ECF-100BC5-16-0051
Revision 0

Calibration of Continuing Source for Strontium 90 in the 100-BC-5 Operable Unit

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

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

P.O. Box 1600
Richland, Washington 99352

Approved for Public Release;
Further Dissemination Unlimited

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Document Type: ENV Program/Project: EP&SP

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Date Published
October 2016

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APPROVED
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Release Approval Date

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ENVIRONMENTAL CALCULATION COVER PAGE

Section 1: Completed by the Responsible Manager

Project: 100-BC Remedial Investigation/Feasibility Study

Date: 03/31/2016

Calculation Title & Description: Calibration of Continuing Source for Strontium-90 in the 100-BC-5 Operable Unit

RELEASE / ISSUE

DATE: Oct 19, 2016 HANFORD RELEASE

Section 2: Completed by Preparer

Calculation No.: ECF-100BC5-16-0051 **Revision No.:** 0

Revision History

Revision No.	Description	Date	Affected Pages ADD ROW
0 RS	Initial issue	03/31/2016	All

Section 3: Completed by the Responsible Manager

Document Control:

Is the document intended to be controlled within the Document Management Control System (DMCS)? ☒ Yes ☐ No

Does document contain scientific and technical information intended for public use? ☒ Yes ☐ No

Does document contain controlled-use information? JRR 10/19/16 ☐ Yes ☒ No

Section 4: Document Review & Approval

	Name /Position	Signature	Date
Preparer:	H Rashid/Modeler TB Hammond/Modeler	H Rashid M. B. Hammond	03/31/2016 3/31/2016
Checker:	MC Weber	Mary C Weber	3/31/2016
Senior Reviewer:	G Ruskauff	G Ruskauff	3/31/2016
Responsible Manager:	AH Aly / Risk & Model Integr. Mngr.	AH Aly	6/1/16

Section 5: Applicable if calculation is a risk assessment or uses an environmental model

PRIOR TO INITIATING MODELING:

Required training for modelers completed:

	Name /Position	Signature	Date
Integration Lead	Not applicable		

Safety Software Approved:

	Name /Position	Signature	Date
Integration Lead	Not applicable		

CALCULATION APPROVED:

	Name /Position	Signature	Date
Risk/Modeling Integration Manager:	AH Aly / Risk & Model Integr. Mngr.	AH Aly	6/1/16

Environmental Calculation File

Calibration of Continuing Source for Strontium-90 in the 100-BC-5 Operable Unit

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Abbreviations

CHPRC	CH2M HILL Plateau Remediation Company
DOE	U.S. Department of Energy
ECF	environmental calculation file
FEPs	features, events, and processes
GWFTM	Groundwater Flow and Transport Model
HEIS	Hanford Environmental Information System (environmental database)
HISI	Hanford Information System Inventory (software database)
MCL	maximum contaminant level
MODFLOW	MODular groundwater FLOW code (software)
MT3DMS	Modular 3-Dimensional Multiple Species transport code (software)
PNNL	Pacific Northwest National Laboratory
PRG	preliminary remediation goal
OU	Operable Unit
SSM	Source/Sink Mixing Package
STOMP	Subsurface Transport Over Multiple Phases (modeling software)

1 Purpose

The objective of this environmental calculation file (ECF) is to provide a source/sink mixing package for strontium-90 that will be used as a continuing source for the 100-BC-5 operable unit (100-BC model) groundwater flow and transport model derived from vadose zone sources. The vadose zone calculation is performed with models implemented in the STOMP©[1] (Subsurface Transport Over Multiple Phases) fate and transport simulation software (PNNL-11216, *STOMP Subsurface Transport Over Multiple Phases: Application Guide*; PNNL-12030, *STOMP Subsurface Transport Over Multiple Phases: Theory Guide*; PNNL-15782, *STOMP Subsurface Transport Over Multiple Phases: Version 4.0: User's Guide*). Calibration of source strength is achieved by using PEST (a parameter estimation software by John Doherty). STOMP 1-D model framework used in this analysis is identical to that used in ECF-Hanford-15-0129, *STOMP 1-D Modeling for Determination of Soil Screening Levels and Preliminary Remediation Goals for Waste Sites in the 100-BC-1 and 100-BC-2 Source Operable Units*. However, a few changes were made to the STOMP 1-D model framework so that the parameters were consistent with the 100-BC groundwater flow and transport model (SGW-59365, *100-BC Scale-Appropriate Fate and Transport Model*).

2 Background

The background information within this ECF is not meant as an exhaustive discussion of the location, hydrogeology, and 100-BC groundwater/sub-surface flow and transport model. A more detailed discussion of each of these can be found in the documents ECF-Hanford-15-0129 and SGW-59365. The information presented here only provides a brief context for discussion of the construction and results of the numerical modeling results associated with this area.

2.1 Site Location and Contaminants of Concern

The 100-BC area is located in the northern portion of the Hanford Site adjacent to the Columbia River. It is the western-most reactor area and is adjacent to the 100-K Area to the east. It covers more than 11.54 km^2 (4.45 mi^2) of land along the southern shore of the Columbia River. The 100-BC boundary at the river is the ordinary low water mark, which is characterized by the presence of the "green line" of algae delineating the permanently inundated portion of the river channel. The 100-BC area is shown in Figure 2-1; the B and C reactors were located in this area. 100-BC is located on the south bank of the Columbia River, upstream from the other Hanford Site reactor areas. Figure 2-2 shows the operable unit (OU) boundaries, facilities, and reactors. The B reactor was shut down in 1968. The C reactor was shut down in 1969.

Two contaminants persist in the groundwater and vadose zone that merited numerical fate and transport simulation. These were hexavalent chromium [Cr(VI)] and strontium-90.

[1] Battelle Memorial Institute (Battelle) retains copyright on all versions, revisions, and operational modes of the Subsurface Transport Over Multiple Phases (STOMP) software simulator, as permitted by the U.S. Department of Energy. STOMP is used here under a limited government use license.

