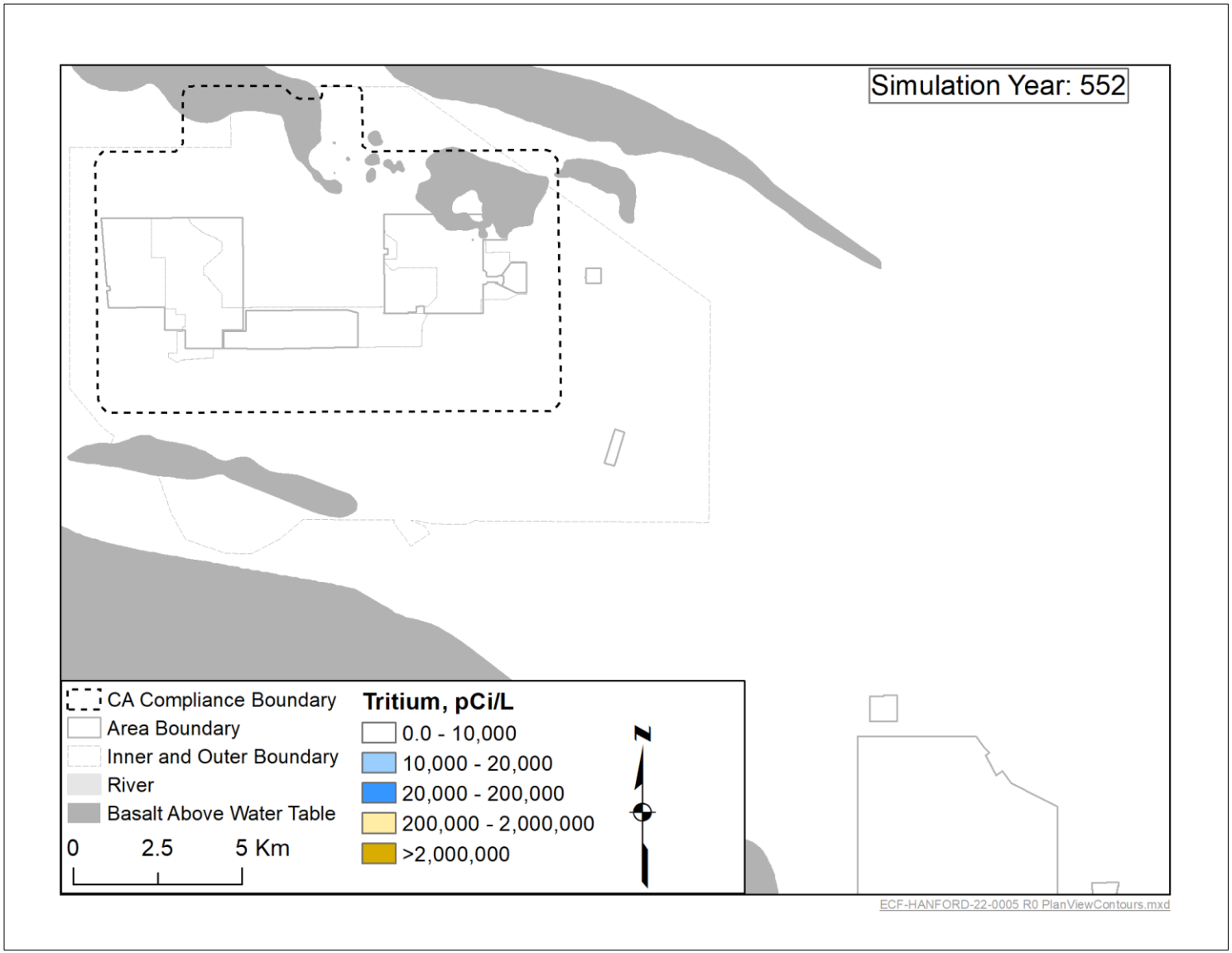

Figure C-27. Plan View Contours of Tritium Concentration Simulated 552 Years (Calendar Year 2570) from the Start of Simulation Assuming the Best Estimate Initial Concentration

