ECF-HANFORD-20-0075
Revision 1

Application of a Null-Space Monte Carlo Flow Model Set to the Composite Analysis Base Case Fate and Transport Modeling

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

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Terms

CA	composite analysis
COPC	contaminant of potential concern
CPCCo	Central Plateau Cleanup Company
ECDF	empirical cumulative distribution function
ECF	environmental calculation file
F&T	fate and transport
HISI	Hanford Information System Inventory
HSS	Hydrocarbon Spill Source package
MODFLOW	MODular Groundwater FLOW modeling code
MT3DMS	Modular Three-Dimensional Multiple Species transport modeling code
NSMC	null space Monte Carlo
P2R	Plateau-to-River (model)

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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 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.

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 the application of the hydraulic property fields and recharge parameters documented in ECF-HANFORD-20-0027, *Null Space Monte Carlo Evaluation of the Plateau to River Model* to the CA flow and F&T simulation results to quantify the uncertainty in the simulated results due to input parameter selection.

Use of numerical groundwater models is always accompanied with uncertainty in the results produced by a model because models are approximations of reality. Thus, by definition, models lack the detail to fully represent observed behavior. Use of numerical techniques, such as a null space Monte Carlo (NSMC) analysis, can help in identifying and quantifying the potential uncertainties associated with a numerical model such as the P2R Model. The result of NSMC analysis is a set of F&T simulations that provide an estimate of the range of possible outcomes, which are used to quantify the uncertainty in simulated concentrations produced using the base case simulations. The simulated concentrations from all simulations will support calculation of the uncertainty of the total dose calculated in a separate calculation.

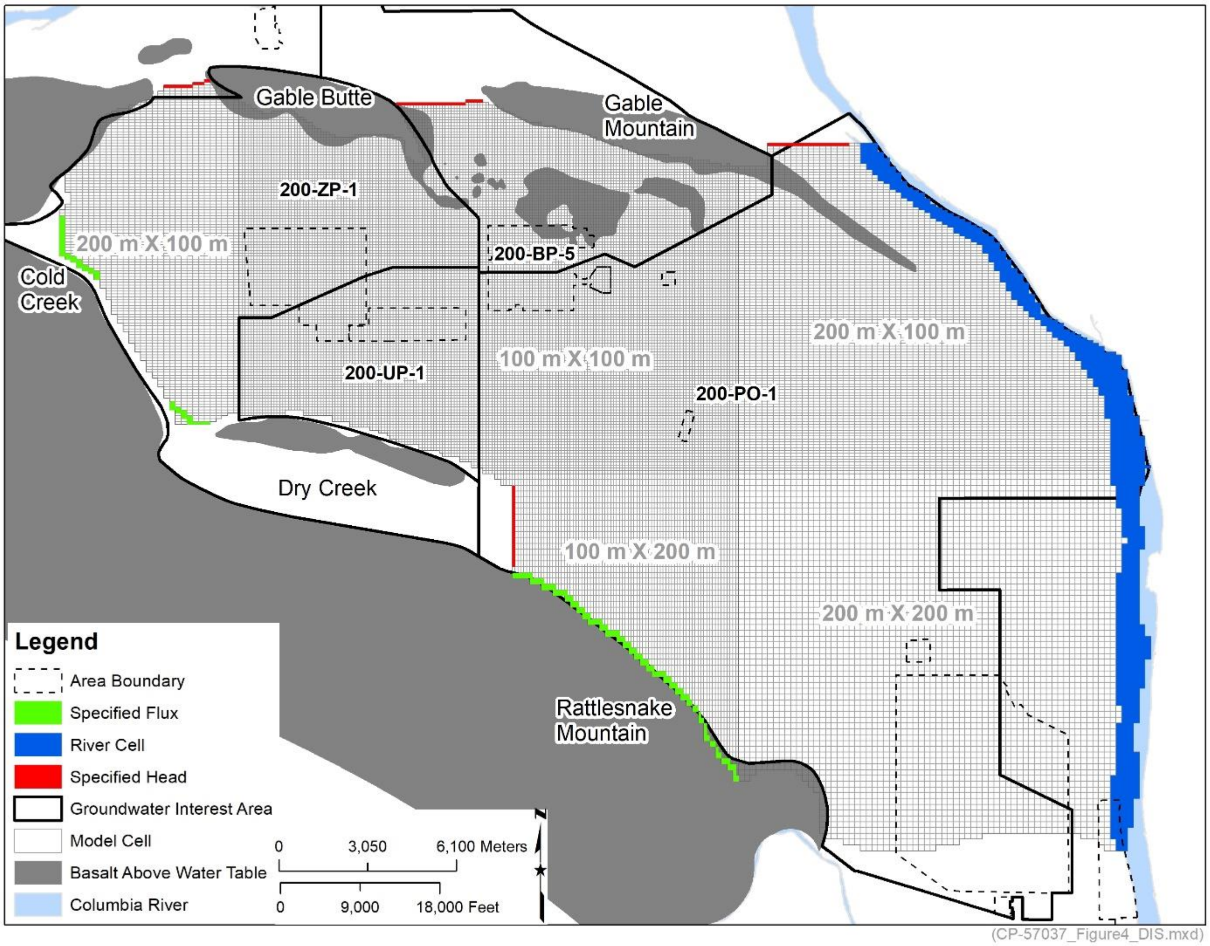


Figure 1. P2R Version 8.3 Model Extent, Discretization, and Boundary Conditions

2 Background

The development of the P2R Model is documented in CP-57037. Uncertainty analysis of the hydraulic properties and recharge parameters was carried out and documented in ECF-HANFORD-20-0027. Application of version 8.3 of the P2R Model for the purpose of the CA is documented in two separate ECFs (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*). These ECFs provide the basis for the model development and specific application to the CA. Simulations conducted for these calculations rely heavily on the input parameters, assumptions, limitations, and data discussed in the ECFs listed above. It is assumed that the reader is familiar with those ECFs as much of the information is not repeated in this calculation. Rather, this calculation focuses on those parameters and simulation outputs that differ from those utilized in the preceding reports and environmental calculations.

To understand the results of the calculation, a brief description of the NSMC approach is provided in this section. NSMC is an algorithm developed to evaluate uncertainty in numerical model predictions. Application of the algorithm as part of groundwater flow and transport modeling can be achieved through use of the PEST software package (Doherty, 2016, *PEST Model-Independent Parameter Estimation User Manual: 6th Edition*) that was used as part of the calibration of the P2R Model version 8.3. This section provides a broad description of what an NSMC evaluation entails by briefly describing traditional Monte Carlo evaluation, the differences between the traditional approach and NSMC, and describe how simulation outputs can be used to understand uncertainty. Details regarding the theory behind NSMC are described in various reports including Doherty et al., 2010, *Approaches to Highly Parameterized Inversion: A Guide to Using PEST for Model-Parameter and Predictive-Uncertainty Analysis*, and Tonkin and Doherty, 2009, "Calibration-constrained Monte-Carlo analysis of highly parameterized models using subspace techniques."

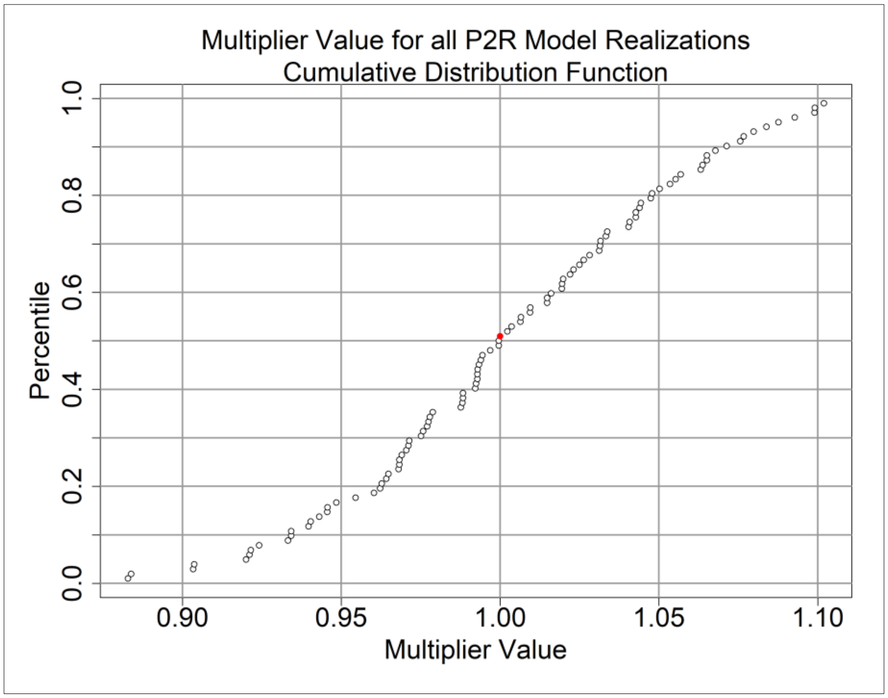
2.1 Traditional Monte Carlo Evaluation

Monte Carlo analysis of a mathematical model includes the creation of variant models by sampling the statistical distributions of input parameters and executing the simulations to produce model outputs (Metropolis, et al., 1953, "Equation of State Calculations by Fast Computing Machines"; Hastings, 1970, "Monte Carlo sampling methods using Markov chains and their applications"; Metropolis, 1987, "The beginning of the Monte Carlo method"). The variation of model inputs result in variations of model outputs that can be used to develop a statistical representation of the simulation results rather than relying only on a deterministic model result. To produce the simulation results necessary for describing the statistics of the output, sampling the input parameter set is typically done hundreds to thousands of times. This is because each sampled input parameter is created at random and is equiprobable to the other model variants.

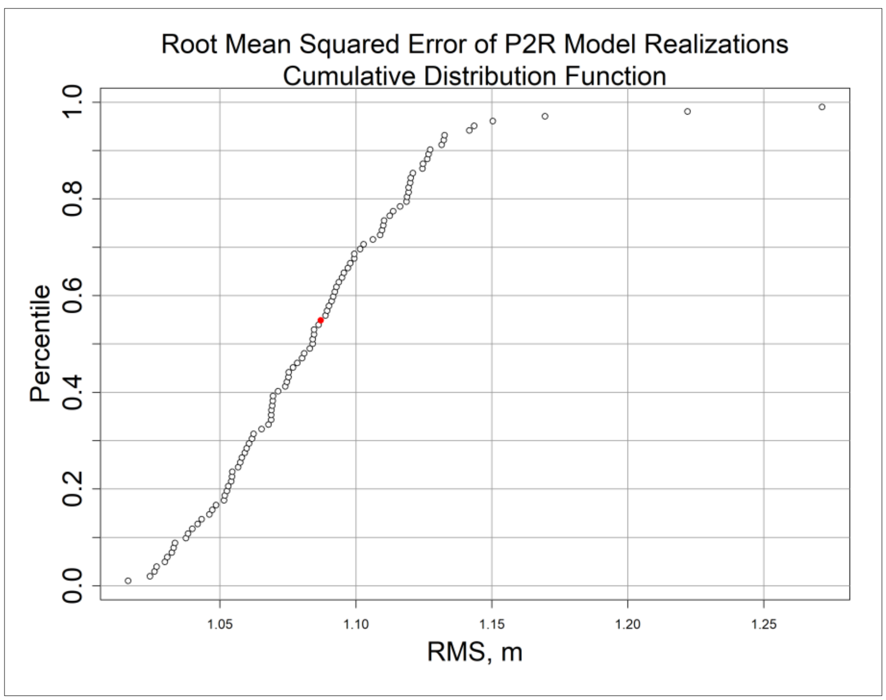
In numerical models, like the P2R Model, where large numbers of input parameters are utilized, the Monte Carlo approach can become difficult to manage. When many input parameters can be varied the traditional Monte Carlo approach can require increased computer resources to store and produce the simulation output. For the calibration of the P2R Model, 1,058 parameters were used to determine the best match to the historic observation data. Thus, for a traditional Monte Carlo Approach where a thousand realizations are not out of the ordinary, the process could require a million simulations in the case of the P2R Model. Furthermore, perturbing any of these parameters in a random fashion does not guarantee a parameter set that produces a reasonable set of inputs, which is well-posed with respect to the governing equations. Unreasonable parameter sets can result in nonconvergence and unusable simulation outputs. Thus, many variant models are typically needed to ensure at least some of the parameter sets produce usable output. Large numbers of variant parameter sets coupled with many input parameters required by traditional Monte Carlo approach can make it infeasible in many cases.

2.2 NSMC Evaluation

The NSMC simplifies the traditional Monte Carlo approach by reducing the number of simulations needed to represent the statistical distributions of the model results. The reduction is achieved by utilizing the information gathered through the calibration process. Automated parameter estimation, as used in the development of the P2R Model, records information regarding changes in input parameters and the effect of those changes on the match to observation values. In the NSMC, the recorded parameter information is used to sample input parameters in such a fashion that each perturbation of the input parameter set results in a model that does not invalidate the calibration with respect to the historic observation data. The initial variant input parameter sets are further adjusted using automated calibration techniques so the statistical match between observed and simulated heads are similar within a specified tolerance. Once the final set of parameter variants are created, each of the models can be executed and the simulation results can be compared to quantify the uncertainty in the model results. Even though the variant simulations each produce a statistically similar calibration, the variation in the inputs and outputs represent ranges of values that are possible while still approximating historical observations. Empirical cumulative distribution functions (ECDF) can be illustrative of the range of variation that exists amongst the set of calibrated models. Figure 1 (insets a and b) show an ECDF of multiplier applied to total recharge flux in the P2R Model and the ECDF of the root mean squared error, respectively, of each simulation result produced by the variant input parameter sets documented in ECF-HANFORD-20-0027. The plot in Figure 1 (inset b) illustrates the range of values that can still produce simulation results that are reasonably calibrated, ranging from a root mean square error of 1.02 to 1.27 m. The plot also illustrates where the calibrated P2R Model ranks in comparison to the variant simulations by showing the results of the calibration as a red dot on the ECDF.



(a)



(b)

Note: The calibrated simulation is shown as a red dot in both insets a and b.

Figure 2. Example ECDFs for (a) Recharge Multiplier and (b) Root Mean Squared Error for with Each of the Variant Simulations Represented as a Separate Point on the Plot

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3 Methodology

Contaminant concentration predictions are simulated using the P2R Model developed using the acquired computer software: the U.S. Geological Survey 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 governing equations of MODFLOW and MT3DMS are solved based on input parameters stored in the model files. The results of the NSMC documented in ECF-HANFORD-20-0027 can be utilized to quantify uncertainty in the simulation results from the CA base case F&T simulations (ECF-HANFORD-19-0120). The steps for generating the variant groundwater flow and F&T simulations to evaluate the P2R Model predictive uncertainty are as follows:

1. Create 100 variant groundwater flow simulations by combining the base case flow simulation (ECF-HANFORD-19-0119) with the model files developed in ECF-HANFORD-20-0027.
   a. Generate 100 copies of the base case groundwater flow simulations.
   b. Adjust each copy of the simulation files for hydraulic conductivity, specific storage, and specific yield to link to the files for the 100 variant simulations documented in ECF-HANFORD-20-0027.
   c. Generate recharge input files matching the CA base case flow simulation temporal domain that match the 100 variant parameters for mountain front and ancillary anthropogenic recharge as well as the overall multiplication factor.
   d. Execute the 100 variant simulations.
   e. Determine any simulations that did not successfully converge and remove them from the set of 100 variant simulations.
2. Simulate F&T using the CA base case simulation files from each of the variant simulations used to generate the groundwater flow field created in the previous step.
   a. Select the contaminants of concern that will be simulated as part of the NSMC application to the CA base case.
   b. Adjust the flow link package to be used by the transport simulation to the correct flow simulation for all variant F&T models.
   c. Based on the simulated hydraulic head from the variant flow simulation, adjust the continuing source term input files to assign the uppermost layer that stays saturated for the entire simulation as the location for the source entering the saturated zone for each row and column in the model.
   d. Create tables and figures that illustrate the variability in the predicted concentrations:
      i. Create a table that illustrates the uncertainty of simulated peak concentration. The table includes the peak concentration of the base case and the highest and lowest value from the variant simulations at the time of the peak calculated in the base case.
      ii. Illustrate the variability in the predicted concentrations through the creation of "horse-tail" plots of peak concentration (see Section 6).

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. Parameter sets representing the 100 variant flow simulations from the NSMC evaluation are documented in ECF-HANFORD-20-0027. Only two types of alterations to these input data were required for this environmental calculation: construction of predictive recharge packages for each of the 100 variant flow simulations and alteration of model layer assignments for the continuing source terms created for the CA base case, documented in ECF-HANFORD-19-0120. Descriptions of the source of inputs documented in other reports, the creation of the variant recharge packages, and the alteration of continuing source term layer assignment are found in the following sections.

4.1 Input Data Source

The input parameters used for the NSMC application to the CA base 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. Most of the input parameters for the NSMC flow and F&T simulations are kept the same as the CA base case model, except for the hydraulic properties and recharge rates. More detailed descriptions of the model inputs and assumptions for the NSMC flow and F&T simulations are given in Table 1.