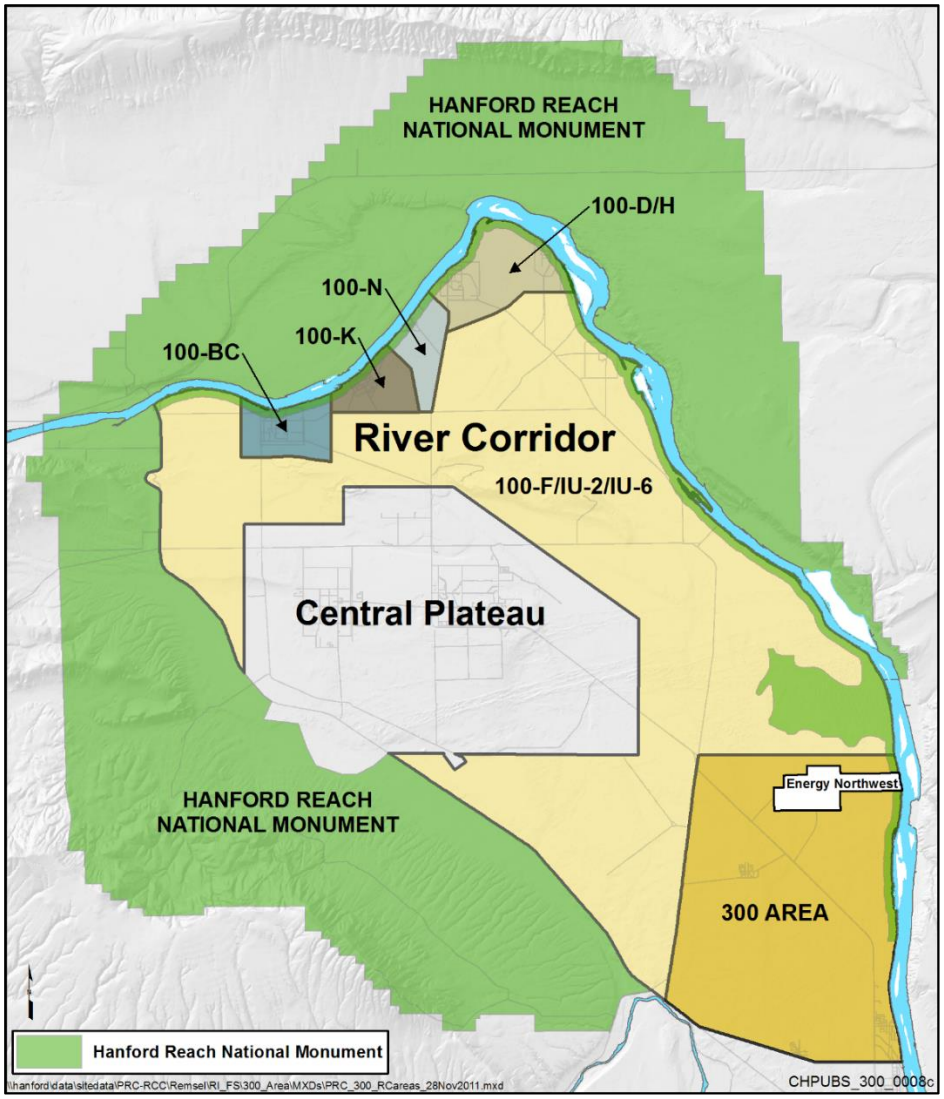

Figure 2-1. Hanford Site

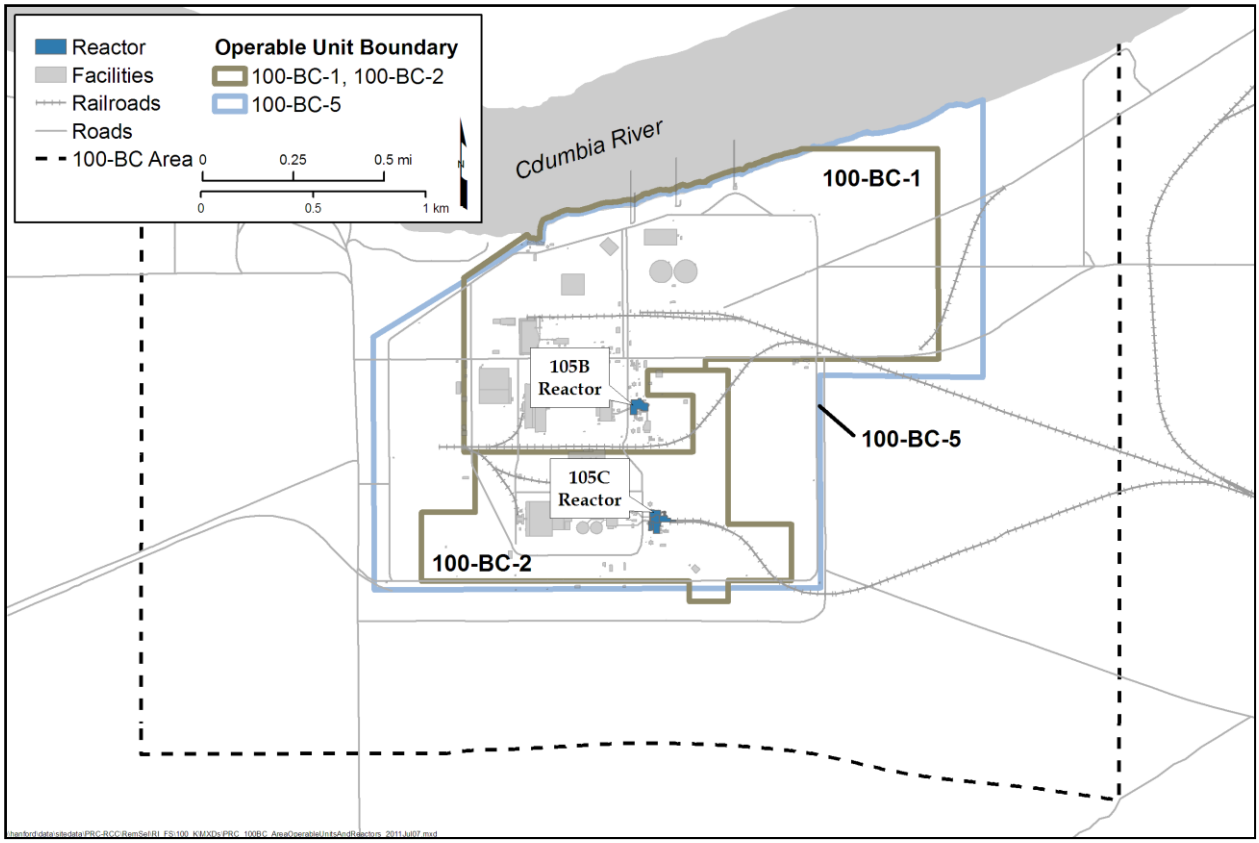

Figure 2-2. 100-BC Reactors and Operable Units

3 Methodology

Persistent strontium-90 groundwater concentrations suggest there is a continuing source. This possibility is investigated using a one-dimensional fate and transport simulation to derive a characteristic breakthrough curve for the strontium-90 release to the aquifer from the vadose zone, and calibrating the soil concentration to the observed groundwater trends. The STOMP code was selected to perform the simulations on the basis of its ability to adequately simulate the vadose zone features, events, and processes (FEPs) relevant to calculating PRGs in the 100-BC OU and to satisfy the other code criteria and attributes identified in DOE/RL-2011-50, *Regulatory Basis and Implementation of a Graded Approach to Evaluation of Groundwater Protection*. Detailed information on the development and basis of the models used in the STOMP 1-D calculation are provided in ECF-Hanford-15-0129.