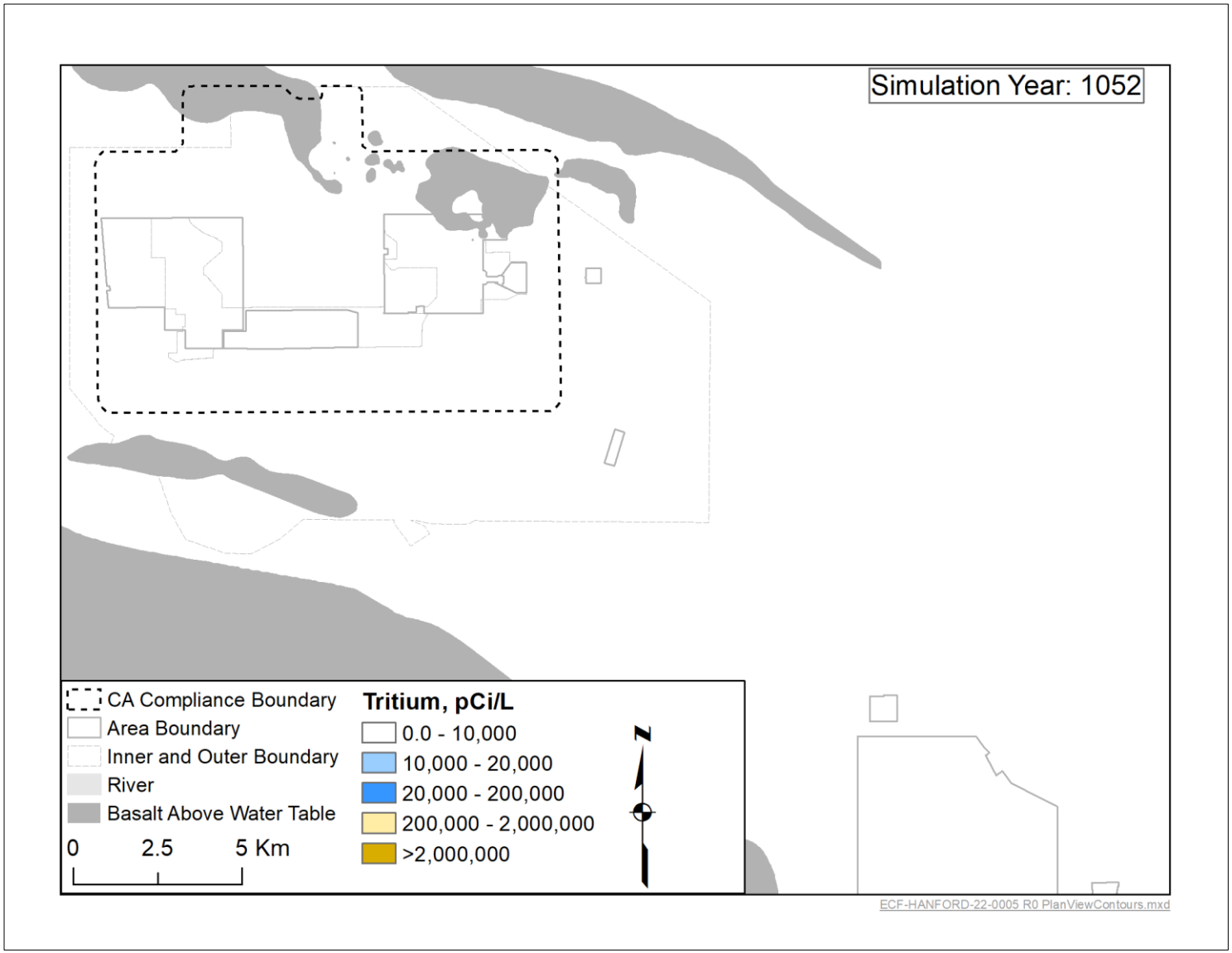

Figure C-28. Plan View Contours of Tritium Concentration Simulated 1052 Years (Calendar Year 3070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