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

Input Type	Input Parameters	Description	Document
Flow Simulation Information			
Model Extents and Discretization	Active Model Domain	The domain and spatial discretization do not change for any variant model.	CP-57037, Section 4.2.1
	Spatial Discretization		CP-57037, Sections 4.2.2 and 4.2.3
	Temporal Discretization	No change between the CA base case and any of the 100 variant simulations.	ECF-HANFORD-19-0120, Section 4.2
Hydraulic Properties	Hydraulic Conductivity, Specific Storage, and Specific Yield	The CA base case hydraulic properties are the same as the calibrated P2R Model. For each variant model, the hydraulic properties are identical to the properties of the 100 variant simulations documented in ECF-HANFORD-20-0027.	CP-57037, Section 4.2 and ECF-HANFORD-20-0027, Attachment B Figures
	May-Junction Fault Hydraulic Characteristic	No changes made to the hydraulic characteristic in any model	CP-57037, Section 4.4.2
Sources and Sinks	Injection/Extraction Rates	Rates match the assumptions presented as part of the CA base case.	ECF-HANFORD-19-0119, Section 4.4
	Columbia River Stage and Bottom Elevation	River stage and bottom elevation match the inputs from the CA base case.	CP-57037, Section 4.4.3 and ECF-HANFORD-19-0119 Section 4.2.1

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

Input Type	Input Parameters	Description	Document
Boundary Conditions	Natural and Anthropogenic Recharge*	Approach to defining recharge is the same as the CA base case. Alterations to the inputs based on the NSMC results are discussed in Section 4.2 of this ECF.	CP-57037, Section 4.4.3 and ECF-HANFORD-19-0119, Section 4.2.3
	Specified Head Boundaries	Specified heads match the assumptions presented as part of the CA base case.	ECF-HANFORD-19-0119, Section 4.2.2
Fate and Transport 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 all model variants as part of the NSMC application to the CA base case.	ECF-HANFORD-19-0120, Section 4.3.1
Aquifer Properties	Effective Porosity and Bulk Density		ECF-HANFORD-19-0120, Section 4.3.2.1
Adsorption and Decay	Linear Adsorption and Radioactive Decay Constants		ECF-HANFORD-19-0120, Section 4.3.2.2
Dispersion	Longitudinal, Transverse, and Vertical Dispersivity		ECF-HANFORD-19-0120, Section 4.3.3
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 and all variant simulations. Changes made to the model layer assignments are described in Section 4.3 in this ECF.	ECF-HANFORD-19-0120, Section 4.3.4

* Portions of the inputs are changed for the application of this environmental calculation and are discussed in Sections 4.2 and 4.3 of this ECF.

Note: Complete reference citations are provided in Section 8 of this ECF.

CA = composite analysis
ECF = environmental calculation file
NSMC = null space Monte Carlo
P2R = Plateau-to-River

4.2 Variant Recharge Input Parameters

Recharge at the water table in the P2R Model includes the contributions to total recharge from the following components:

- **Natural recharge:** Deep percolation of precipitation that is not evaporated/transpired and is not retained in storage in the vadose zone.
- **Mountain-front recharge:** Contribution to the groundwater flux from upgradient sources to the aquifer including Rattlesnake Mountain and the Dry Creek and Cold Creek watersheds (see Figure 1).
- **Anthropogenic recharge:** Historical wastewater discharges at the Hanford Site.

For each stress period of the model, these individual components are summed to create the total recharge to the aquifer. The summed values are input into a MODFLOW recharge package for inclusion in the model simulation. The recharge components for the NSMC application to the CA base case are consistent with the methodologies documented in CP-57037 and ECF-HANFORD-19-0119. Changes were made to values in the recharge package based on the 100 variant NSMC simulations documented in ECF-HANFORD-20-0027. Table 2 provides a statistical summary of the values used for the variant simulations. Recharge parameters that were allowed to differ as part of the NSMC included the following:

- The recharge array multiplication factor scaled the total recharge at each timestep of the CA base case simulation. The value ranged from 0.88 to 1.10 times the calibrated value of 1.0.
- Recharge parameters representing mountain-front recharge were adjusted from the value used in the CA base case to match the values from each 100 variant simulations documented in ECF-HANFORD-20-0027. Locations receiving mountain-front recharge included Rattlesnake Mountain, Cold Creek or Dry Creek areas shown as specified flux locations in Figure 1. Minimum, maximum, and average values of mountain-front recharge for each of the three areas are shown in Table 2.
- Ancillary anthropogenic recharge variant simulation results were applied to cells designated in the model in the 200 East and 200 West Areas. The minimum, maximum, and average values of ancillary recharge are shown in Table 2.

4.3 Alteration of Continuing Source.

An adjustment was made to the MODFLOW/MT3D model layer assignment for the continuing source term. The adjustment was necessary to align the model layer assignment to the simulated groundwater flow field from each of the variant NSMC simulations. The CA base case saturated zone simulations utilized the Hydrocarbon Spill Source (HSS) package to simulate continuing activity flux from the vadose zone to the saturated zone over time. Although named for use with hydrocarbons, the package does not explicitly simulate only hydrocarbon sources. It can be used for any contaminant. As part of the input the model layer at each model row and column must be specified as the location for injecting contaminant mass from the vadose zone to the aquifer. For the CA base case, the mass is injected in the uppermost layer that stays active throughout the simulation. The same approach is used for the NSMC variant simulations. However, because the flow simulations differ in hydraulic properties and recharge, the model layer that stays active from location to location can change. Thus, for each variant simulation the HSS package was altered so the uppermost model layer that remained active throughout the simulations was correctly assigned.

Table 2. Statistical Summary of 100 Variant Model Recharge Parameters Used in NSMC

Recharge Parameters	Units	Calibrated Value	Minimum	Maximum	Average
Overall Recharge Multiplication Factor	--	1.00	0.882835	1.102000	1.004868
Ancillary Anthropogenic Recharge					
200 East Area	mm/yr	130	0.731	146	60.2
200 West Area	mm/yr	9	0.731	18.3	2.37
Mountain-Front Recharge					
Dry Creek	mm/yr	1,727	95	2,036	1,276
Cold Creek	mm/yr	667	48	1,363	705
Rattlesnake Mountain	mm/yr	197	67	391	246

5 Software Applications

MODFLOW, MT3DMS, Excel®, ArcGIS®, and R software programs were used for this calculation. MODFLOW and MT3DMS are 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. A copy of the *Software Installation and Checkout Form* for the MT3DMS installation used for this calculation is provided in Attachment A to this ECF.

The GAIA F&T Modeling Platform, owned by CPCCo and operated by Mission Support Alliance, consists of 12 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/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.

® Excel is a registered trademark of the Microsoft Corporation in the United States and other countries.

® ArcGIS is a registered trademark, or service mark, of ESRI in the United States, the European Community, or certain other jurisdictions.

® Dell and PowerEdge are registered trademarks of the Dell Corporation, Round Rock, Texas.

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

5.1 Approved Software

For approved calculation software used in this calculation, the required descriptions are provided below.

5.1.1 Description

MODFLOW

- **Software Title:** MODFLOW
- **Software Version:** CHPRC Build 0008 (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:** GAIA F&T Modeling Platform, DOE #WF43109
- **Authorized User:** S. Tomusiak
- **CPCCo 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 Build 8*
  - CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report: CHPRC Build 8*

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:** GAIA F&T Modeling Platform, DOE #WF43109
- **Authorized User:** S. Tomusiak
- **CPCCo 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 Build 8*
- CHPRC-00261, *MODFLOW and Related Codes Acceptance Test Report: CHPRC Build 8*

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 A to this ECF.

5.1.3 Statement of Valid Software Application

The preparers of this calculation attest that the software identified above, and used for the calculations described in this calculation, 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 MT3DMS are graded is Level C software, use of this software is required to be logged in the HISI. Accordingly, this environmental calculation has been logged by the software owner in the HISI under Identification Numbers 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 set of simulations created to support the NSMC application to the CA base case includes simulations for nine contaminants of potential concern (COPCs) using 96 variant simulations. This section describes the organization and execution of the simulation sets, and the figures and charts that describe the results obtained.

6.1 Simulation Organization

Simulations developed in support of the NSMC application to the CA base case were grouped based on variant flow simulation established during the NSMC documented in ECF-HANFORD-20-0027. Each of the 100 variant hydraulic properties and recharge parameter sets documented in ECF-HANFORD-20-0027 were assigned a unique numeric value from 0 to 99. The simulation files were organized by simulation under separate directories using the naming convention of “nsXX,” where “ns” means “null-space” and “XX” represents the unique numeric value assigned to the input parameter set 0 to 99. Flow simulations were conducted for each variant set. The 100 flow simulations were executed and evaluated to ensure each simulation completed successfully. As is common with Monte Carlo based analysis several of the 100 variant simulations resulted in parameter sets that were ill-posed to converge on a solution to the flow simulation. These were “ns12,” “ns27,” “ns49,” and “ns58.” Due to the nonconvergence on a solution, these parameter sets were removed from the analysis resulting in a total of 96 variant flow simulations that were used to simulate F&T.

A total of 16 COPCs were identified for the CA base case. However, results from the base case indicated that several of the original 16 would not significantly contribute to the final dose calculation. Concentration cutoff levels for each contaminant to assess whether the concentration was included in the final dose calculation were determined as part of Section 5.3.2.1 in DOE/RL-2019-52, *Composite Analysis for Low-Level Waste Disposal in the Hanford Site (FY 2020)*. Therefore, only nine COPCs were simulated, tritium, carbon-14, chloride-36, iodine-129, technetium-99, uranium-233, uranium-234, uranium-235, and uranium-238. Table 6-1 shows a comparison of the peak concentration at or beyond the compliance boundary for all 16 COPCs to the calculated cutoff values. The table also describes the reason for excluding those COPCs that were not included in the NSMC application to the CA base case.

Table 3. Comparison of Estimated Concentration from the CA Base Case to the Dose Calculation Cutoff Concentration

COPC	Cutoff (pCi/L)	Peak at or Outside Compliance Boundary	Reason for Exclusion
Carbon-14	4.24E+01	2.47E+03	--
Chlorine-36*	7.21E+00	7.83E-01	Peak concentration below cutoff
Tritium	6.25E+02	4.46E+05	--
Iodine-129	1.28E-01	7.36E+00	--
Neptunium-237	3.31E-01	9.56E-03	Peak concentration below cutoff
Radium-226	8.11E-02	1.73E-05	Peak concentration below cutoff
Strontium-90	3.03E-01	1.37E+02	Limited geographic impact/peak occurs from initial condition
Technetium-99	3.56E+01	2.27E+03	--
Thorium-230	1.19E-01	4.55E-07	Peak concentration below cutoff
Uranium-232	6.25E-02	1.78E-03	Peak concentration below cutoff
Uranium-233*	6.82E-01	1.68E-01	Peak concentration below cutoff
Uranium-234	7.08E-01	1.25E+01	--
Uranium-235*	7.43E-01	5.66E-01	Peak concentration below cutoff
Uranium-236	7.50E-01	1.08E-01	Peak concentration below cutoff
Uranium-238	7.21E-01	3.48E+02	--

*Although not required to be included based on concentration cutoff, simulations for these COPCs were conducted based on an initial evaluation and results are included as part of the analysis.

6.2 Assessing Plume Migration for Existing Plumes

The NSMC simulated concentrations from the 96 variant model and nine COPCs mentioned previously were processed to create a set of figures to illustrate the variability in estimated peak concentration. The P2Rv8.3 Model extent was subdivided into three zones as a means of presenting plume migration from the Central Plateau towards the Columbia River. These zones are based on the boundary CA Compliance Boundary of the Hanford Central Plateau (Figure 3). The three zones are designated signifying the areas within the CA Compliance Boundary (Within_Boundary), at the CA Compliance Boundary (At_Boundary), and the remaining modeled extent of the Hanford Site (Beyond_Boundary). Peak concentration (pCi/L) time-series plots are generated for each zone and COPC conducted as part of this calculation, including the NSMC sensitivity variants as well as the base case (total of 27). The CA base case results are also shown in red overlying the results of all 96 variant F&T simulation results. Peak concentration is defined as the maximum concentration at any point within a zone for a given point in time. Figure 4 provides an example time-series plot for technetium-99 peak concentration values for the ”Beyond_Compliance_Boundary” zone. A full set of figures for all of the COPCs and zones is included in Attachment B.

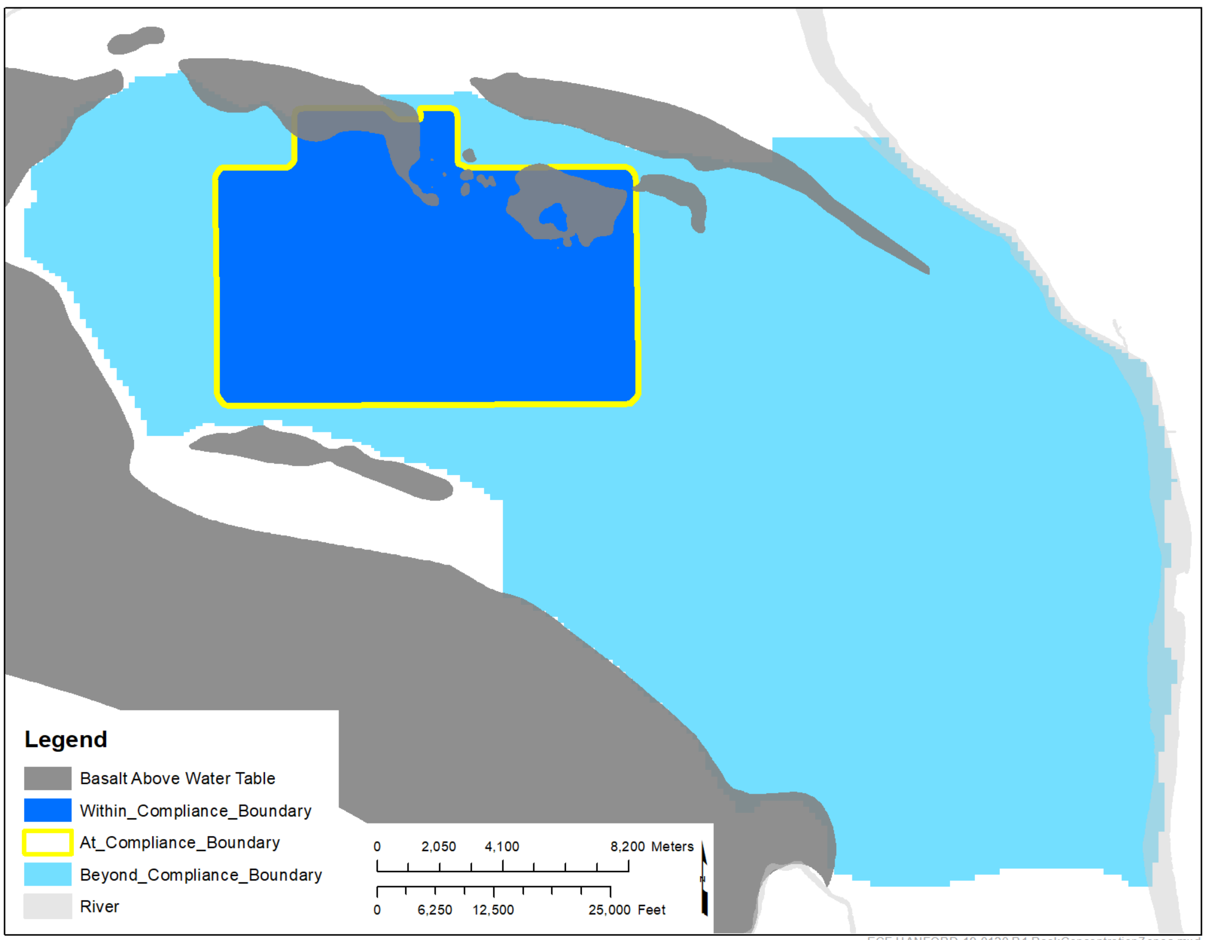

Figure 3. P2R Version 8.3 Peak Concentration Summary Zonation Extents

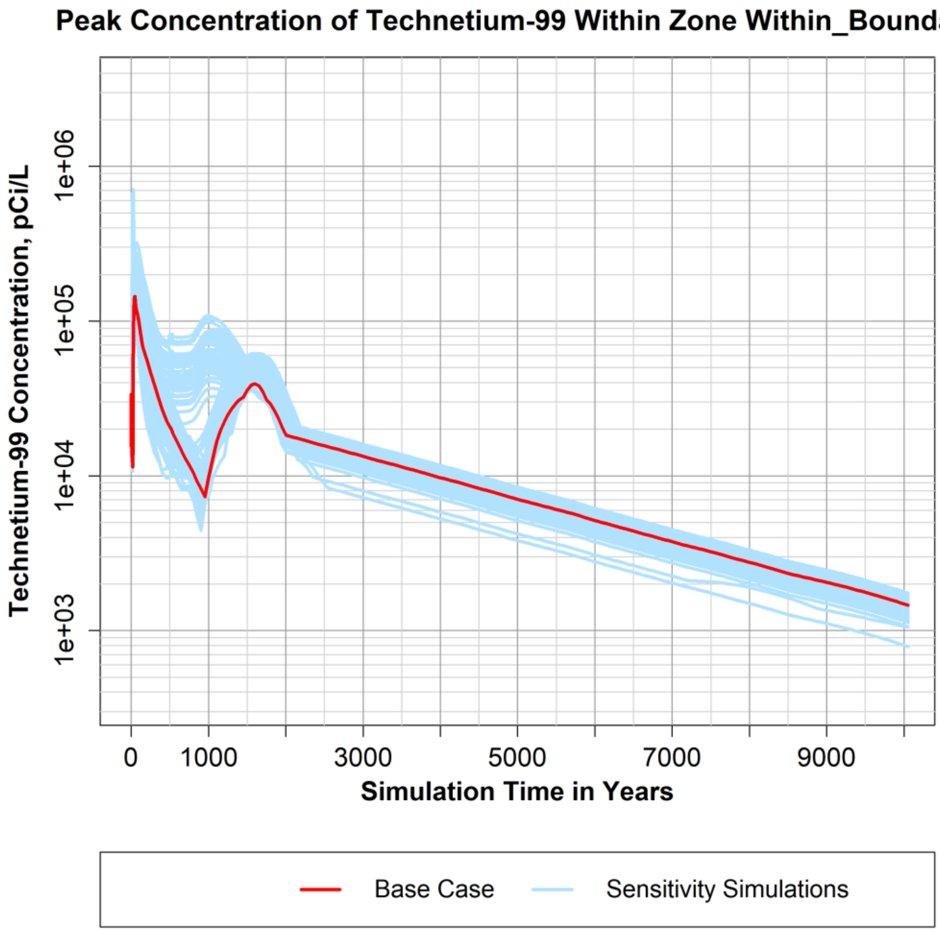

Figure 4. Simulated Maximum Concentrations of Technetium-99 Over Time Within the "Within_Compliance_Boundary" Zone from the P2R Model Version 8.3 for the CA Base Case (red) Overlying the NSMC Variant Simulation Results (Blue)

7 Results/Conclusions

NSMC analysis results consist of a series of graphics and tables showing the simulated outputs from the 96 variant simulations and the CA base case. Horse-tail plots, as described in Section 6.2, are available in Attachment B for the three zones (see Figure 4) and each of the nine COPCs simulated as part of the calculation. Table 4 summarizes the NSMC simulation results including peak concentration and the time they occurred for each of the three zones. The table also presents the highest and lowest value from all 96 variant simulations at the time the base case peak occurred.