PEST (Doherty, 2007) was used to calibrate the mass of strontium-90 entering the saturated zone at a rate similar to breakthrough curve derived from STOMP 1-D simulation. Strontium-90 soil concentrations in the vadose zone was parameterized by pilot points interpolated over the model grid via ordinary kriging. This approach is termed the “pilot point” method of parameterization (Doherty, 2003).

To derive a source/sink mixing package for MT3D, the continuing source is considered to be the amount of contamination that is predicted to reach the saturated zone within a 125 year simulation time frame. This section describes the steps in developing the source term. These steps include: 1) evaluating ^{90}Sr groundwater trends to estimate potential source locations and for calibration purposes, 2) constructing a representative hydrogeologic section, 3) estimating the amount of activity in the vadose zone, 4)

estimating the timing of activity entry into the saturated zone, and 5) creating the model inputs to deliver the estimated activity at the correct time.

3.1 Identification of Vadose Zone Source Area

Liquid wastes from reactor operations and associated facilities in the 100-BC OU were released to the vadose zone and the Columbia River. Solid wastes were disposed in burial grounds associated with the facilities. Waste sites above the strontium-90 annual groundwater plume could be the possible vadose zone sources. Analyzing the strontium-90 concentration history over time at groundwater wells within the groundwater plume may identify a continuing source. Strontium-90 concentrations at some monitoring wells are not declining as it is expected with radioactive decay. It indicates that a continuing source is present at around the monitoring wells and possibly near the waste sites. A detailed analysis on the strontium-90 concentration at the monitoring wells is discussed in section 4.3.1. A source zone was assumed which includes the area within the monitoring wells and nearby waste sites where strontium-90 concentrations are declining slower than the decay rate. Figure 3-1 shows the waste sites, strontium-90 plume, monitoring wells, and possible source zones within the 100-BC OU.

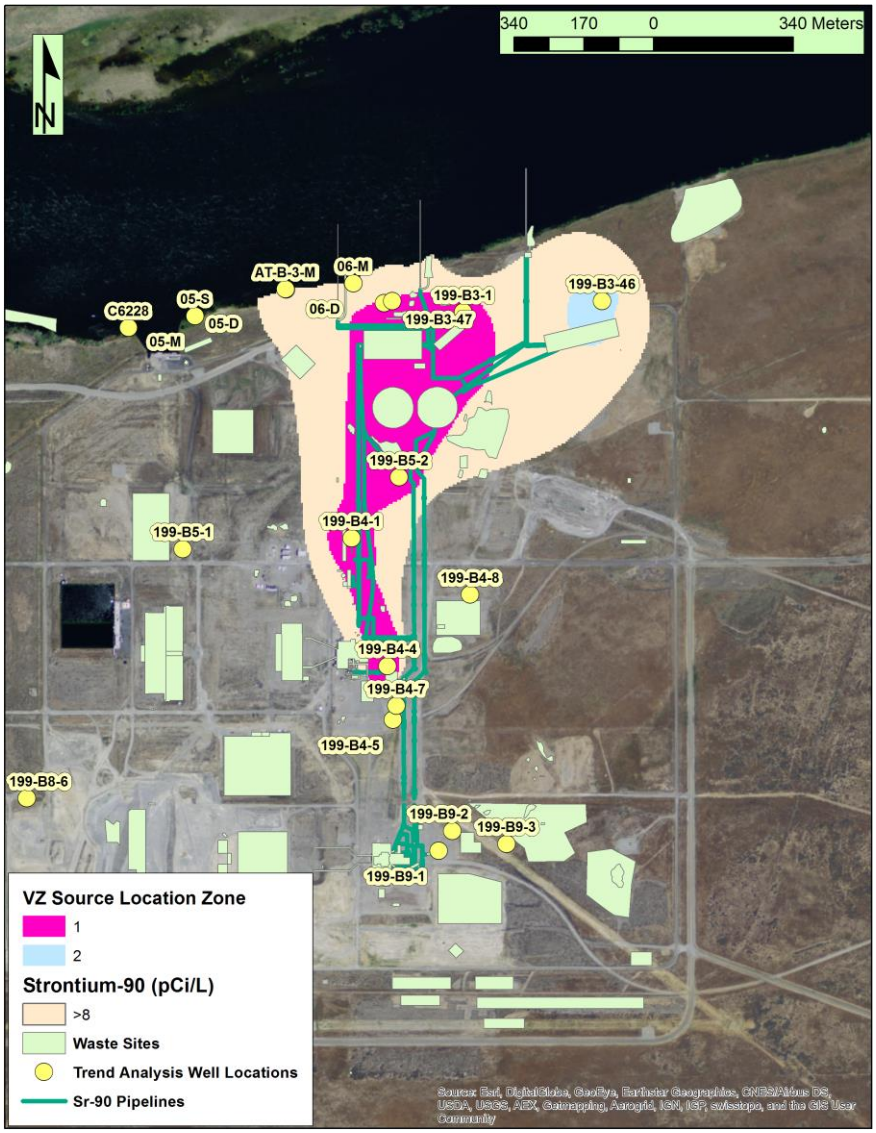

Figure 3-1. Strontium-90 Plume, Waste Sites, Monitoring Wells, and Potential Source Zones in the 100-BC Operable Unit

3.2 Identification of Representative Stratigraphic Columns

ECF-Hanford-15-0129 identifies seven representative stratigraphic columns to represent vadose zone in the 100-BC OU. However, probable source locations and the strontium-90 plume (Figure 3-1) mostly lie beneath representative column 1, column 3, column 6, and column 7. These four representative columns (Figure 3-2) from ECF-Hanford-15-0129 were selected for 1-D STOMP simulation.