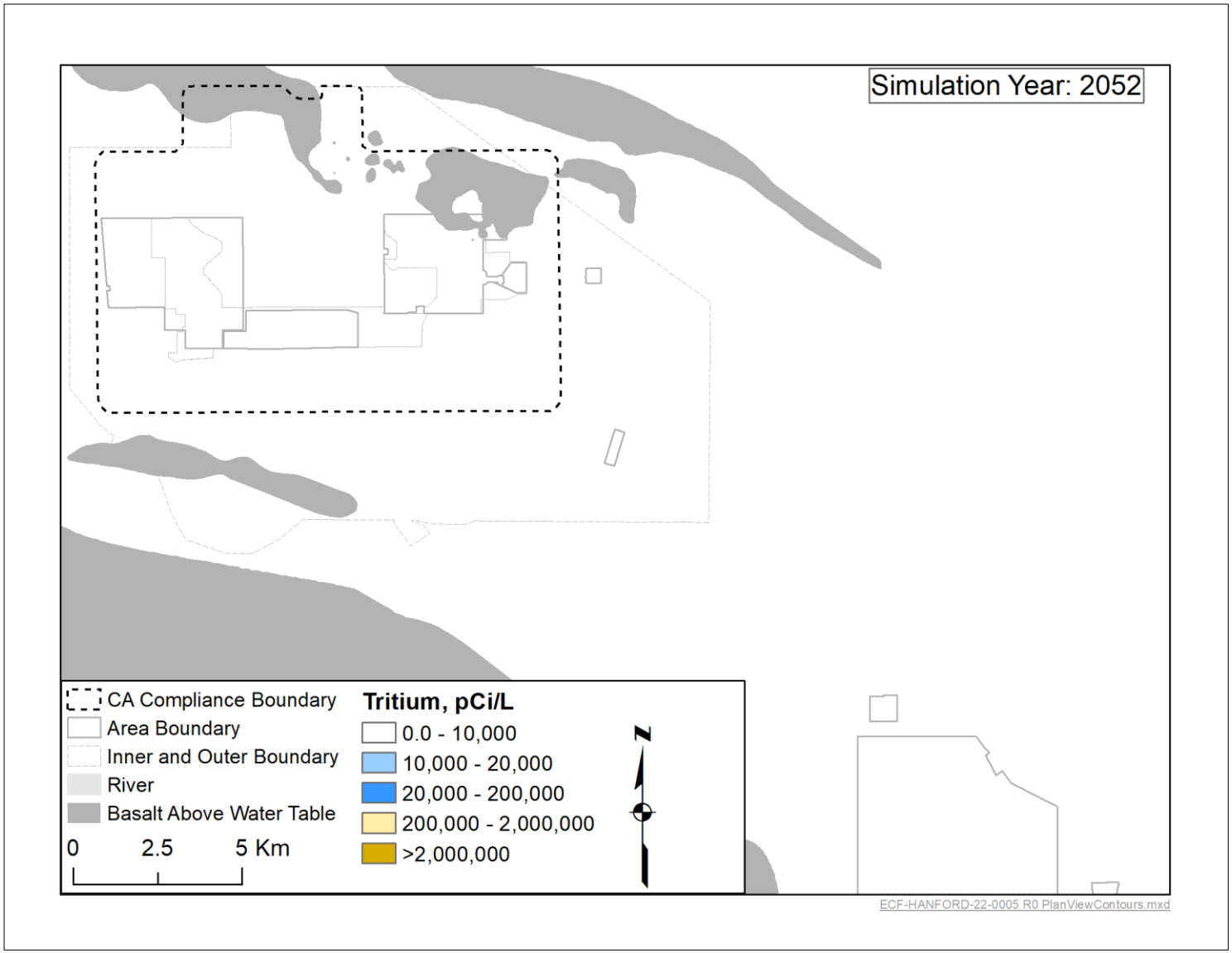

Figure C-29. Plan View Contours of Tritium Concentration Simulated 2052 Years (Calendar Year 4070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