Table 4. Summary of NSMC Simulation Results Illustrating the Variation in Peak Concentration Described by the Inner and Outer Area Boundaries on the Central Plateau of the Hanford Site

Zone	COPC	Iodine-129	Technetium-99	Tritium
Beyond_Boundary	Time, years	0	0	0
	Base case, pCi	7.36E+00	1.78E+03	4.46E+05
	Maximum of variants, pCi	7.36E+00	1.78E+03	4.46E+05
	Minimum of variants, pCi	7.36E+00	1.78E+03	4.46E+05
At_Boundary	Time, years	9	0	5
	Base case, pCi	3.86E+00	2.27E+03	3.87E+04
	Maximum of variants, pCi	4.13E+00	2.27E+03	5.27E+04
	Minimum of variants, pCi	2.83E+00	2.27E+03	2.86E+04
Within_Boundary	Time, years	10052	45	19
	Base case, pCi	1.11E+03	1.44E+05	3.90E+06
	Maximum of variants, pCi	1.33E+03	2.78E+05	4.19E+06
	Minimum of variants, pCi	6.04E+02	9.30E+04	2.27E+06
Zone	**COPC**	**Uranium-238**	**Uranium-233**	**Uranium-234**
Beyond_Boundary	Time, years	0	30	60
	Base case, pCi	3.48E+02	1.60E-01	1.24E+01
	Maximum of variants, pCi	3.48E+02	3.25E-01	1.33E+01
	Minimum of Variants, pCi	3.48E+02	4.86E-02	2.24E-01
At_Boundary	Time, years	58	29	59
	Base case, pCi	1.29E+01	1.68E-01	1.25E+01
	Maximum of variants, pCi	1.37E+01	3.25E-01	1.34E+01
	Minimum of variants, pCi	4.55E-01	8.12E-02	1.95E-01
Within_Boundary	Time, years	2.74E-05	112	1502
	Base case, pCi	1.24E+03	1.44E+01	8.41E+02
	Maximum of variants, pCi	1.24E+03	2.53E+01	1.18E+03
	Minimum of variants, pCi	1.24E+03	4.85E+00	2.10E+02

Table 4. Summary of NSMC Simulation Results Illustrating the Variation in Peak Concentration Described by the Inner and Outer Area Boundaries on the Central Plateau of the Hanford Site

Zone	COPC	Uranium-235	Carbon-14	Chlorine-36
Beyond_Boundary	Time, years	60	117	1502
	Base case, pCi	5.60E-01	2.35E+03	7.52E-01
	Maximum of variants, pCi	6.01E-01	2.49E+03	1.46E+00
	Minimum of variants, pCi	8.60E-03	2.00E+03	6.93E-01
At_Boundary	Time, years	59	80	1502
	Base case, pCi	5.66E-01	2.47E+03	7.83E-01
	Maximum of variants, pCi	6.07E-01	3.85E+03	1.51E+00
	Minimum of variants, pCi	7.48E-03	2.33E+03	7.40E-01
Within_Boundary	Time, years	1502	1352	1452
	Base case, pCi	3.74E+01	6.92E+05	1.27E+03
	Maximum of variants, pCi	5.27E+01	7.65E+05	1.52E+03
	Minimum of variants, pCi	9.33E+00	5.92E+05	6.89E+02

COPC = contaminant of potential concern

8 References

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Attachment A

Software Installation and Checkout Forms for Approved Software Installations

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A1 Introduction

This appendix 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.

A2 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.

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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):

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

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]/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)

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 B

Plots of Simulated Peak Concentration Over Time for Base Case and Sensitivity Simulations

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Figures

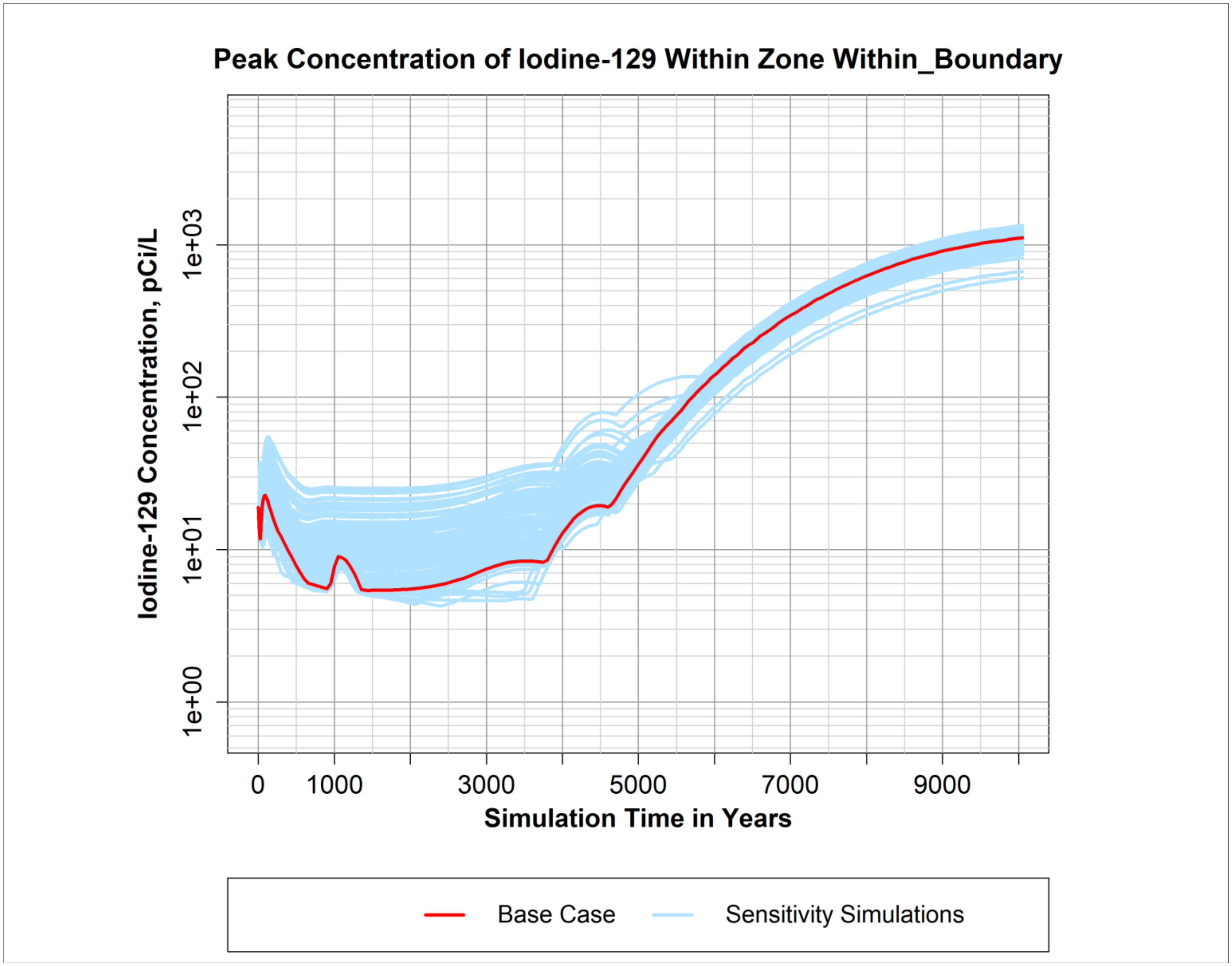

Figure B-1. Peak Simulated Concentration of Iodine-129 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

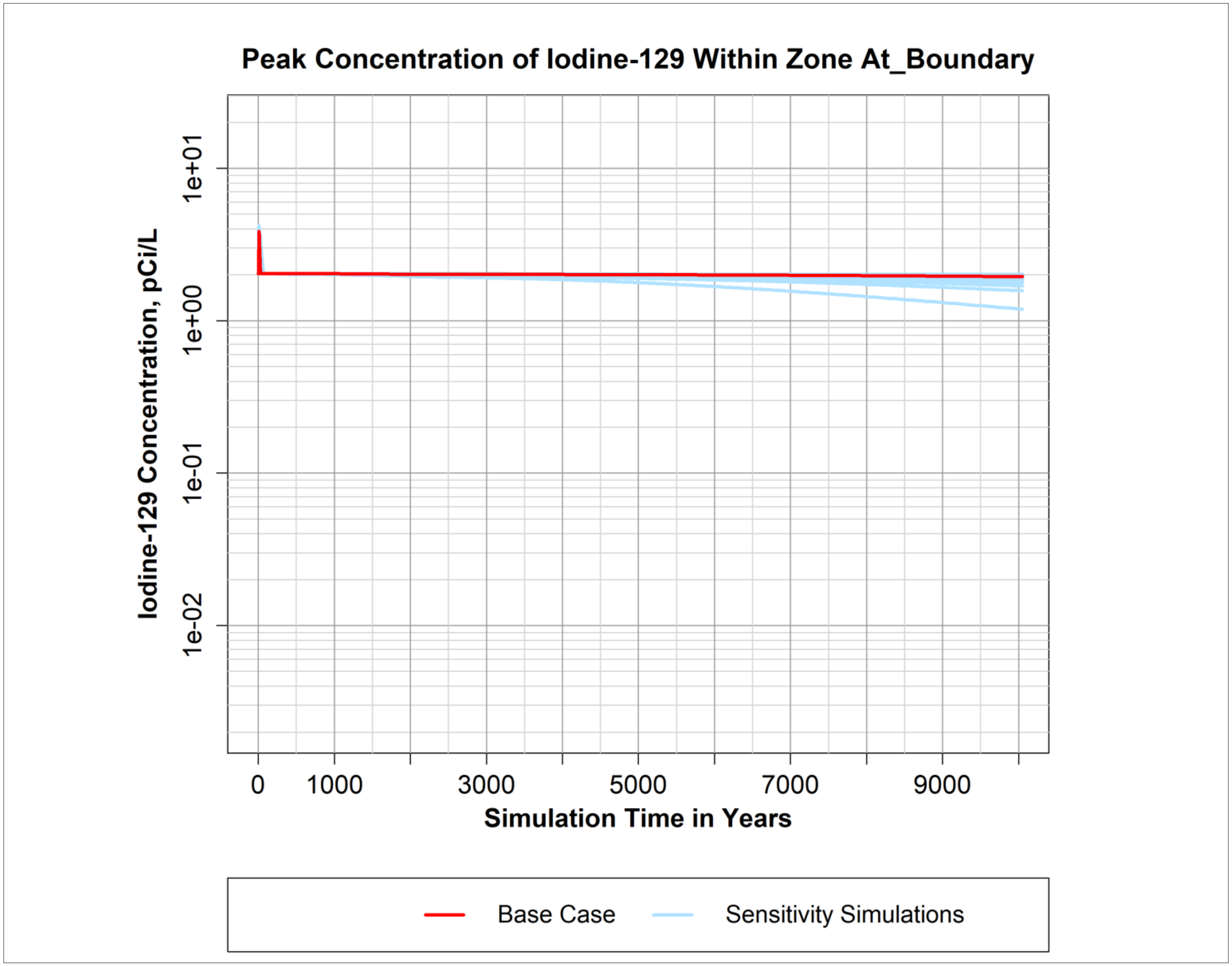

Figure B-2. Peak Simulated Concentration of Iodine-129 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

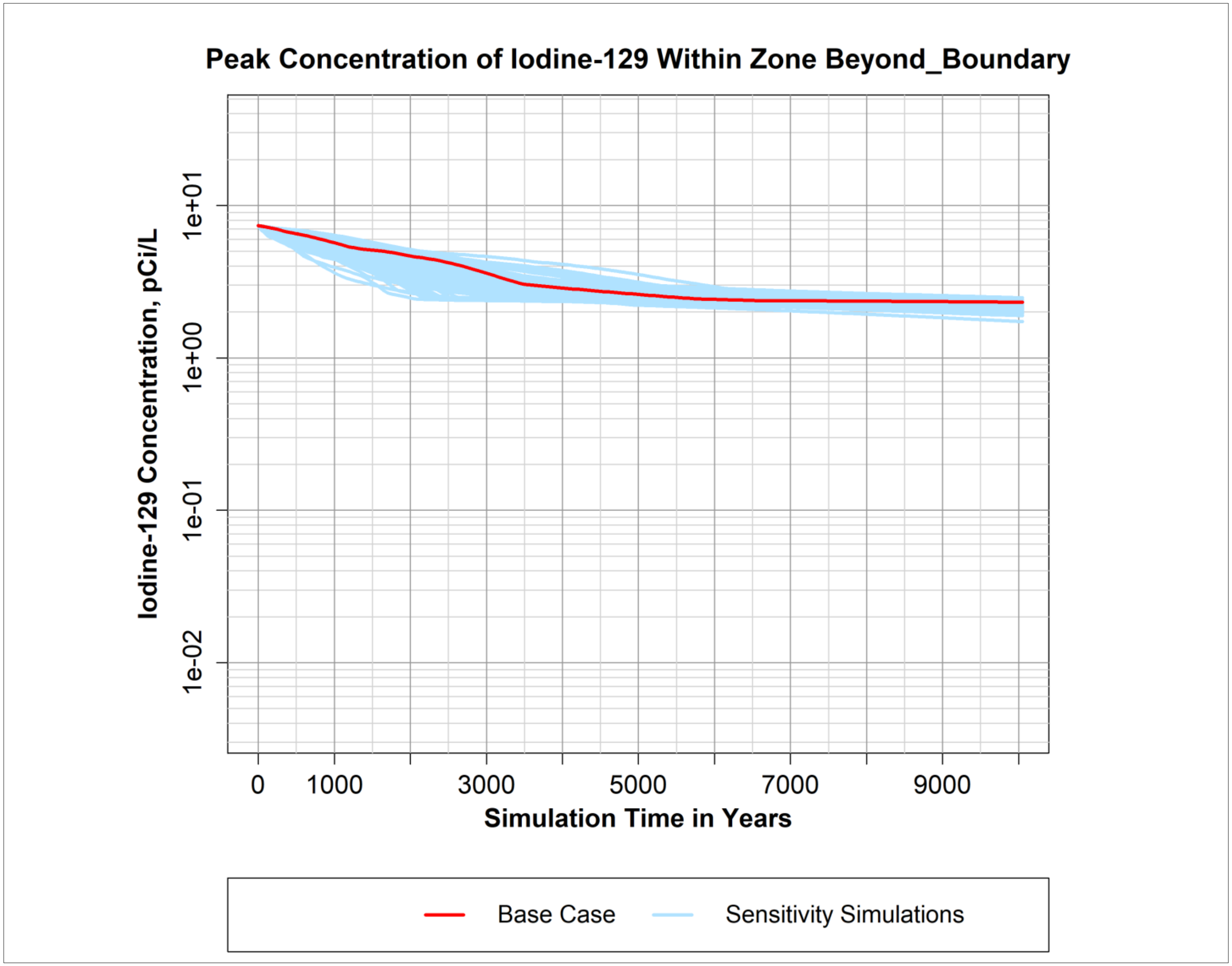

Figure B-3. Peak Simulated Concentration of Iodine-129 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

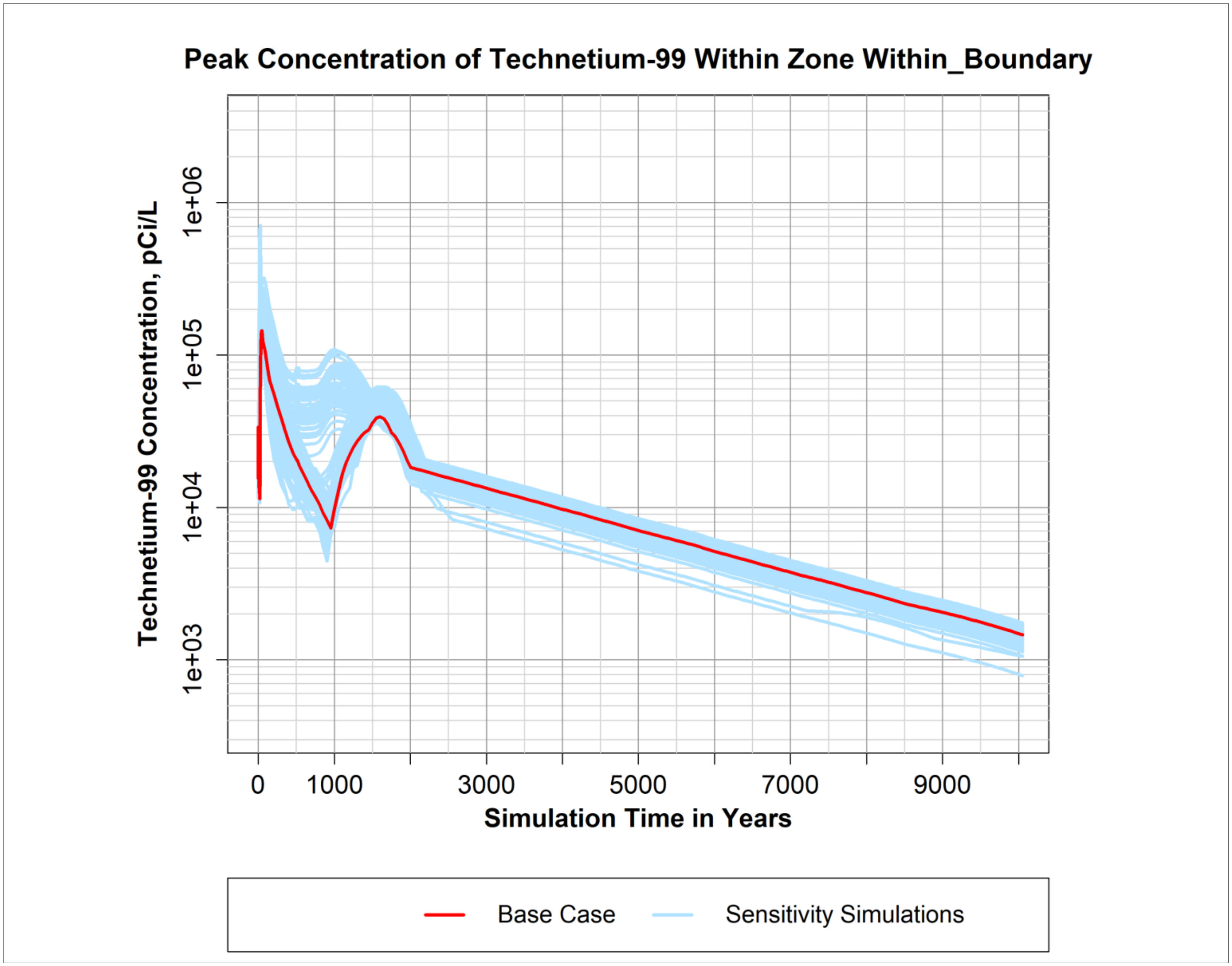

Figure B-4. Peak Simulated Concentration of Technetium-99 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