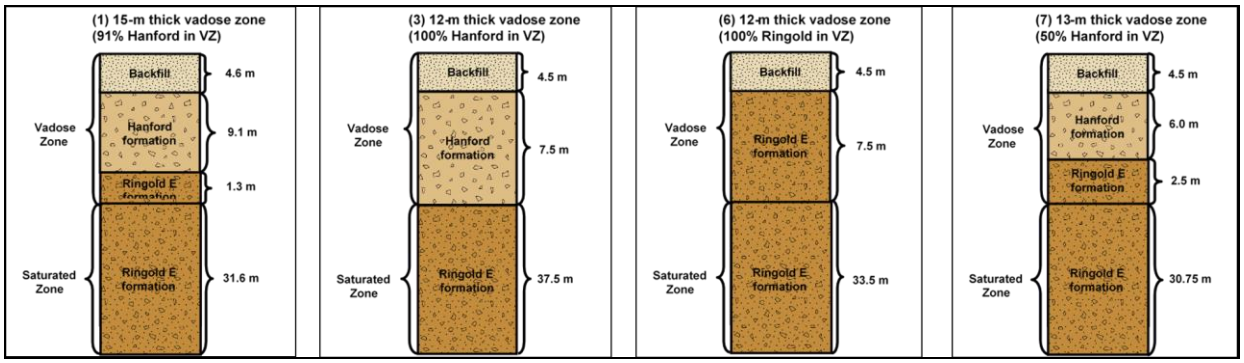

Figure 3-2: Selected Representative Columns from ECF-Hanford-15-0129 for 1-D STOMP Simulations

3.3 Vadose Zone Mass

Some depth discrete data for strontium-90 in the vadose zone were available as described in section 4.3. However, a vadose zone plume for strontium-90 that can be used to calculate total vadose zone activity available was not available in the 100-BC OU. Therefore, PEST was used to estimate a spatially distributed soil concentration (i.e., pCi/g) over the assumed source zone. The soil concentration is then converted to total activity available in the vadose zone as described in section 6 of this document.

3.4 Temporal Distribution of Mass

The STOMP 1-D simulation calculates time-series of activity entering the saturated zone from the vadose zone. The time-series represents the mass expected to enter the saturated zone based on a unit soil concentration over a unit area. Therefore, the unit temporal distribution curve or characteristic breakthrough curve must be scaled based on the amount of activity estimated to be present in the vadose zone.

Table 3-1 illustrates the process of scaling the temporal distribution based on the estimated vadose zone activity. The activity from the STOMP output is summed to determine the total activity that enters the aquifer over the 1,000 years of simulation for STOMP. In the table for simplicity, the hypothetical time-series is presented to illustrate this concept using only five periods. The actual simulated results used 675 stress periods based on the results from the 1-D STOMP simulation. Based on the total activity that entered the aquifer in the STOMP simulation, the time series is normalized using the total activity to provide the percent of total activity that enters the aquifer in each period. Finally, the normalized temporal distribution is multiplied by the total activity in the aquifer in order to estimate the amount of activity that will enter the saturated zone during the simulated period of 125 years.

The predictive simulations for the 100-BC GWFTM provide estimates for 125 years into the future. The STOMP simulations have a total simulated period of 1,000 years while the MT3D simulated time length is only 125 years. Thus, for strontium-90 with a high adsorption value, the total simulated activity entering the aquifer is less than the total activity in the aquifer over the 1,000-year simulation. In this case, the total activity found in Table 3-1 is scaled based on the amount of the estimated percent of total that enters the aquifer in the first 125 years of the STOMP simulation. The total activity that enters the saturated zone is also affected by radioactive decay for strontium-90. This estimated percent of total that enters the aquifer in the first 125 years of the STOMP simulation is also calibrated using the PEST framework.

Table 3-1. Example of Scaling of Total Activity to the Unit Temporal Distribution from STOMP

Estimated Total Activity: 55 pCi			
Time Period	**STOMP 1-D Output (pCi)**	**Percent of Total from STOMP**	**Simulated MT3D Activity Input (pCi)**
1	30	7	3.8
2	220	51	27.8
3	112	26	14.2
4	50	11	6.3
5	23	5	2.9
Total	435	100	55

3.5 Construction of Source/Sink Mixing Package

In order to input the continuing source data into the 100-BC GWFTM files the activity must be converted to a concentration. The time varying recharge rate from the MODFLOW recharge package and the area of each numerical cell in the 100-BC GWFTM were used to convert the activity into a concentration. These concentration values are arranged into the correct format for the Source/Sink Mixing (SSM) package in MT3D. Once added to the SSM package the pre-processing is complete.

4 Assumptions and Inputs

All the features and processes of 1-D STOMP model (e.g., hydraulic properties, saturation function parameters, boundary conditions, and initial conditions) were kept as same as ECF-Hanford-15-0129 with few exceptions so that 1-D STOMP model is consistent with the groundwater flow and transport model. PEST was used for calibrating the continuing source using the 100-BC groundwater flow and transport model as described in SGW-59365.

4.1 Model Domain

1-D STOMP model represents a column of sediments that comprise a vadose zone underlain by an aquifer. Recharge-driven flow moves downward through the vadose zone, where it encounters contamination that is eventually transported to an underlying aquifer. The contamination that reaches the aquifer serves as a continuing source for the transport simulation in the 100-BC groundwater flow and transport model. The assumed strontium-90 source zone falls in the northern side of the 100-BC GWFTM and can be represented by representative stratigraphic columns mentioned in section 3.2 of this ECF. The details on these representative columns can be found at section 3.1 of ECF-Hanford-15-0129. These representative columns were used for 1-D STOMP simulation to derive a characteristic breakthrough curve.

The 100-BC GWFTM extends to the Columbia River on the north side of the model, basalt above water table (no flow boundary) to the south, and uses a general head boundary on the east and west sides of the model. Land surface is the top of the model and the bottom of Ringold Formation Unit E comprises the

lower model boundary. The 100-BC GFM is restricted to approximately center of the Columbia River. The details on the 100-BC GWFTM model domain can be found in Section 3.2 in SGW-59365.

4.2 Boundary and Initial Conditions

All the boundary and initial conditions for the 1-D STOMP model were retained from ECF-Hanford-15-0129 except the time-varying upper boundary conditions (i.e., recharge rates). It was done so that recharge rates in the vadose zone model is consistent with the groundwater model.

4.3 Model Parameters

All the model parameters for 1-D STOMP and groundwater flow and transport model were kept as same as ECF-Hanford-15-0129 and SGW-59365, respectively. One exception was distribution coefficient (K_d) of strontium which was changed to 15 mL/g from 25 mL/g in the 1-D STOMP model. It was done so that the vadose zone model is consistent with the groundwater model.