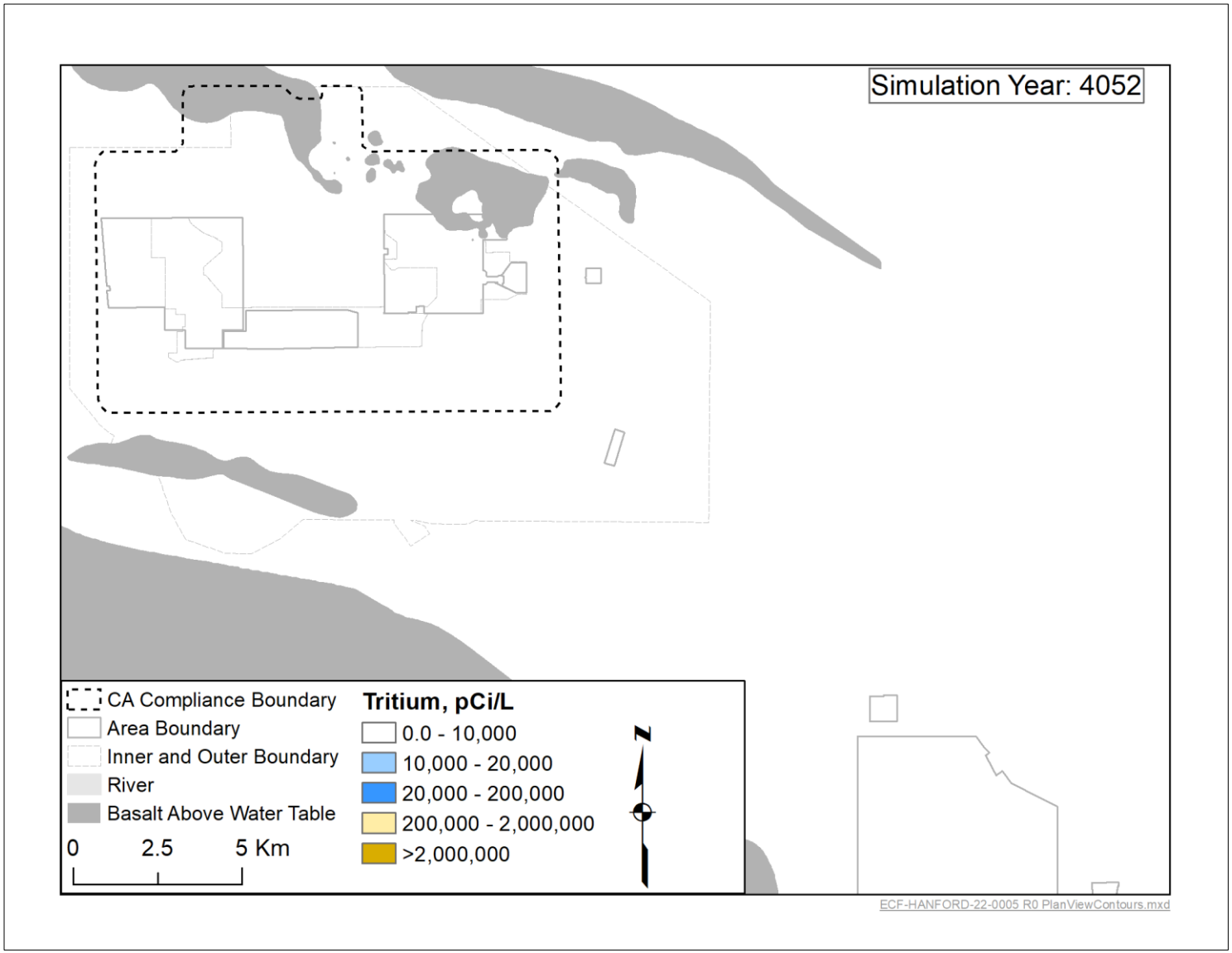

Figure C-30. Plan View Contours of Tritium Concentration Simulated 4052 Years (Calendar Year 6070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