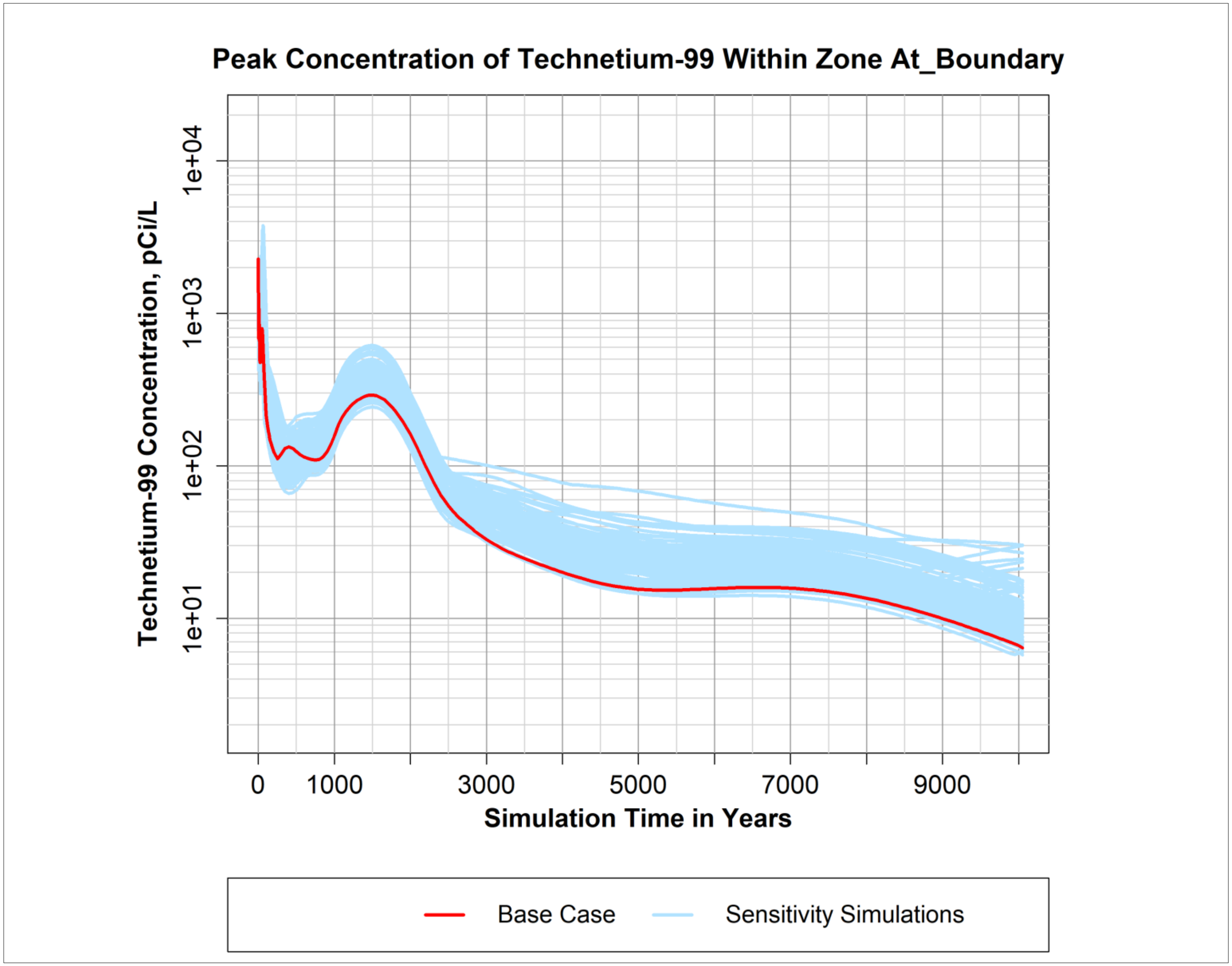

Figure B-5. Peak Simulated Concentration of Technetium-99 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

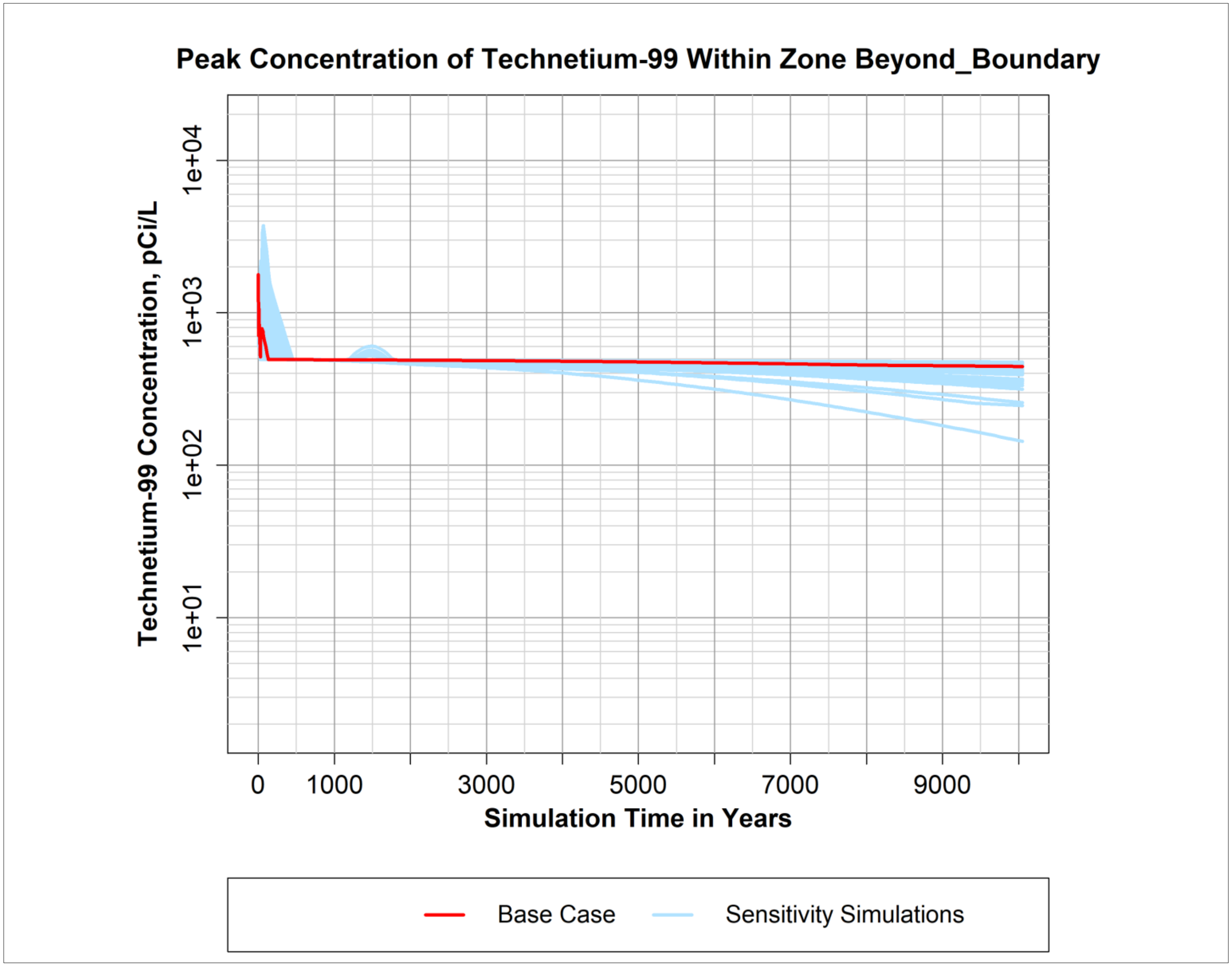

Figure B-6. Peak Simulated Concentration of Technetium-99 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

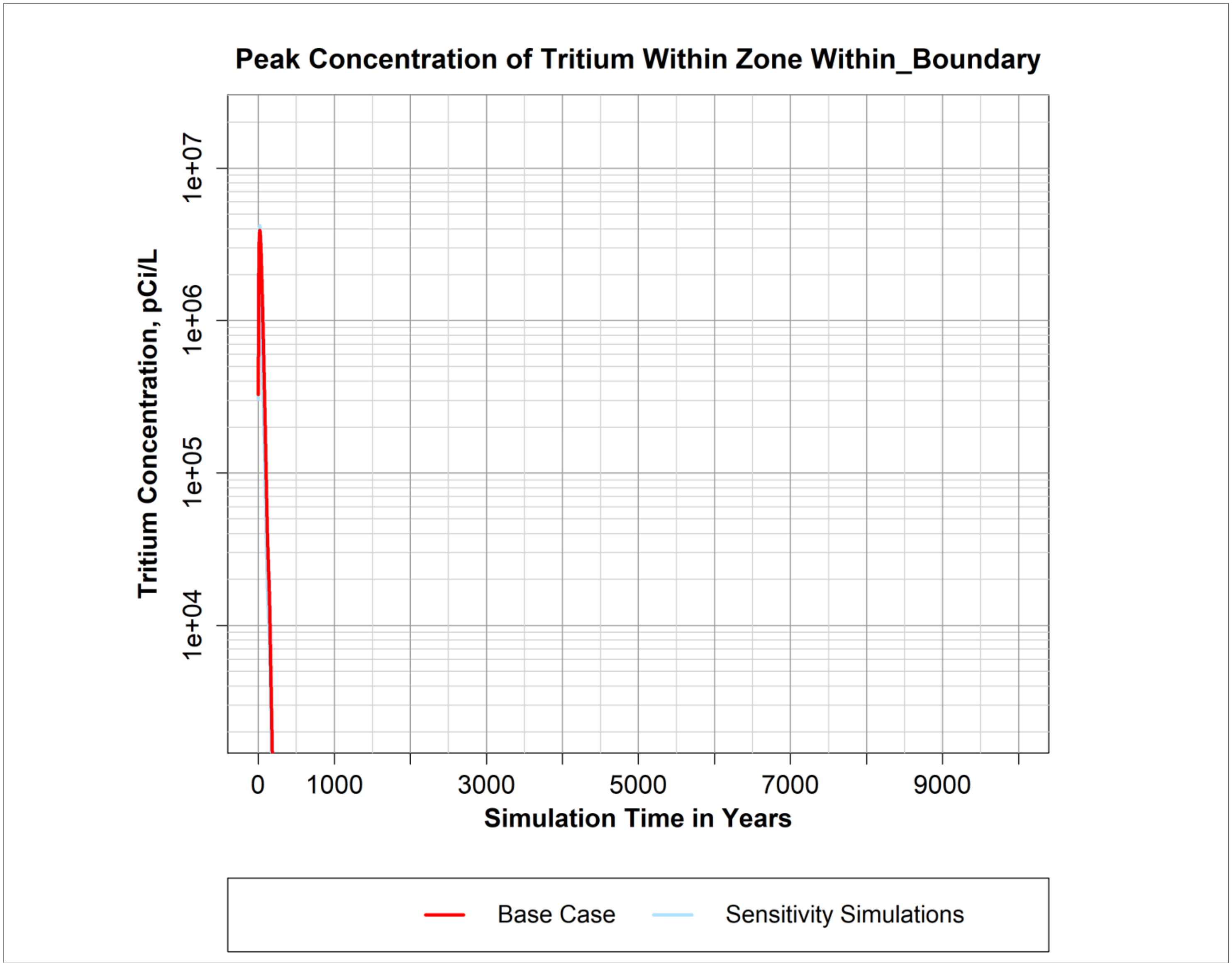

Figure B-7. Peak Simulated Concentration of Tritium Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

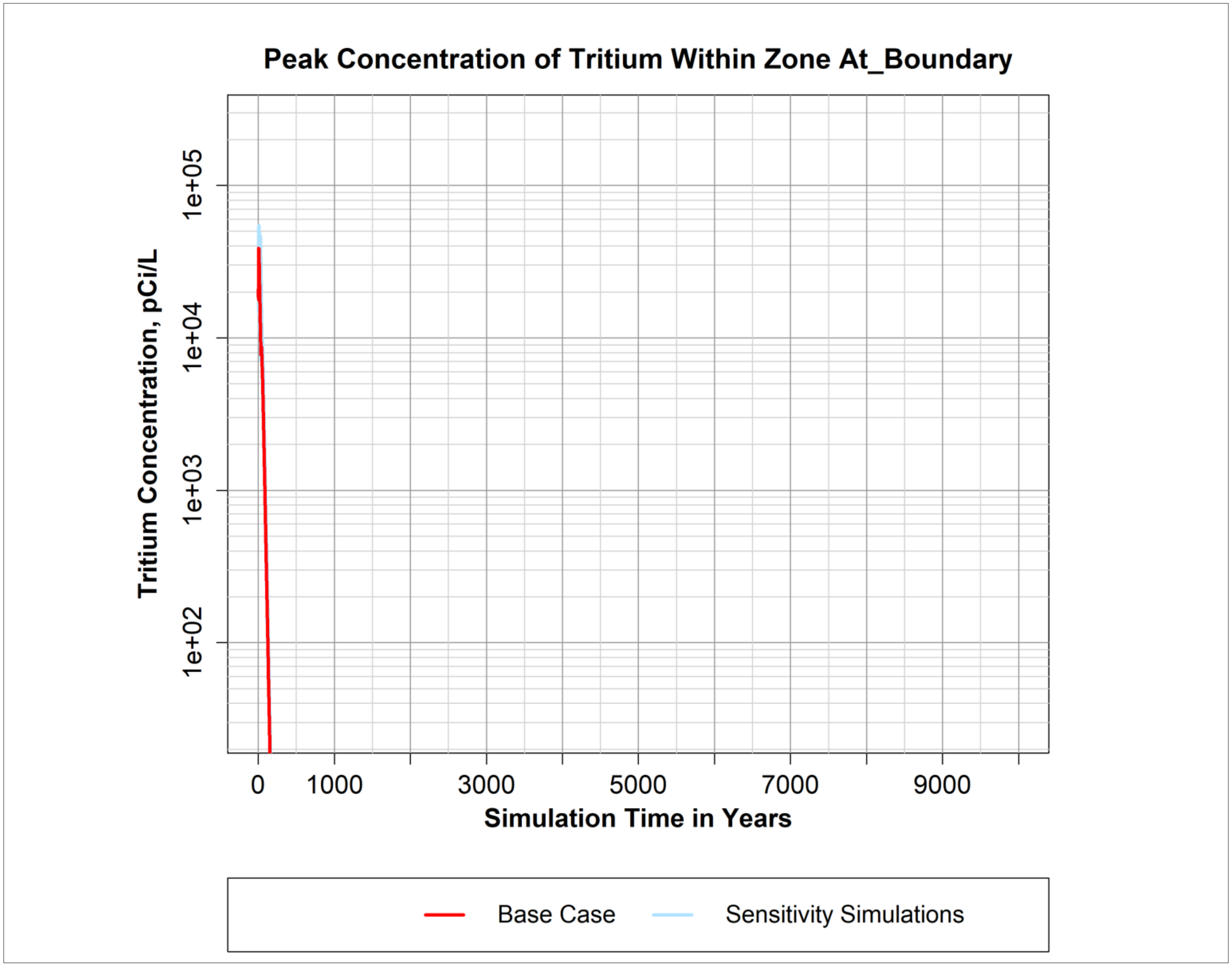

Figure B-8. Peak Simulated Concentration of Tritium Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