PEST uses pilot points to generate soil concentrations at each source location. Soil data collected during drilling of monitoring wells within the 100-BC OU were downloaded from the Hanford Environmental Information System (HEIS). The dataset was used to estimate strontium-90 soil concentration at the beginning of calendar year 2015 by using decay equation (equation 2 in section 4.3.1.1). The HEIS dataset and estimated soil concentrations are shown in Table 4-1. The estimated results suggested that the estimated decayed soil concentration at the beginning of calendar year 2015 would be around 1 pCi/g. PEST was setup such a way that soil concentration at any cell cannot be more than 1 pCi/g. Pilot points within the source zone are placed based on the following criteria:

1. Uniform distribution of the pilot points over the entire source zone so that at least 1-3 points are available for interpolation within the correlation scale (range).
2. High density of pilot points in vicinity of calibration targets (e.g., monitoring wells)

Table 4-1. Estimated Strontium-90 Soil Concentration in the Vadose Zone

Well Name	Sample Date	Depth (m)	Result (pCi/g)	Lab Qualifier	Decayed to 1/1/2015
199-B3-46	2/24/1992	9.8	0.40	J	0.23
	2/24/1992	11.3	7.80	J	4.5
199-B3-47	2/21/1992	9.9	1.20		0.69
	2/24/1992	13.0	0.88	J	0.51
199-B3-51	1/14/2011	9.8	0.31		0.28
	1/17/2011	11.1	0.63		0.57
	1/17/2011	13.1	0.33		0.3
199-B5-2	4/6/1992	16.8	2.90		1.68
	4/6/1992	17.4	2.60		1.5
199-B2-14	1/20/2010	9.45	0.96	U	0.85
	1/20/2010	9.45	0.81	U	0.72
	1/20/2010	9.45	0.97	U	0.86
	1/20/2010	9.45	0.98	U	0.87
	1/20/2010	10.76	0.97	U	0.86
	1/20/2010	10.76	0.98	U	0.87

Table 4-1. Estimated Strontium-90 Soil Concentration in the Vadose Zone

Well Name	Sample Date	Depth (m)	Result (pCi/g)	Lab Qualifier	Decayed to 1/1/2015
	1/20/2010	12.44	0.97	U	0.86
	1/20/2010	12.44	0.99	U	0.88
	1/20/2010	13.2	0.96	U	0.85
	1/20/2010	13.2	0.98	U	0.87
	1/21/2010	13.96	0.97	U	0.86
	1/21/2010	13.96	0.91	U	0.81
199-B3-52	9/17/2010	11.4	1.53		1.38
	9/17/2010	12.28	1.32		1.19
	9/20/2010	12.86	0.81		0.73
	9/20/2010	13.81	0.97		0.87
199-B4-15	11/2/2010	9.27	2.89		2.61
	11/2/2010	10.76	3.88		3.51
	11/2/2010	12.34	6.43		5.82
	11/2/2010	13.81	2.26		2.04
	11/3/2010	15.33	5.02		4.52
	11/3/2010	16.95	5.56		5.03
	11/4/2010	18.5	4.65		4.21
	11/4/2010	21.49	1.42		1.28
	11/4/2010	22.98	0.49		0.44

J = Estimated
U = Undetected

In the context of this application, the correlation scale (range) of the semivariogram represents an influence distance for interpolation, not the actual correlation scale of soil concentration; insufficient data exists to determine the correlation scale of soil concentration. The PEST groundwater utility PPK2FAC was used to generate kriging factors from the pilot points for all the cells within the source zone. A spherical variogram with a correlation range of 250 m was used to characterize spatial variability of soil concentration. The PEST groundwater utility FAC2REAL was used to calculate soil concentration at each source cell based on the pilot point values and kriging factors generated by PPK2FAC program. PEST was run with regularization constraints computed from the PPKREG utility so that FAC2REAL program always generates soil concentration values based on smoothness constraints.

4.3.1 Strontium-90 Trend Evaluation

Groundwater sample data for strontium-90 concentration over time at monitoring wells within 100-BC (extracted from the HEIS database) were evaluated for trends over time to aid in potential source area delineation and as calibration data.

Only groundwater sampling locations within the study area containing enough measurements (at least 8) were considered in the analysis. Two sets of trend analyses were performed for the observed data 1) trend analysis with all the data available and 2) trend analysis with data from May 1999 and later. These two periods were chosen because there is clearly a break in the slope that may be related to waste site

remediation. Table 4-2 lists the well locations from which strontium-90 concentrations used in the trend analysis were sampled.

The method for performing the trend analysis and creating the trend plots is as follows:

1. Create a well list text file containing a single column of all the wells to be considered for trend analysis in the study area. Call this file "welllist.txt". This file should contain the header WELLID.
2. Create an observed data text file (comma separated) titled "Sr90_100BC_GW_Data.txt" with column headers and corresponding information for:
    - SAMP_SITE_NAME – Well name
    - SAMP_DATE_TIME – Date and time formatted as mm/dd/yyyy 00:00:00
    - STD_VALUE_RPTD – Strontium-90 concentration in pCi/L
    - LAB_QUALIFIER – Either "U" for non-detects or blank for detections.

    These formats are identical to the headers and columns of data tables exported from HEIS.
3. Read simulated output and title the file "simulated_Sr90_output.dat".
4. Ensure that the previously created text files are located in the same working directory as the R scripts "MakeHydroPlots_SR90_obs_model_new.R" and "TheilSen.R" (EPA 530/R-09-007, *Statistical Analysis of Groundwater Monitoring Data at RCRA Facilities Unified Guidance*).
5. Run the R script "MakeHydroPlots_SR90_obs_model_new.R" which will also call script "TheilSen.R" to create the trend plots and table listing the slopes and intercepts of the observed strontium-90 trends at each well location.

Table 4-2. Well Locations for Strontium-90 Trend Analysis

Well	X-Coord	Y-Coord	Sample Loc. Type	Initial Observed Concentration (pCi/L)
199-B2-12	565368.4	145363.7	GROUNDWATER WELL	0.19
199-B3-1	565561.5	145342.1	GROUNDWATER WELL	49
199-B3-46	565899.6	145369	GROUNDWATER WELL	57
199-B3-47	565388.7	145369	GROUNDWATER WELL	21
199-B4-1	565289.8	144791.5	GROUNDWATER WELL	23
199-B4-4	565377.1	144479.7	GROUNDWATER WELL	51
199-B4-5	565390.5	144349.2	GROUNDWATER WELL	7.51
199-B4-7	565398.9	144382.8	GROUNDWATER WELL	9.55
199-B4-8	565578.5	144653.8	GROUNDWATER WELL	1.3
199-B5-1	564878.1	144764.9	GROUNDWATER WELL	1.8
199-B5-2	565405.4	144939.7	GROUNDWATER WELL	15
199-B8-6	564498.8	144157.8	GROUNDWATER WELL	Not Detected
199-B9-1	565502	144029.7	GROUNDWATER WELL	2.7