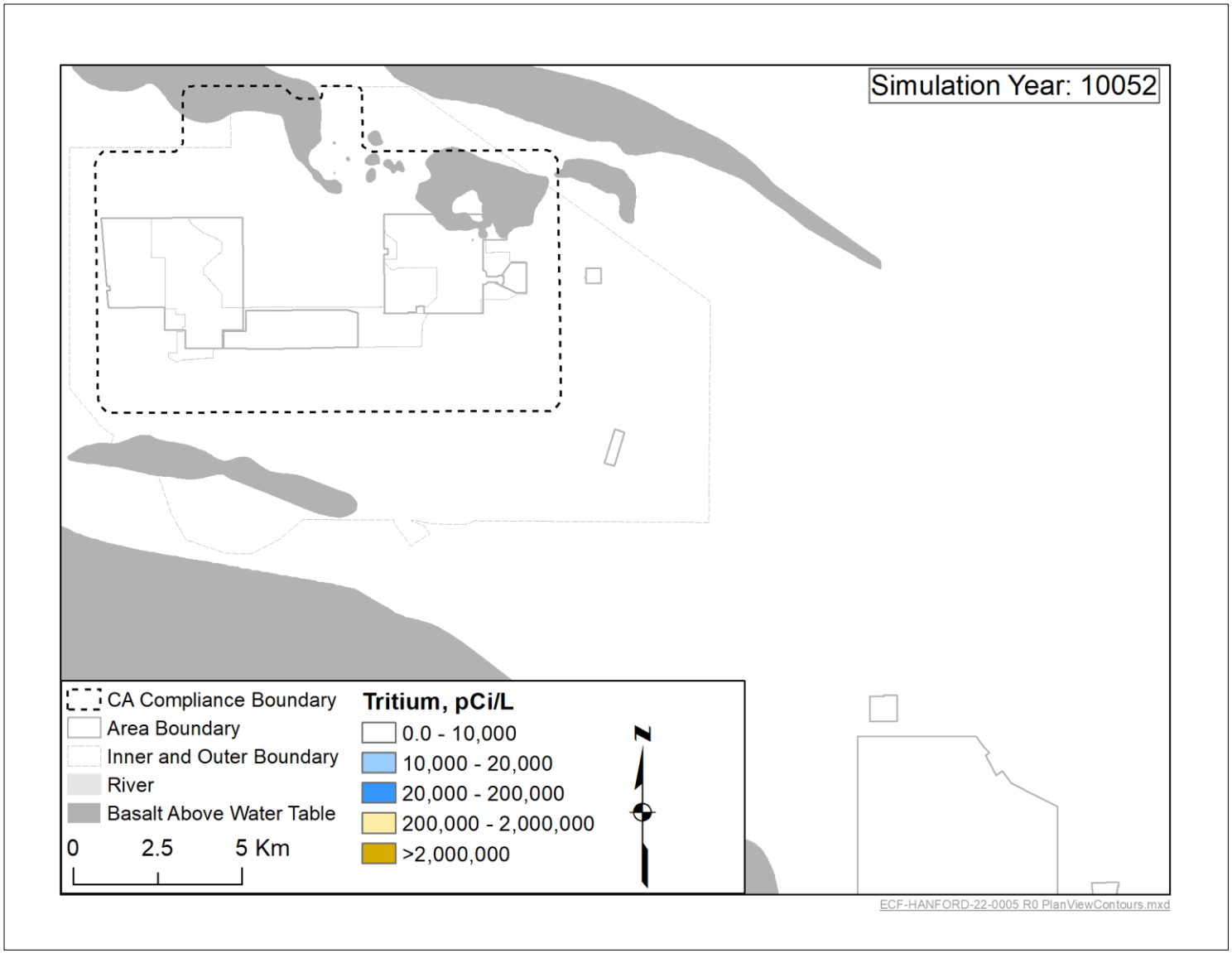

Figure C-31. Plan View Contours of Tritium Concentration Simulated 10052 Years (Calendar Year 12070) from the Start of Simulation Assuming the Best Estimate Initial Concentration