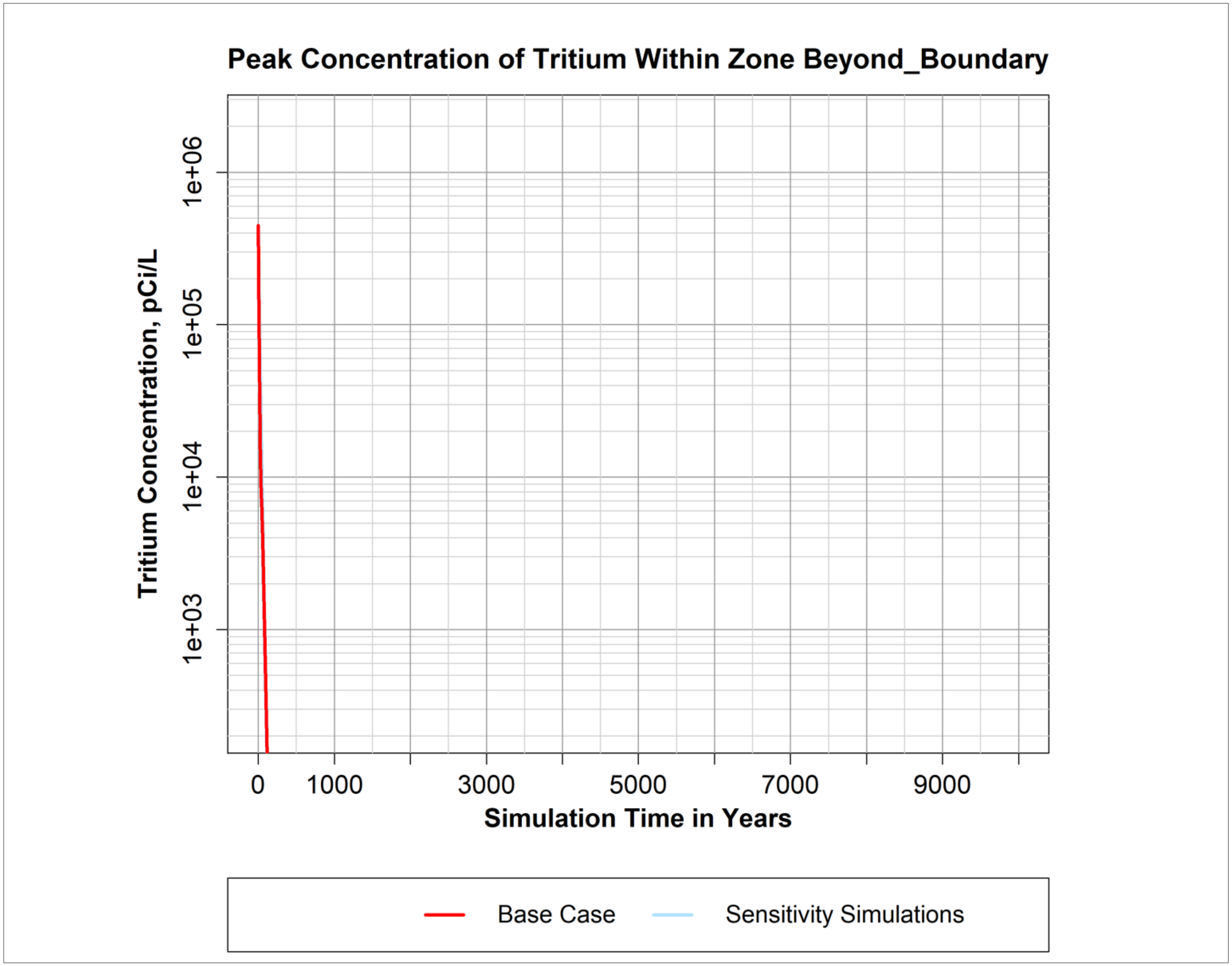

Figure B-9. Peak Simulated Concentration of Tritium Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

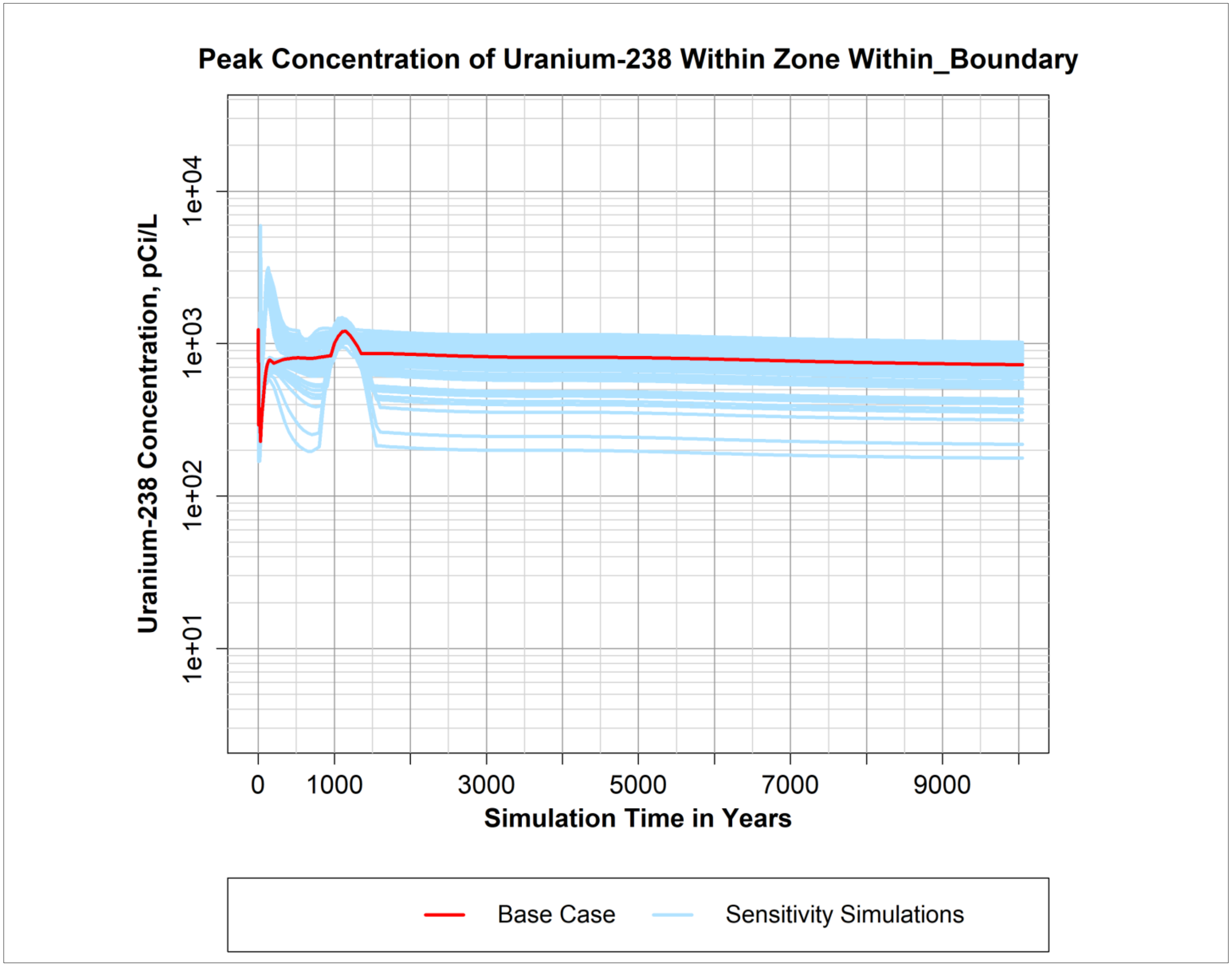

Figure B-10. Peak Simulated Concentration of Uranium-238 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

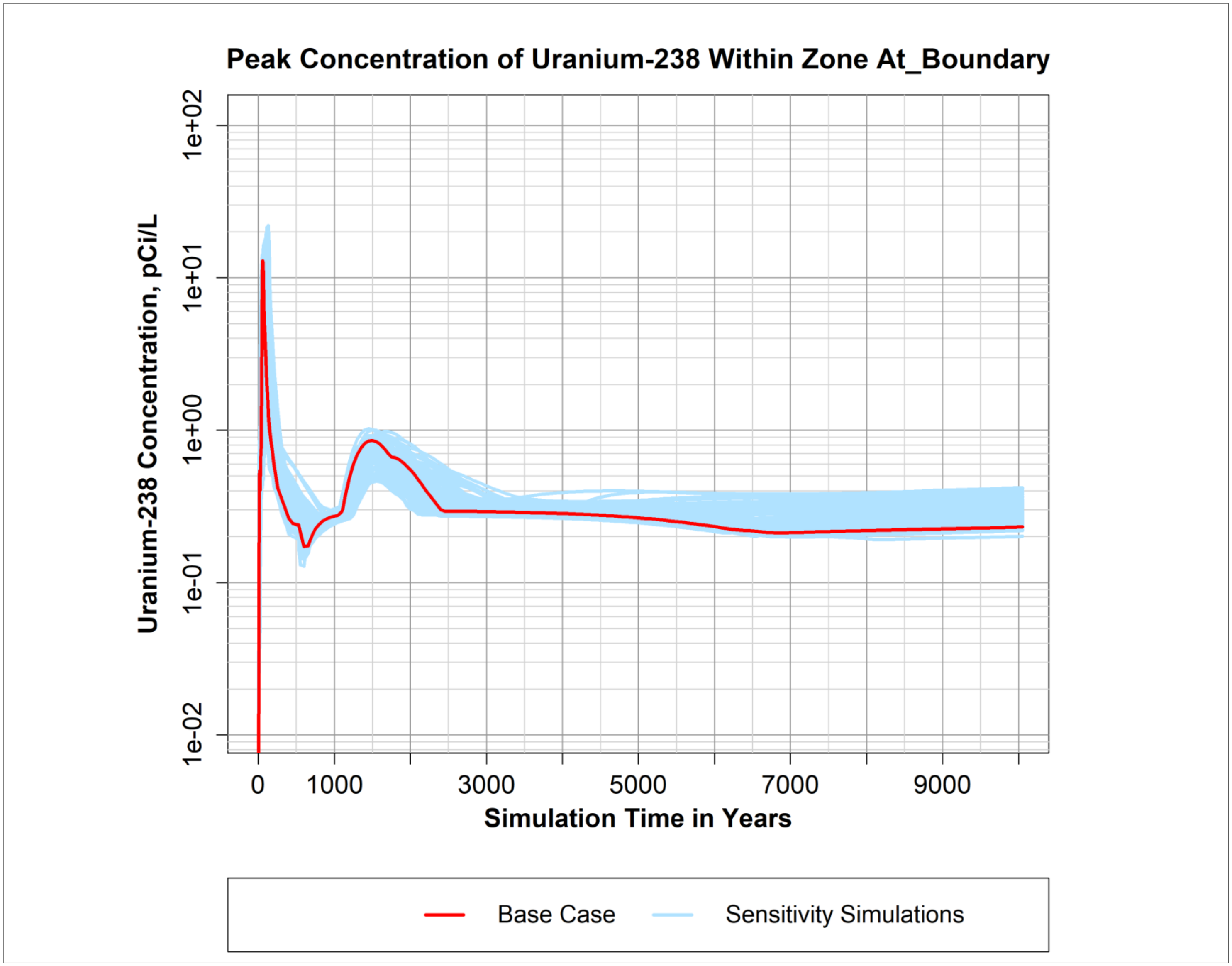

Figure B-11. Peak Simulated Concentration of Uranium-238 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

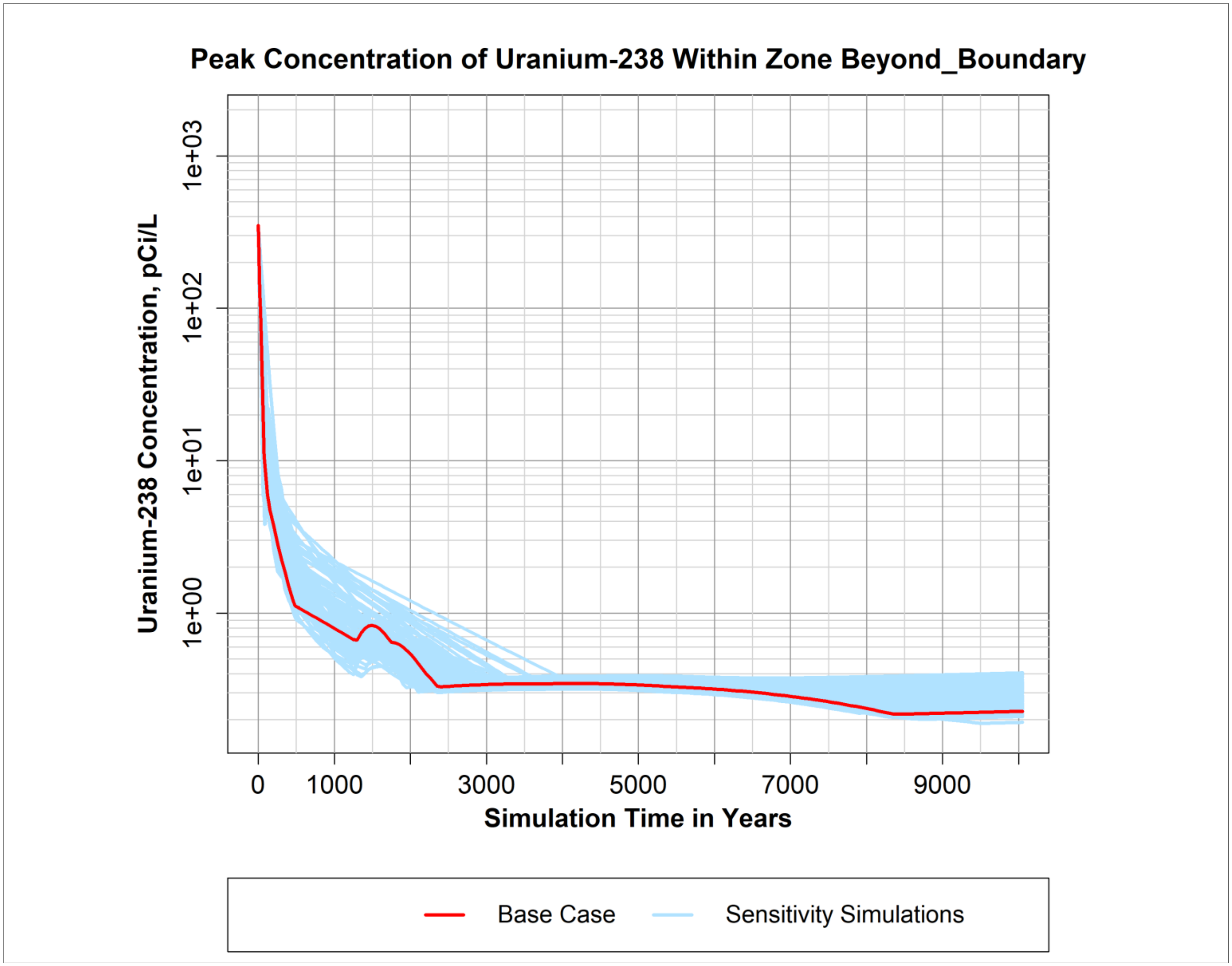

Figure B-12. Peak Simulated Concentration of Uranium-238 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

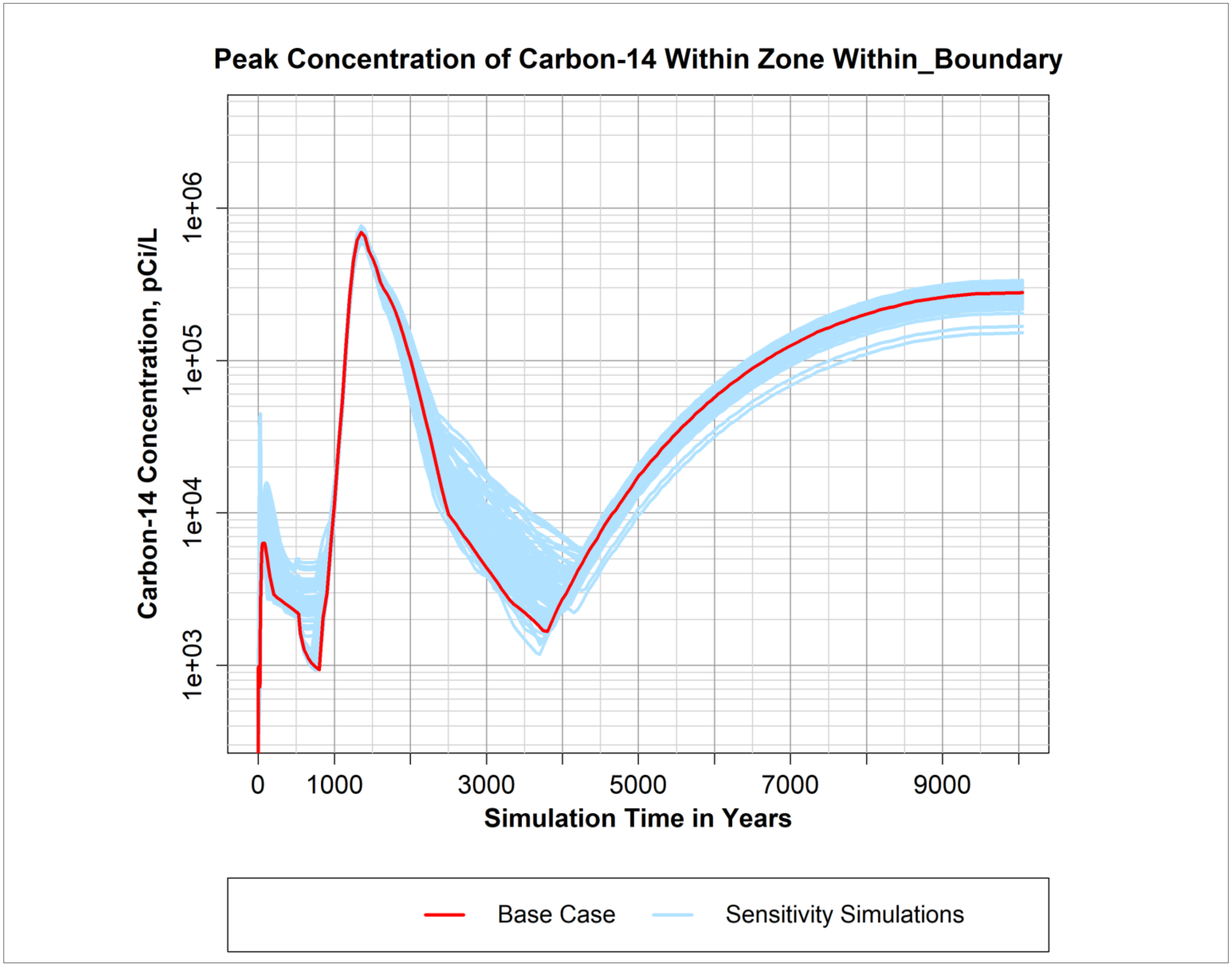

Figure B-13. Peak Simulated Concentration of Carbon-14 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