Table 4-2. Well Locations for Strontium-90 Trend Analysis

Well	X-Coord	Y-Coord	Sample Loc. Type	Initial Observed Concentration (pCi/L)
199-B9-2	565534.8	144078.1	GROUNDWATER WELL	0.16
199-B9-3	565667.4	144046.7	GROUNDWATER WELL	Not Detected
699-65-83	564590.5	143249.1	GROUNDWATER WELL	0.022
AT-B-3-D	565130.5	145397.3	AQUIFER TUBE	Not Detected
AT-B-3-M	565128.6	145397.7	AQUIFER TUBE	0.736
05-D	564908.3	145332.3	AQUIFER TUBE	Not Detected
05-M	564908.3	145332.3	AQUIFER TUBE	17
05-S	564908.3	145332.3	AQUIFER TUBE	4.68
06-D	565293.9	145412.1	AQUIFER TUBE	19
06-M	565293.9	145412.1	AQUIFER TUBE	15.2
C6228	564746.3	145303.8	AQUIFER TUBE	Not Detected

4.3.1.1 Decay Trend

For the decay trend calculation, the initial measured strontium-90 concentration at each well in Table 4-2 was used as a surrogate for the number of decays (N_0) in the equation

$$N(t) = N_0\, e^{-\lambda t} \qquad (1)$$

where $N(t)$ is the concentration of strontium-90 at time t in years and N_0 is the strontium-90 concentration of the first measured data point (t=0). The decay constant of 2.380313E-02 1/yr for strontium-90 was used in equation 1 for the value of λ. The decay line trend is drawn through N_0 , t_0 and $N(t)$ at any given time in years t.

4.3.1.2 Theil-Sen Estimator for the Observed Trend

The observed trend calculation using the Theil-Sen estimator method was carried out in the script "TheilSen.R". Theil-Sen trend line is non-parametric, so the underlying data need not be normal or follow a particular distribution. Furthermore, data ranks are not used, so no special adjustment for ties is needed. Although non-parametric, the Theil-Sen slope estimator does not use data ranks but rather the concentrations themselves. The method is non-parametric because the median pairwise slope is utilized, thus ignoring extreme values that might otherwise skew the slope estimate. The Theil-Sen trend line does not require any special adjustment for ties (e.g., non-detects). The "TheilSen.R" script computes the observed trend for each measuring point by following these basic steps:

1. Observed data is sorted by date/time of sampling.
2. Computes the simple pairwise slope for each pair of distinct sampling events.
3. Sorts the list of slopes and sets the overall slope estimate (Q) as the median slope in this list.
4. Compute the median concentration and the median date/time of sampling.

5. Construct the Theil-Sen trend as the line passing through the median scatter point from Step 4 with slope *Q*.

Two calculations were performed as part of the trend analysis within the R scripts mentioned above. The equation for the strontium-90 decay trend is calculated in a sub-routine within the "MakeHydroPlots_SR90_obs_model_new.R" script and the Theil-Sen estimators for the observed and simulated trends are calculated within the "TheilSen.R" script. The regression lines calculated for both the decay and Theil-Sen trend estimator are drawn on the trend plots output by the script "MakeHydroPlots_SR90_obs_model_new.R".

4.3.1.3 Calibration Targets

PEST was used to derive a SSM package that simulates a similar slope as the trend analysis. For observed and simulated data trend analysis, a set of two scripts (Attachment B) written in the R programming language was used to first calculate the Theil-Sen observed data trend estimator and then create trend plots displaying the observed trend, strontium-90 natural decay trend, observed strontium-90 concentration data points and simulated strontium-90 concentration over time.

Because of the data-limiting factor of having less than eight data points above detection limits, trend analysis was feasible only for a subset of six wells from the 24 wells listed in Table 4-2. These wells include 199-B3-1, 199-B3-46, 199-B3-47, 199-B4-1, 199-B4-4 and 199-B5-2 (Figure 4-1). Figure 4-2 through Figure 4-7 illustrate the observed and decay trends for the six wells. All of the wells except for 199-B3-46 show observed trends that are decreasing slower than their respective decay trends. The more slowly decreasing trend patterns are suggestive of continuous strontium-90 vadose zone sources in the vicinities of these wells. With an estimated groundwater velocity in the area between 2 and 7 m/day (PNNL-21845, *Investigation of Hexavalent Chromium Flux to Groundwater at the 100-C-7:1 Excavation Site*), a source presence would be required to maintain an observed trend that is decreasing more slowly than the decay trend. Even though well 199-B3-46 is located in an area of high strontium-90 groundwater concentrations, the observed data trend at that location follows the decay trend that is not suggestive of a continuing source.