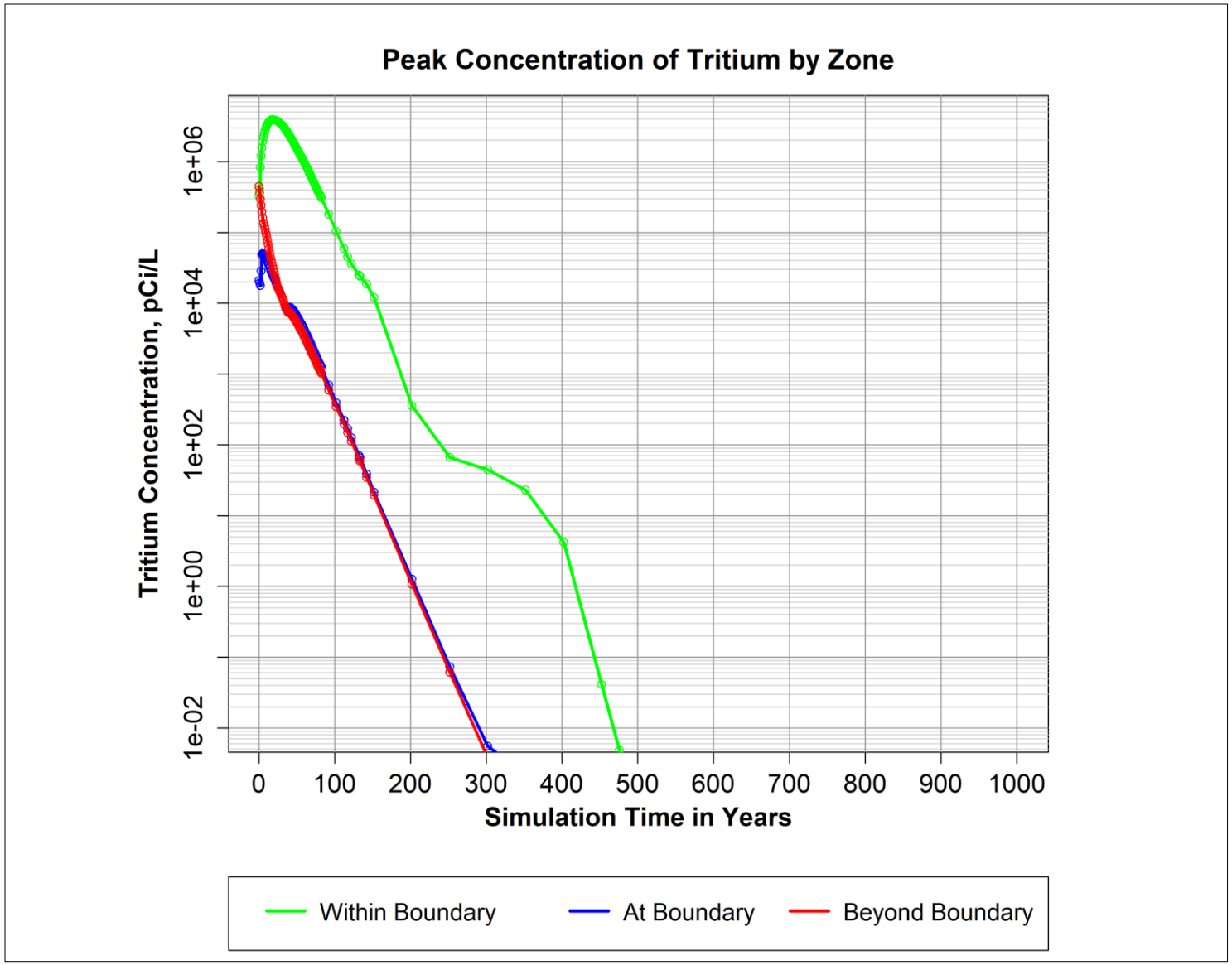

Figure C-32. Peak Concentration of Tritium from the Start of Simulation Until the End of the Compliance Period Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