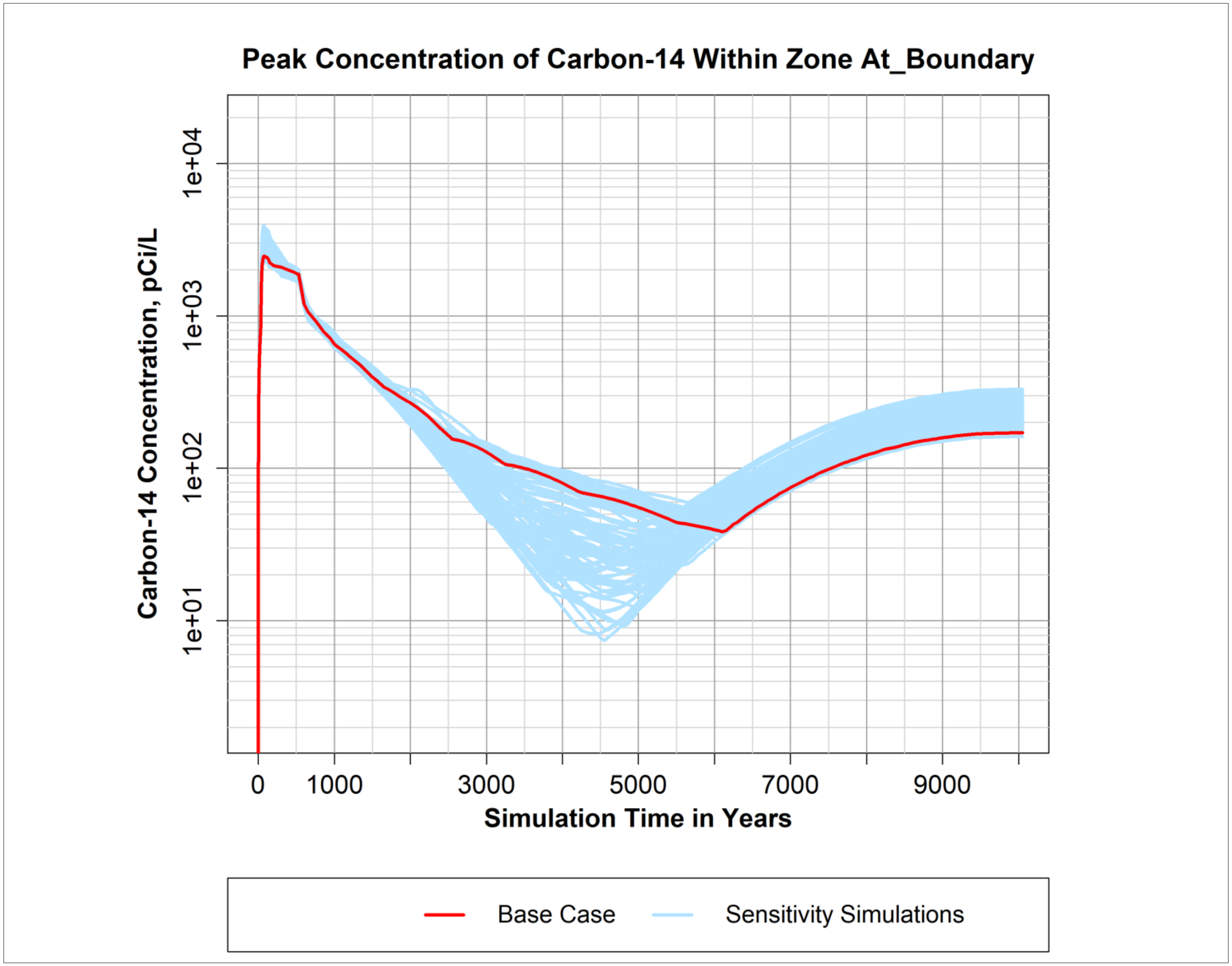

Figure B-14. Peak Simulated Concentration of Carbon-14 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

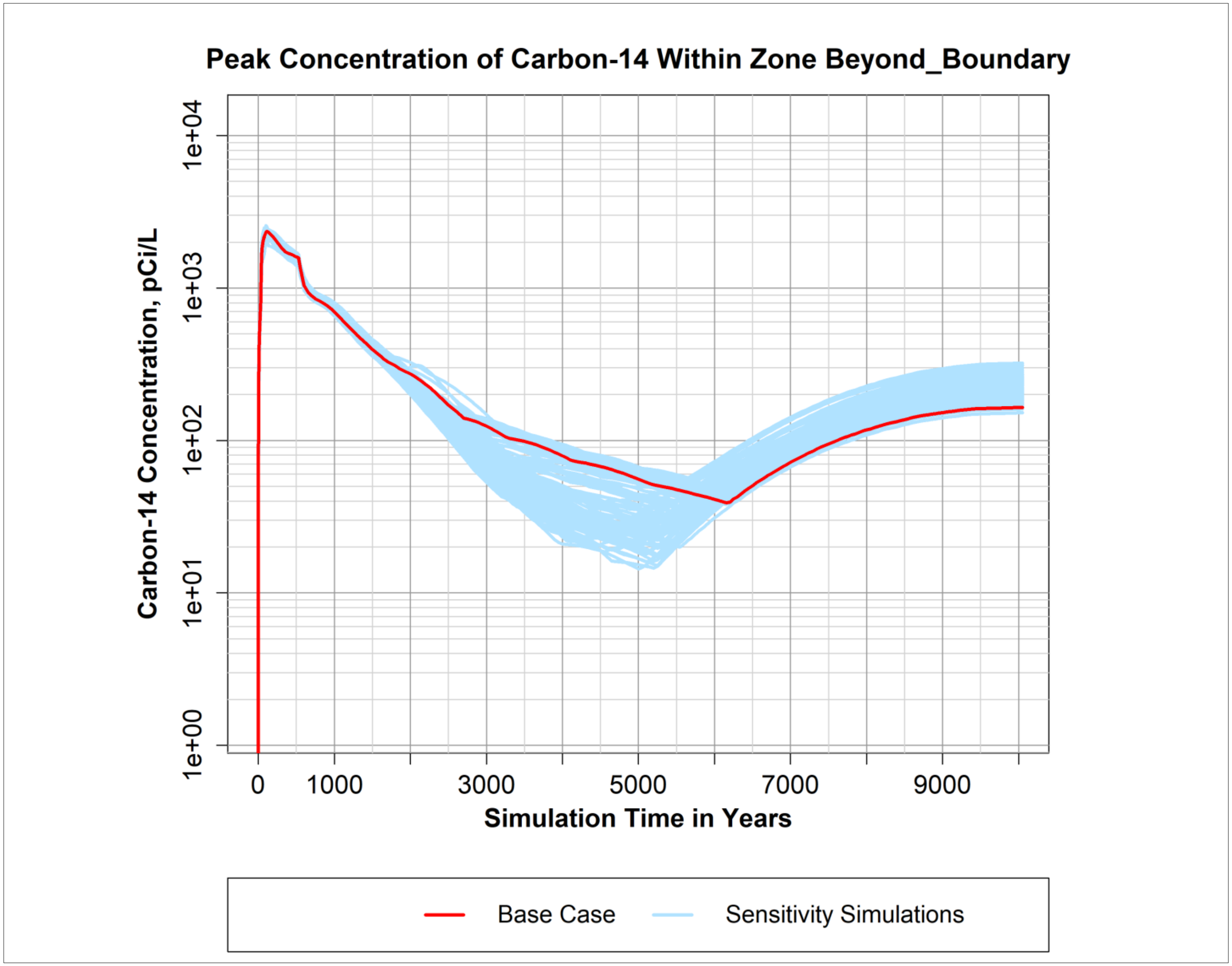

Figure B-15. Peak Simulated Concentration of Carbon-14 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

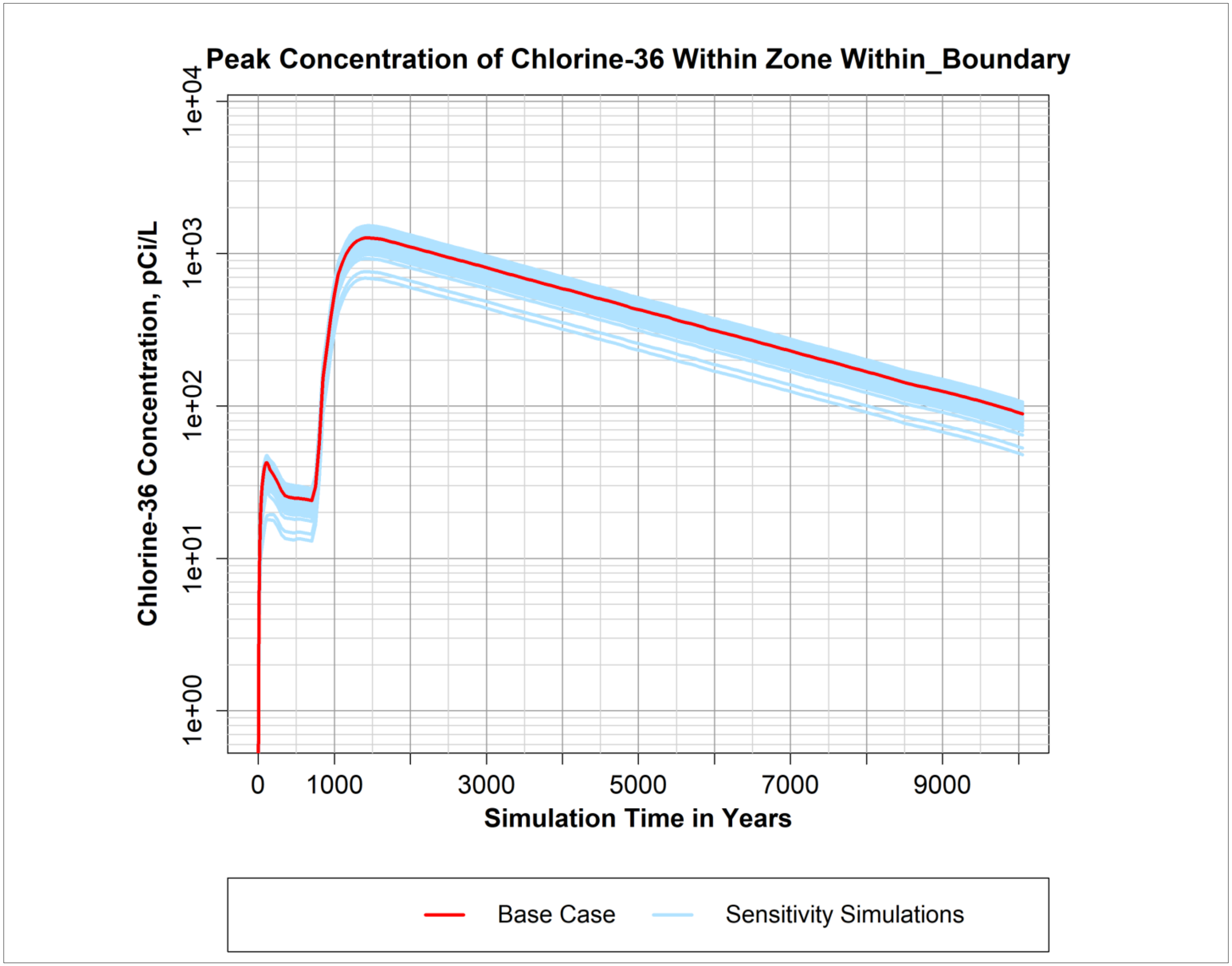

Figure B-16. Peak Simulated Concentration of Chlorine-36 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

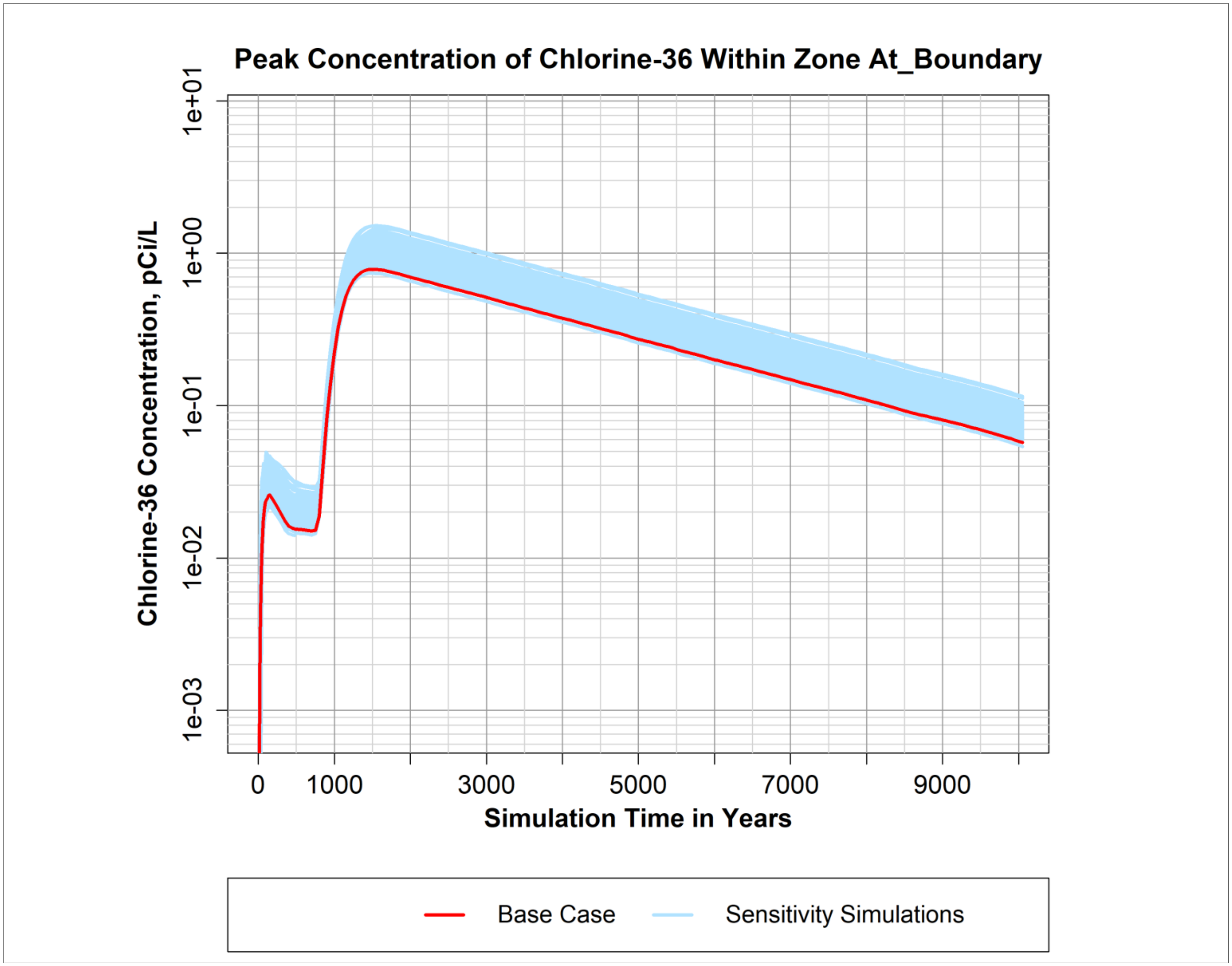

Figure B-17. Peak Simulated Concentration of Chlorine-36 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

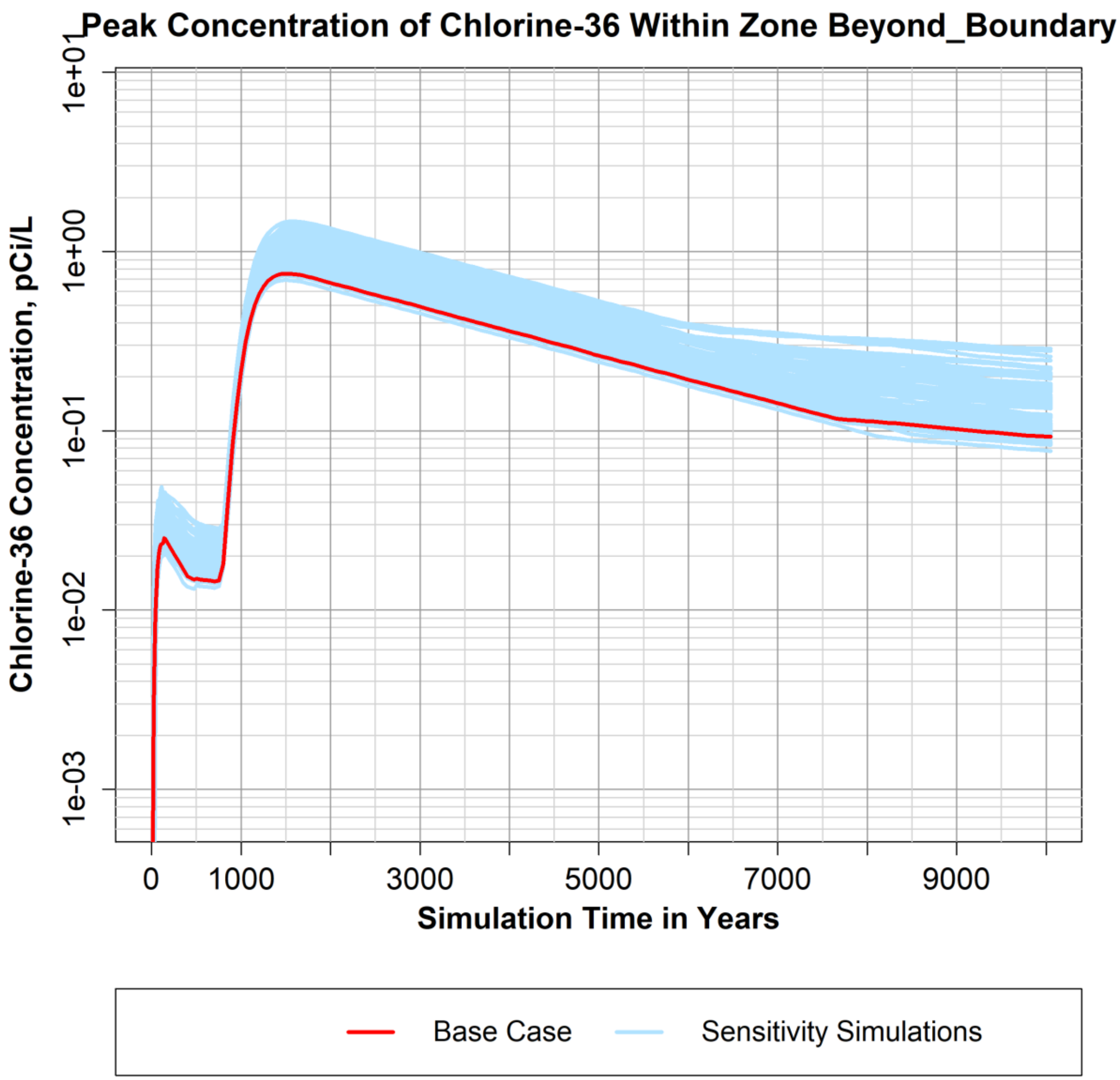

Figure B-18. Peak Simulated Concentration of Chlorine-36 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