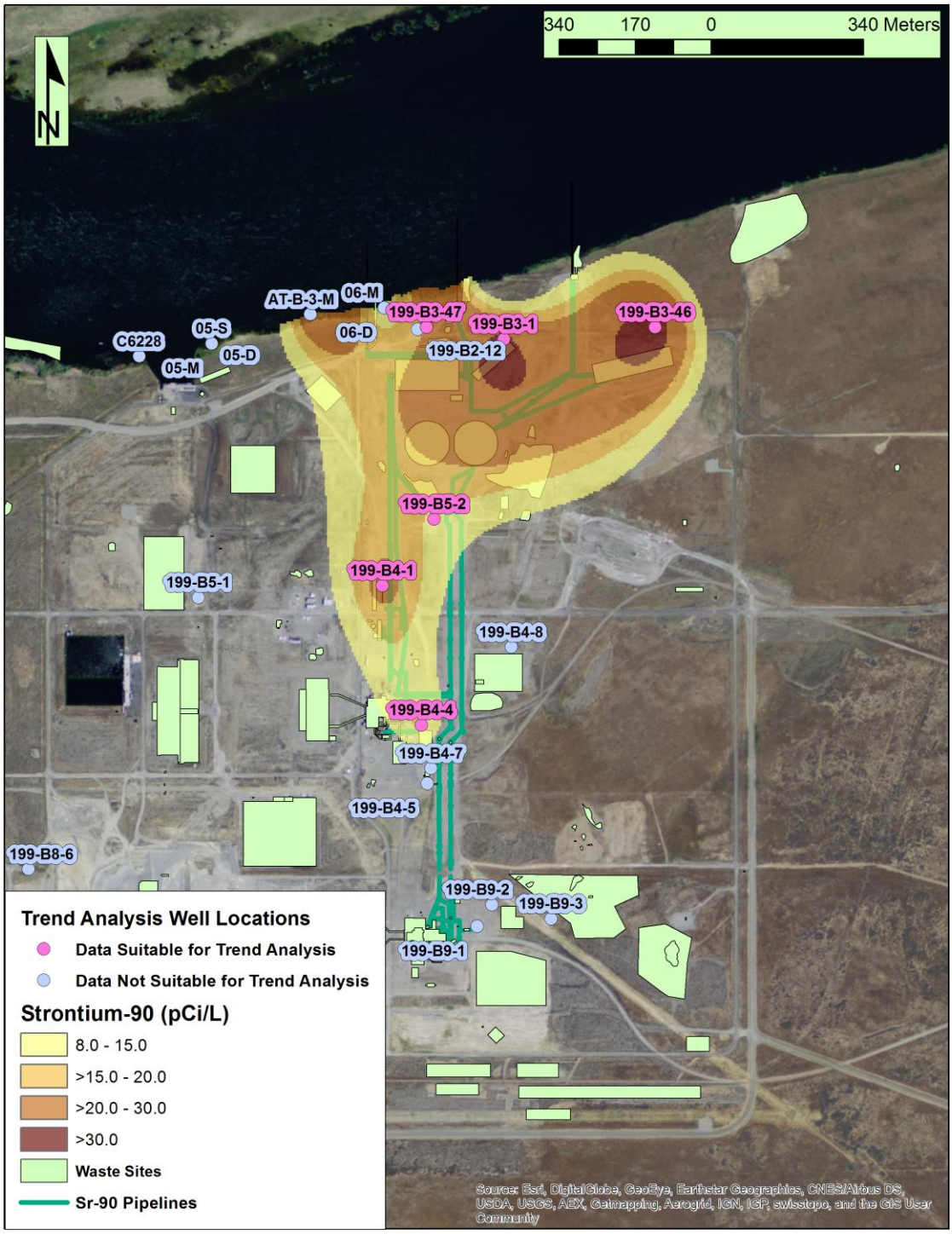

Figure 4-1. 100-BC Strontium-90 Trend Analysis Well Locations

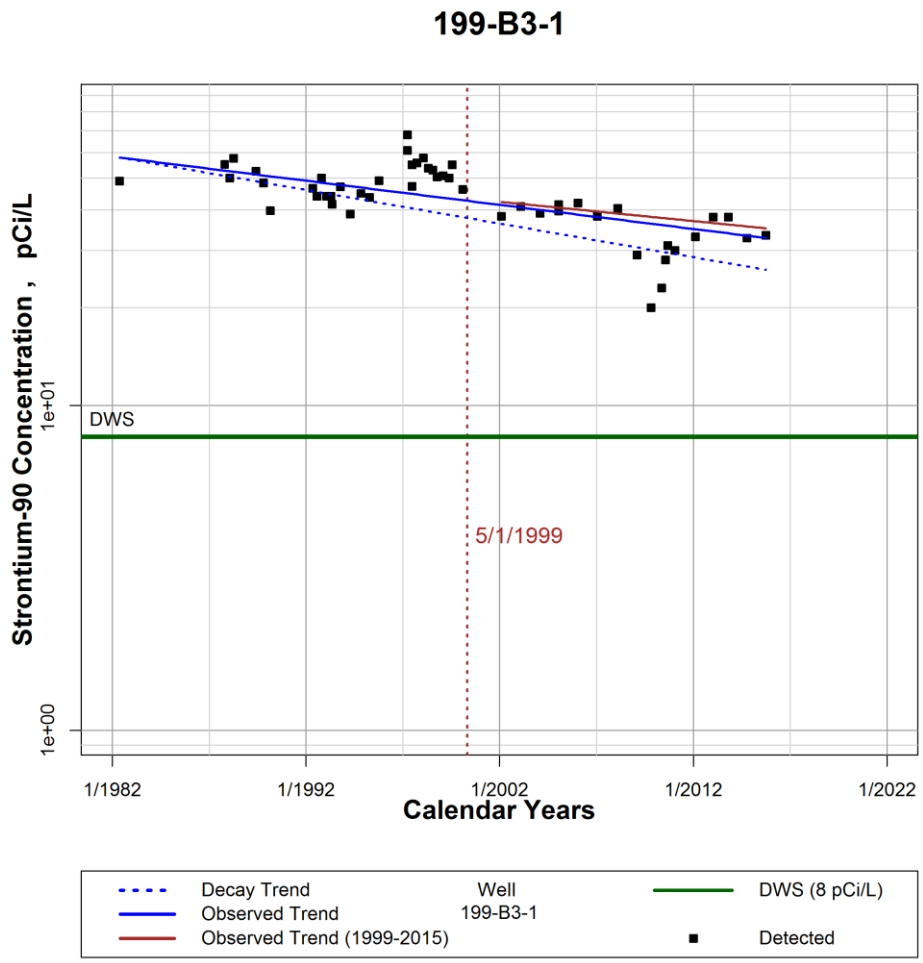

Figure 4-2. Observed Trend Analysis Plot for Well 199-B3-1

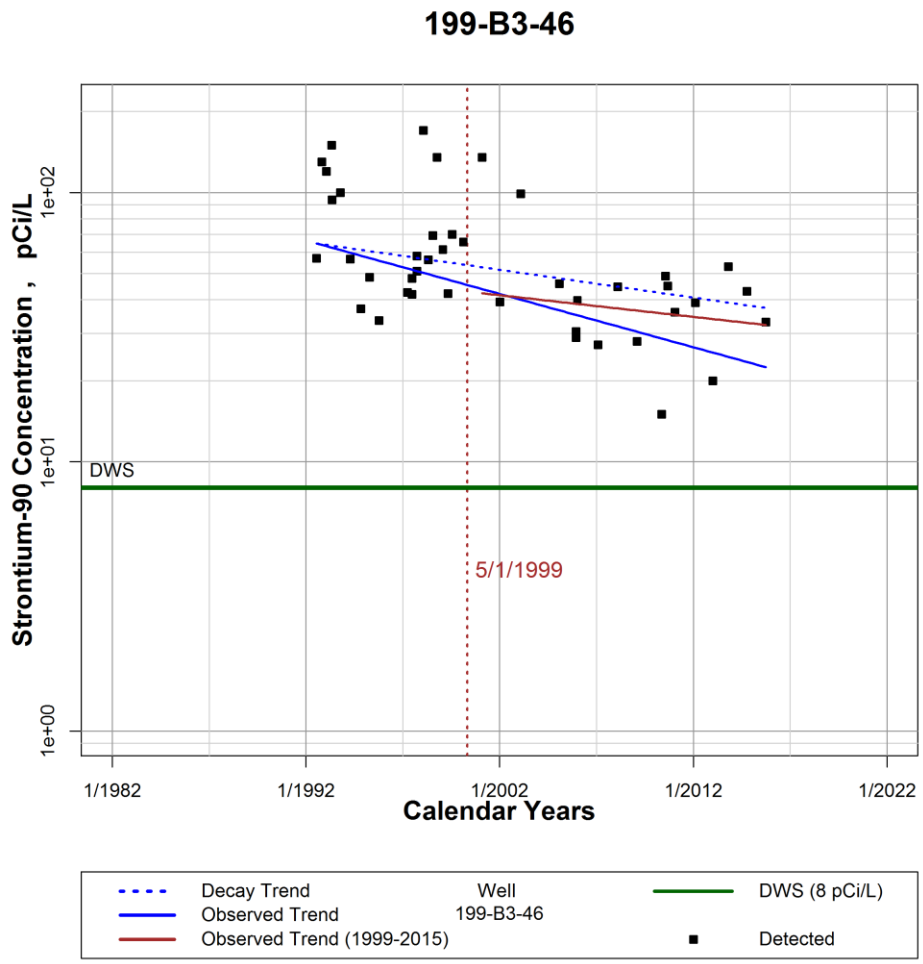