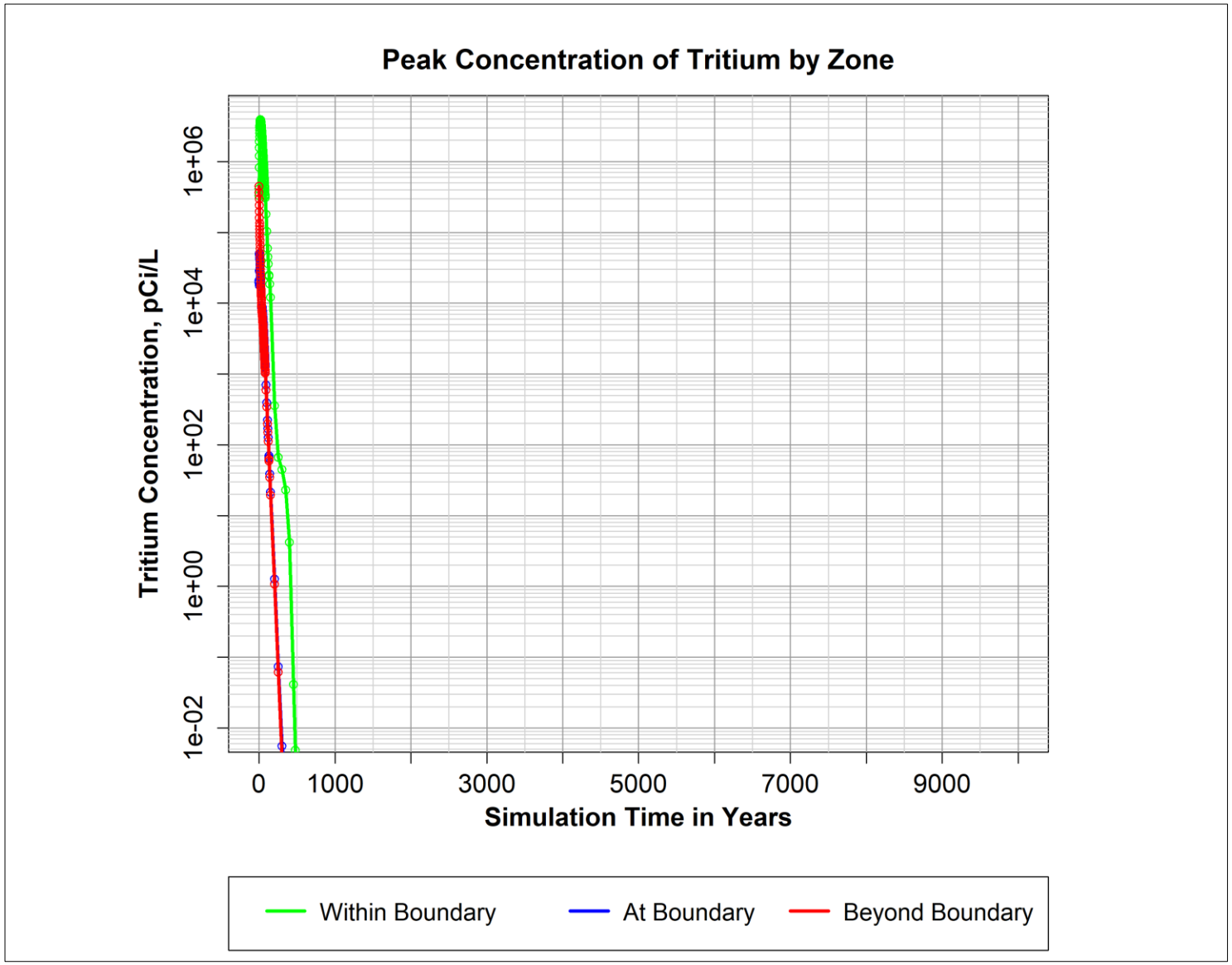

Figure C-33. Peak Concentration of Tritium from the Start of Simulation to the end of the Simulation Within, At, and Beyond the Compliance Boundary Assuming the Best Estimate Initial Concentration

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