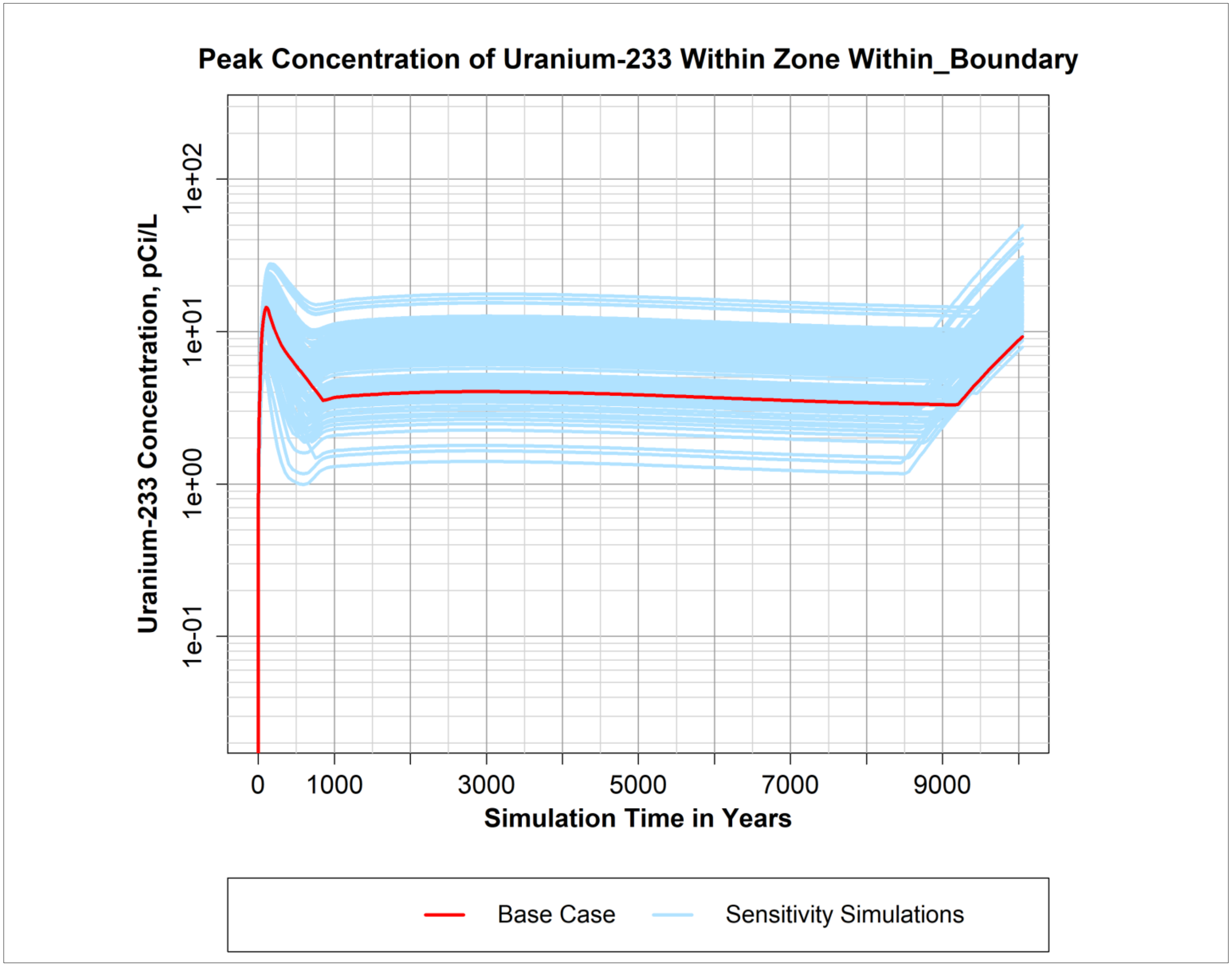

Figure B-19. Peak Simulated Concentration of Uranium-233 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

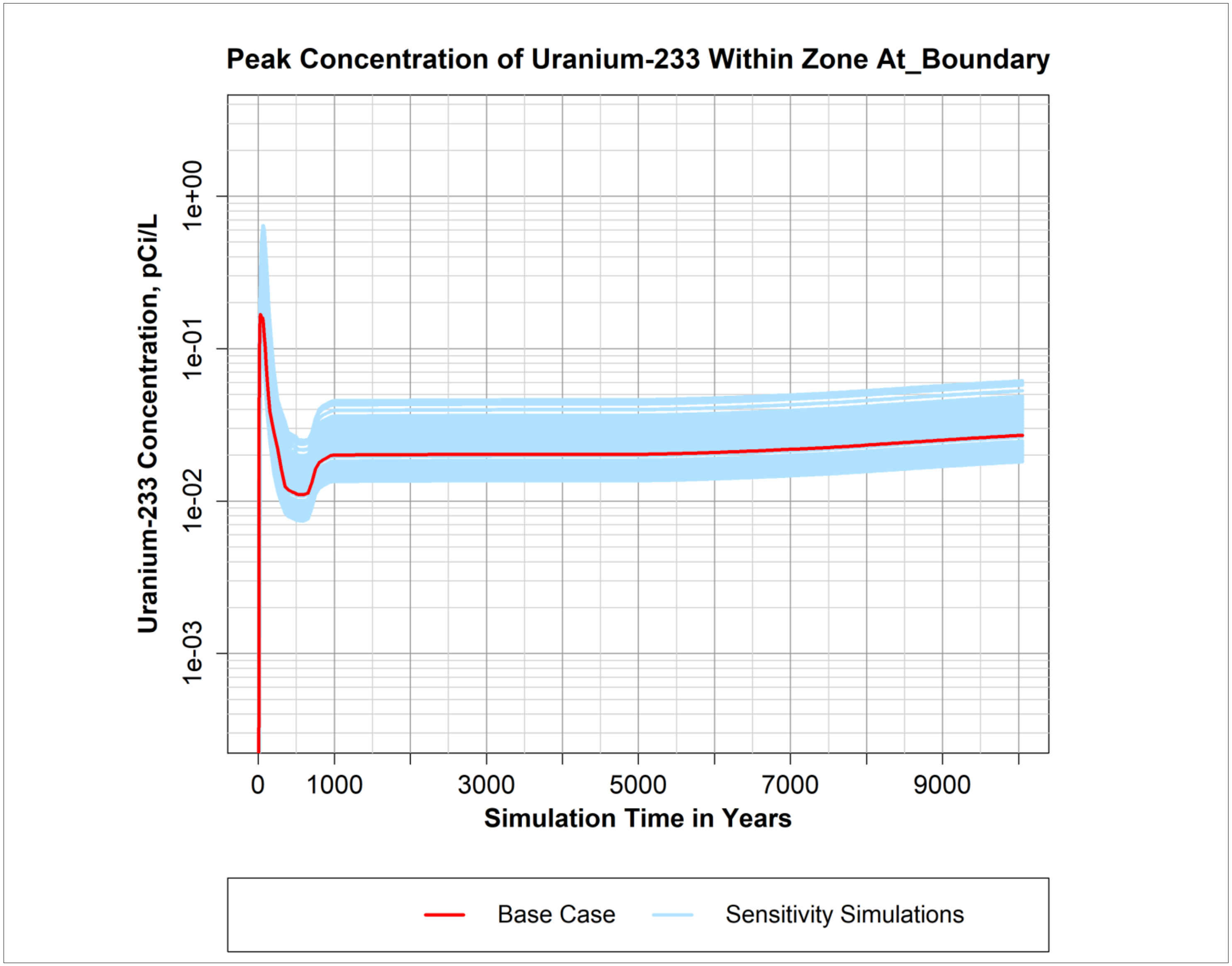

Figure B-20. Peak Simulated Concentration of Uranium-233 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

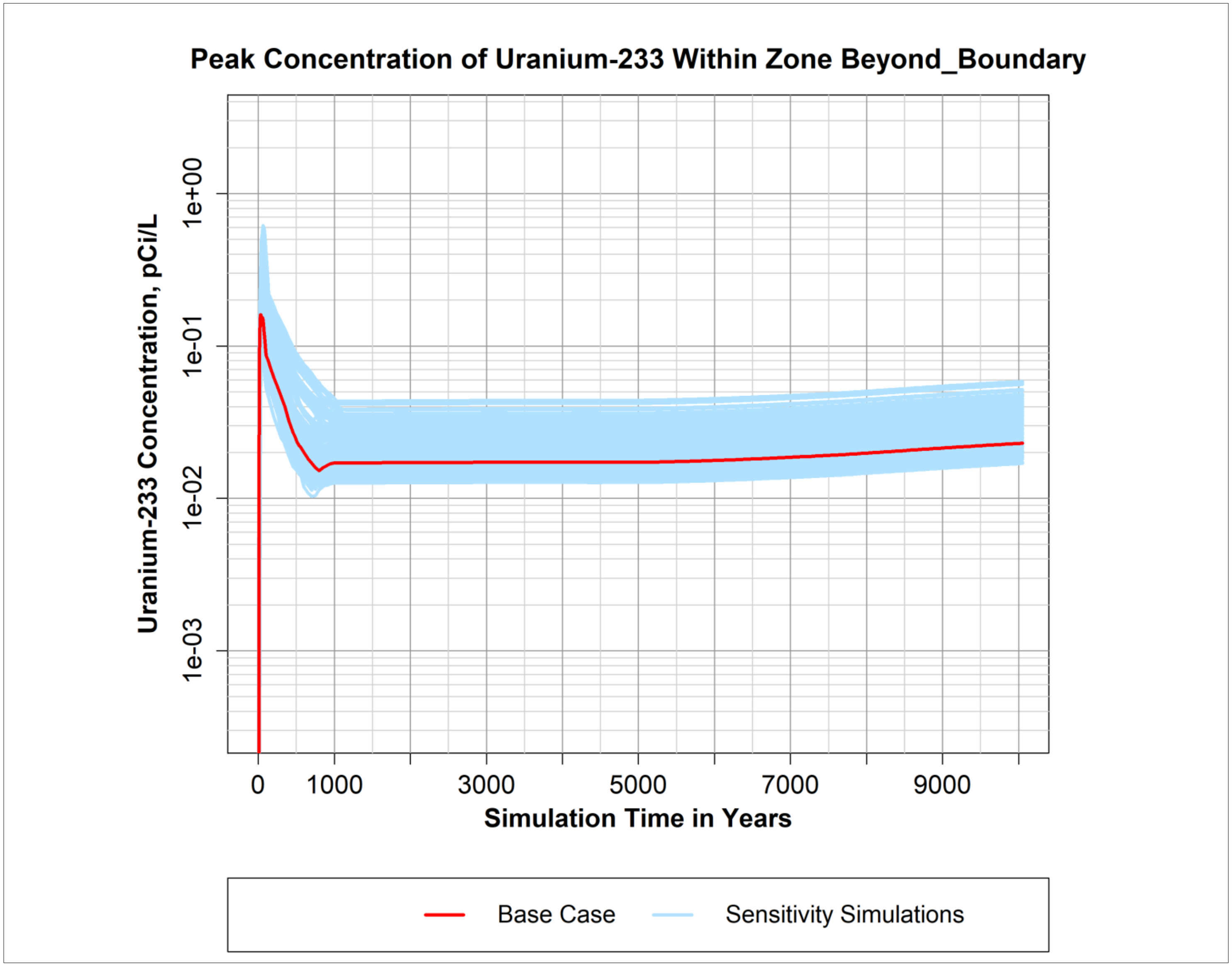

Figure B-21. Peak Simulated Concentration of Uranium-233 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

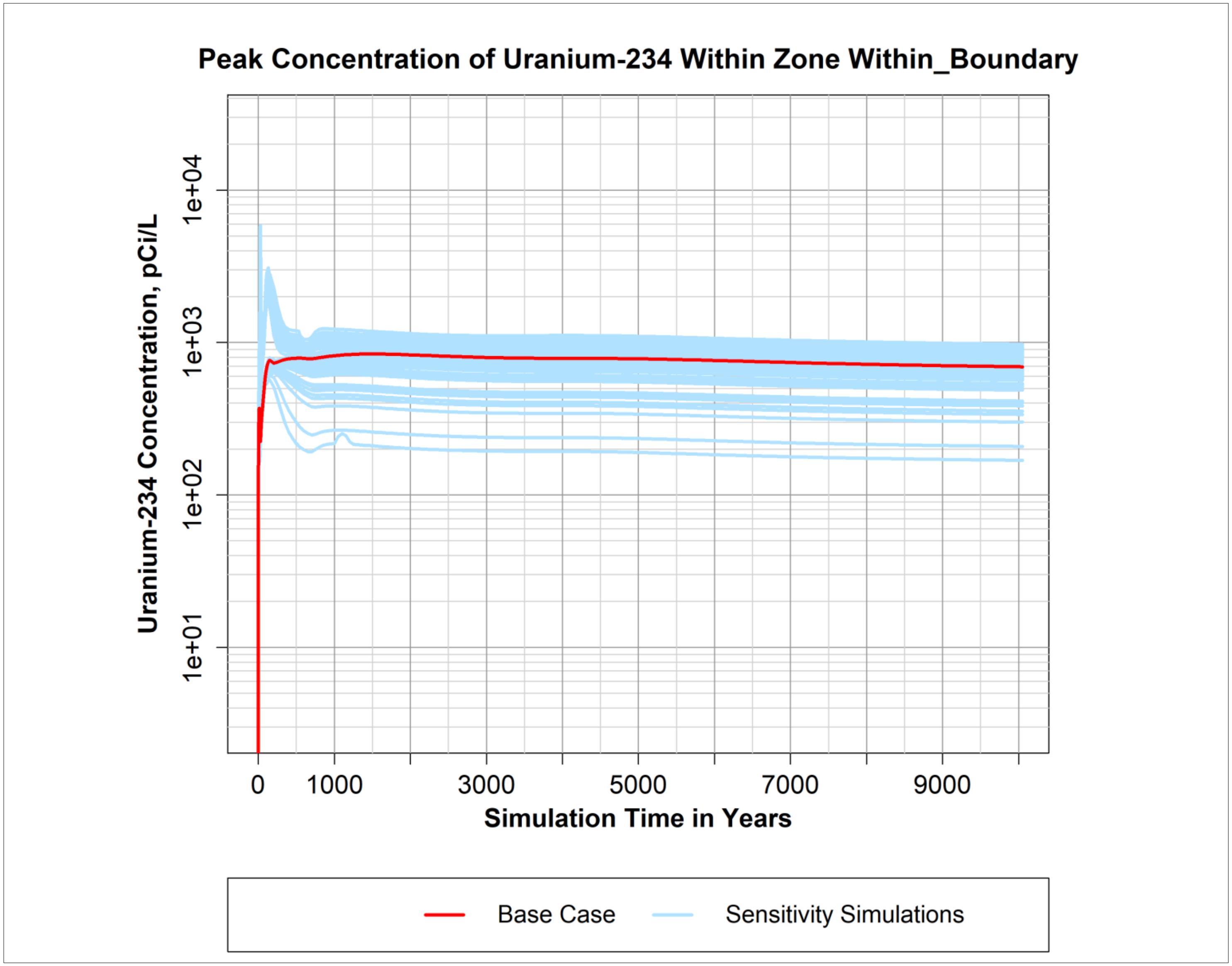

Figure B-22. Peak Simulated Concentration of Uranium-234 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

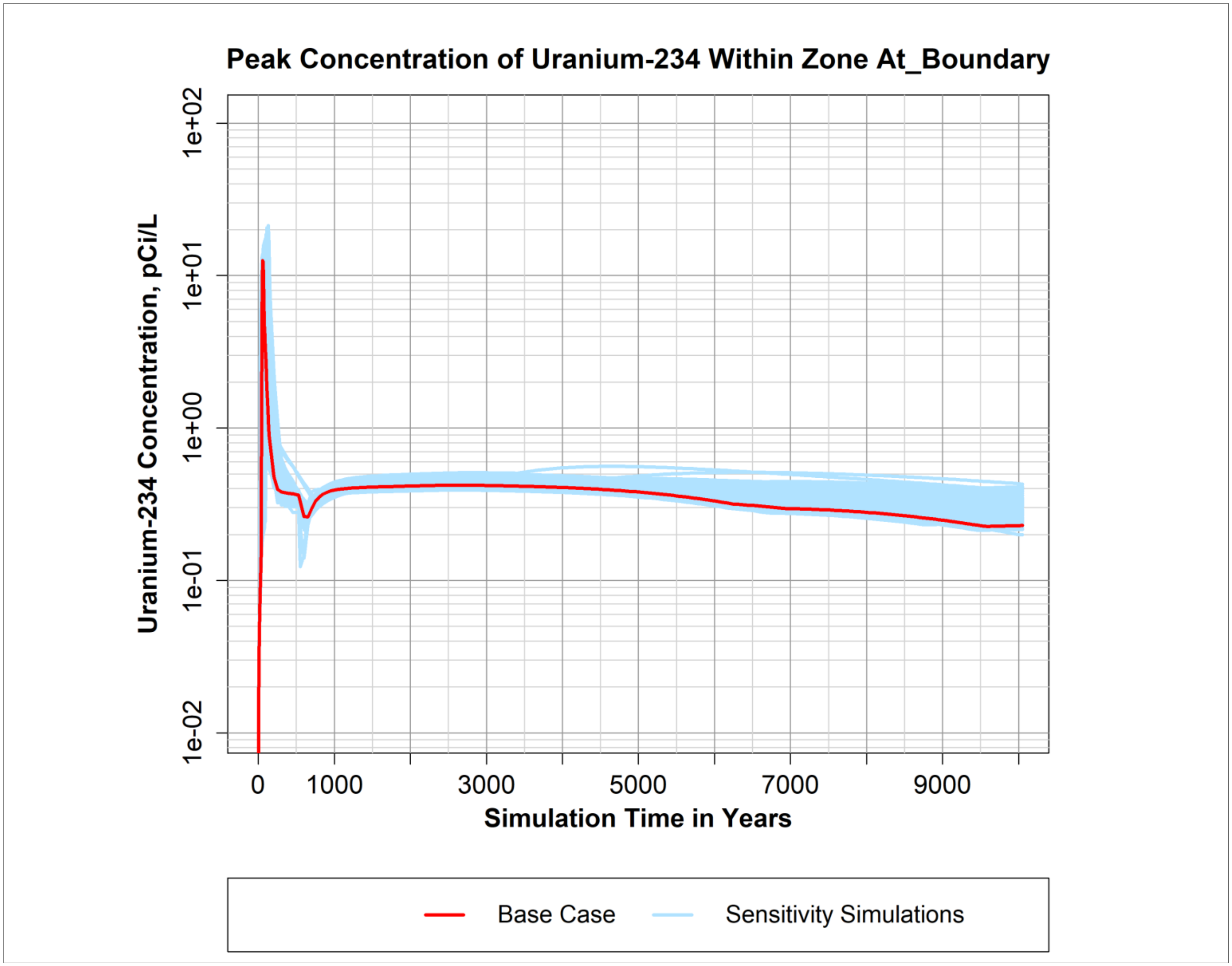

Figure B-23. Peak Simulated Concentration of Uranium-234 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

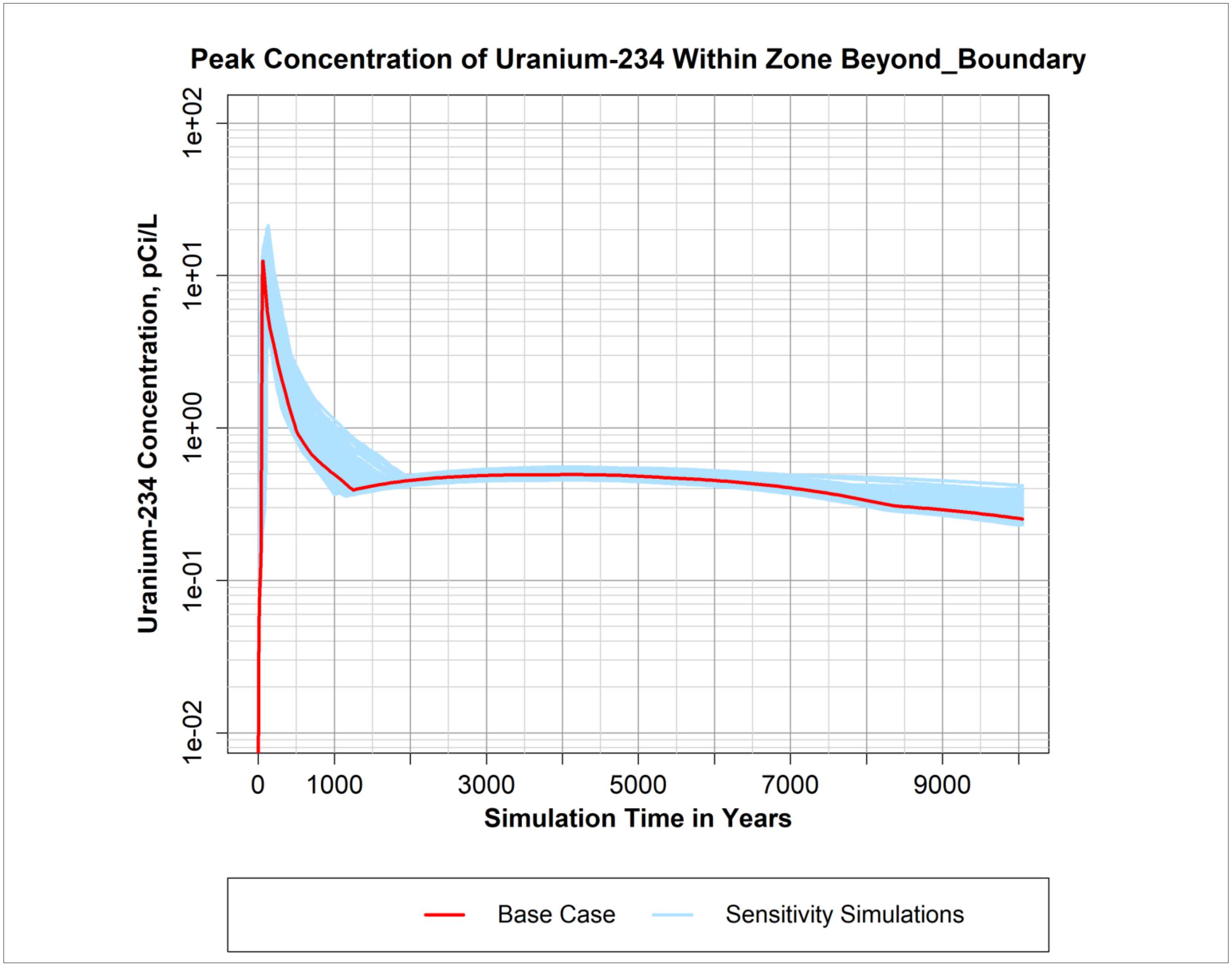

Figure B-24. Peak Simulated Concentration of Uranium-234 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

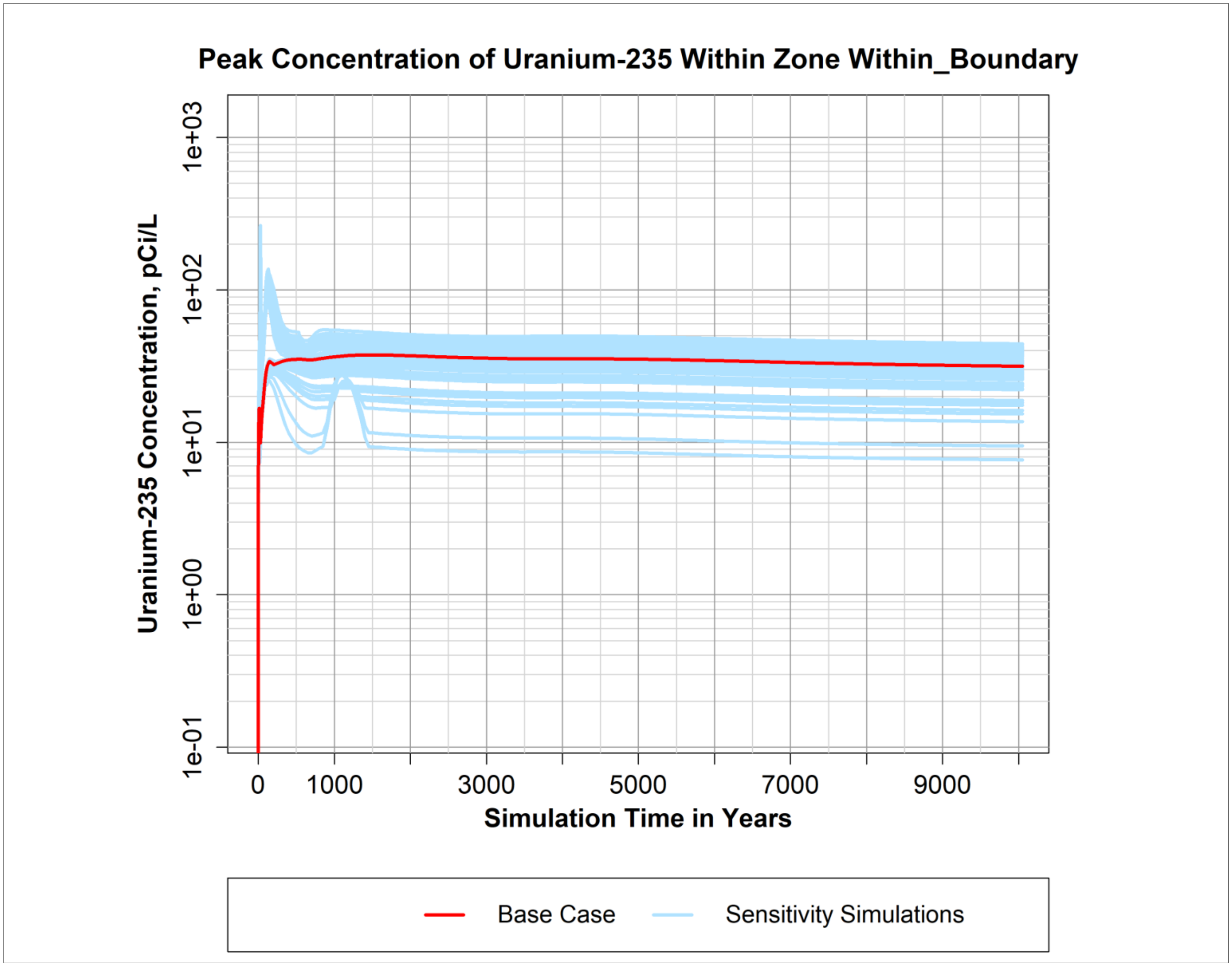

Figure B-25. Peak Simulated Concentration of Uranium-235 Over Time Within the 'Within_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

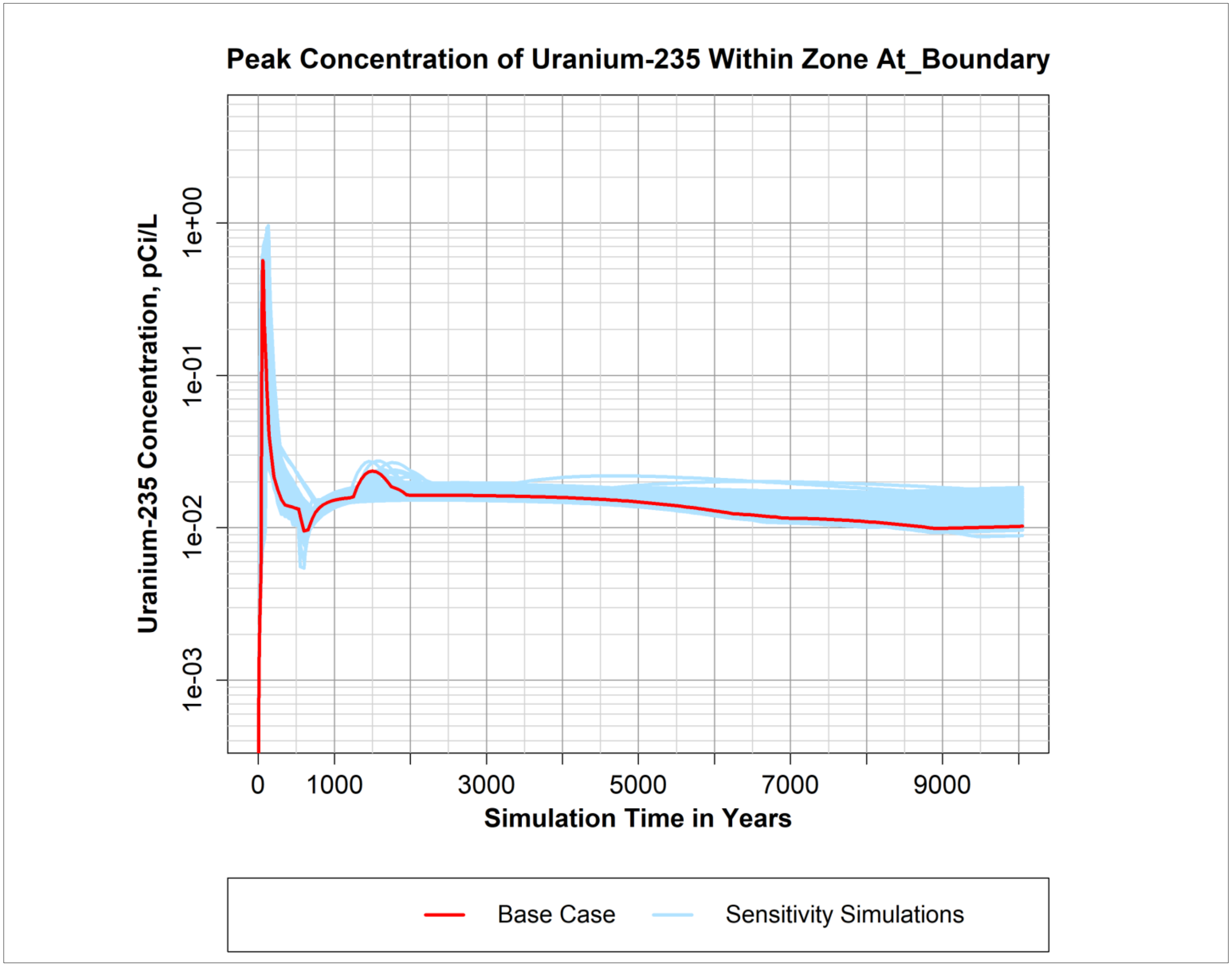

Figure B-26. Peak Simulated Concentration of Uranium-235 Over Time Within the 'At_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

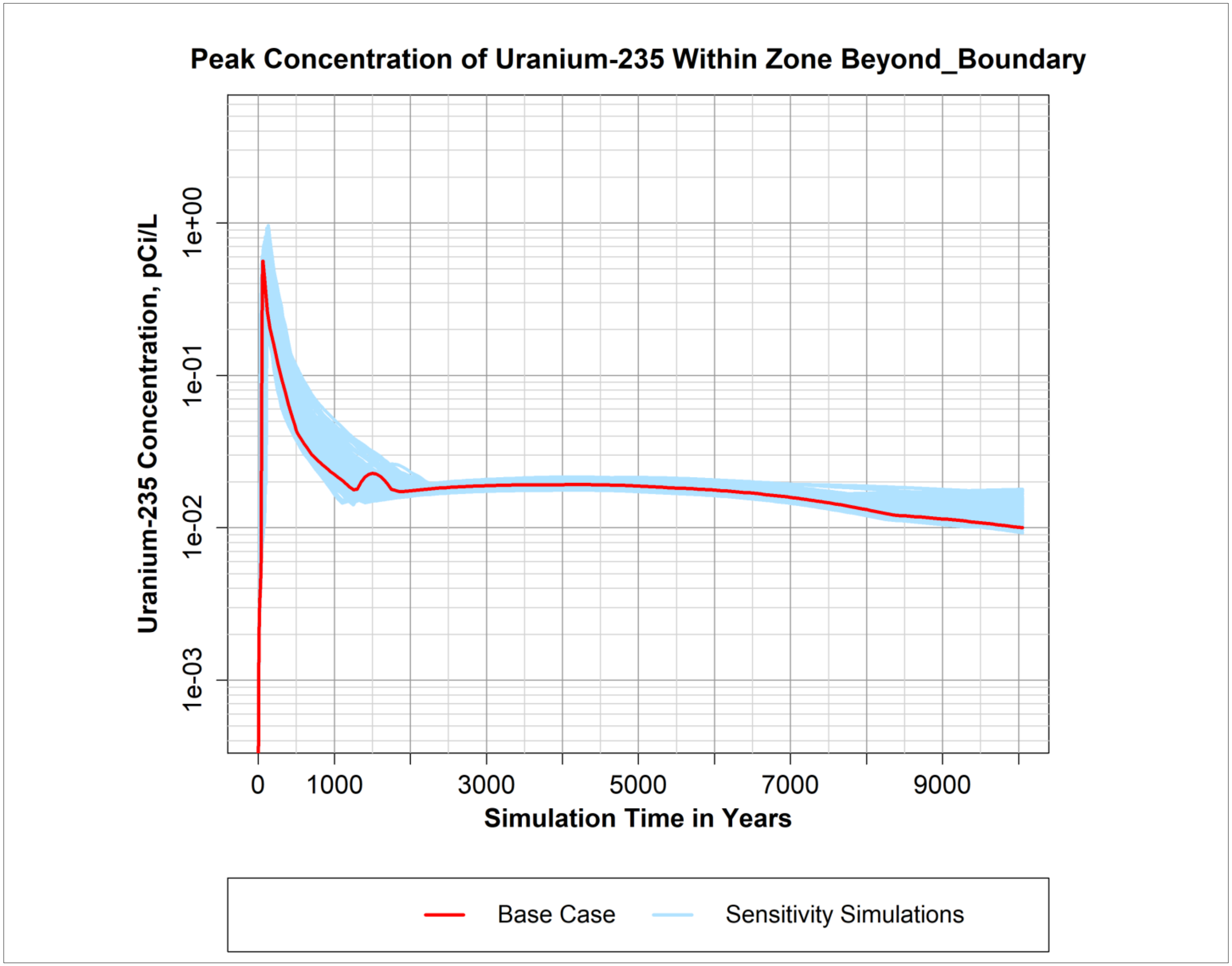

Figure B-27. Peak Simulated Concentration of Uranium-235 Over Time Within the 'Beyond_Boundary' Zone Defined Within the P2R Model Version 8.3 Domain

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