Figure 4-3. Observed Trend Analysis Plot for Well 199-B3-46

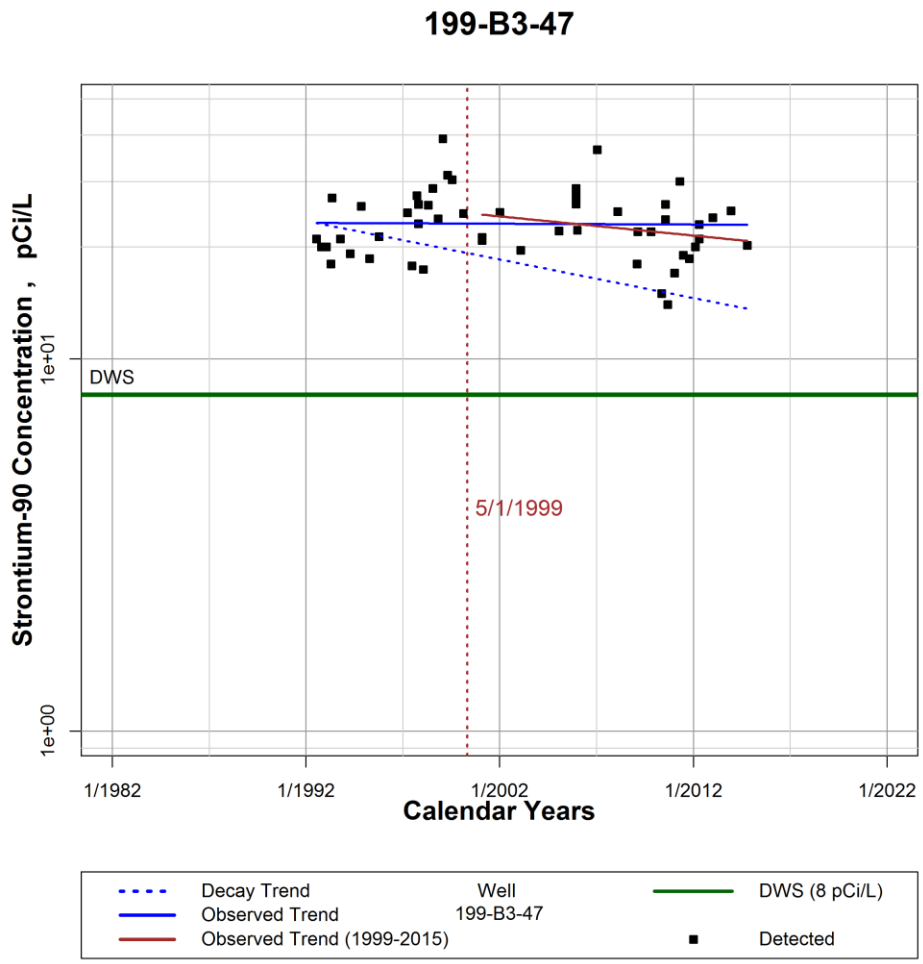

Figure 4-4. Observed Trend Analysis Plot for Well 199-B3-47

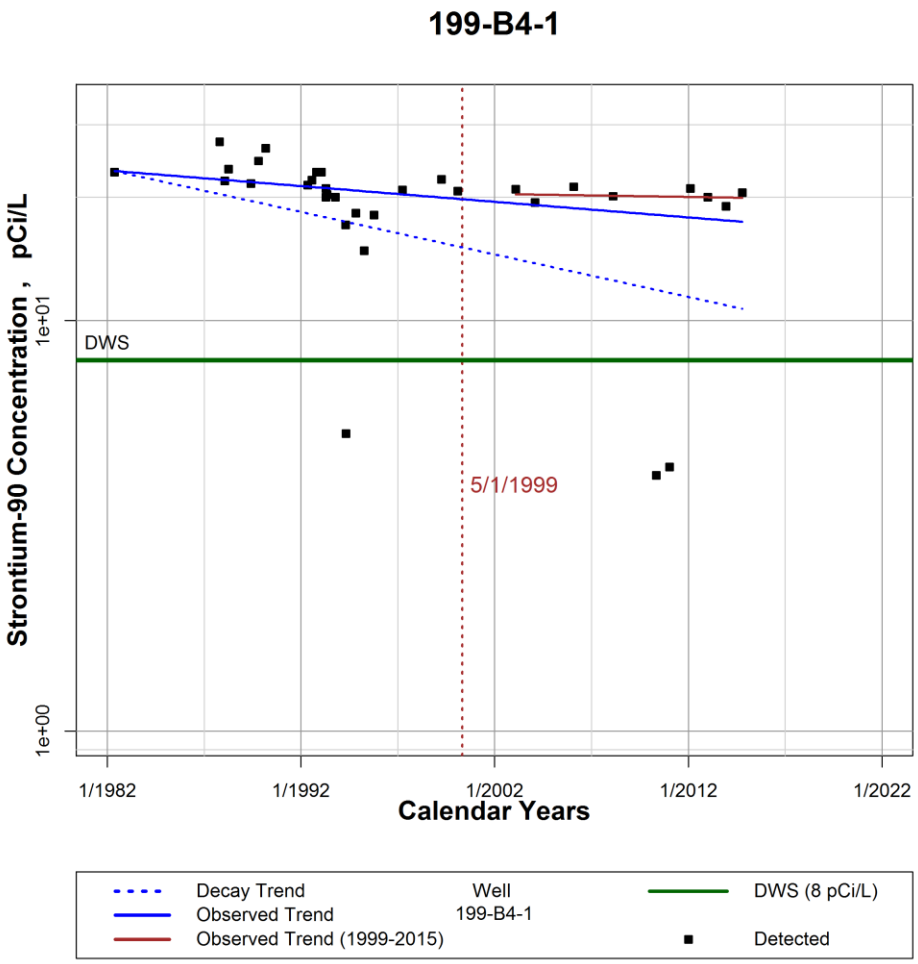

Figure 4-5. Observed Trend Analysis Plot for Well 199-B4-1

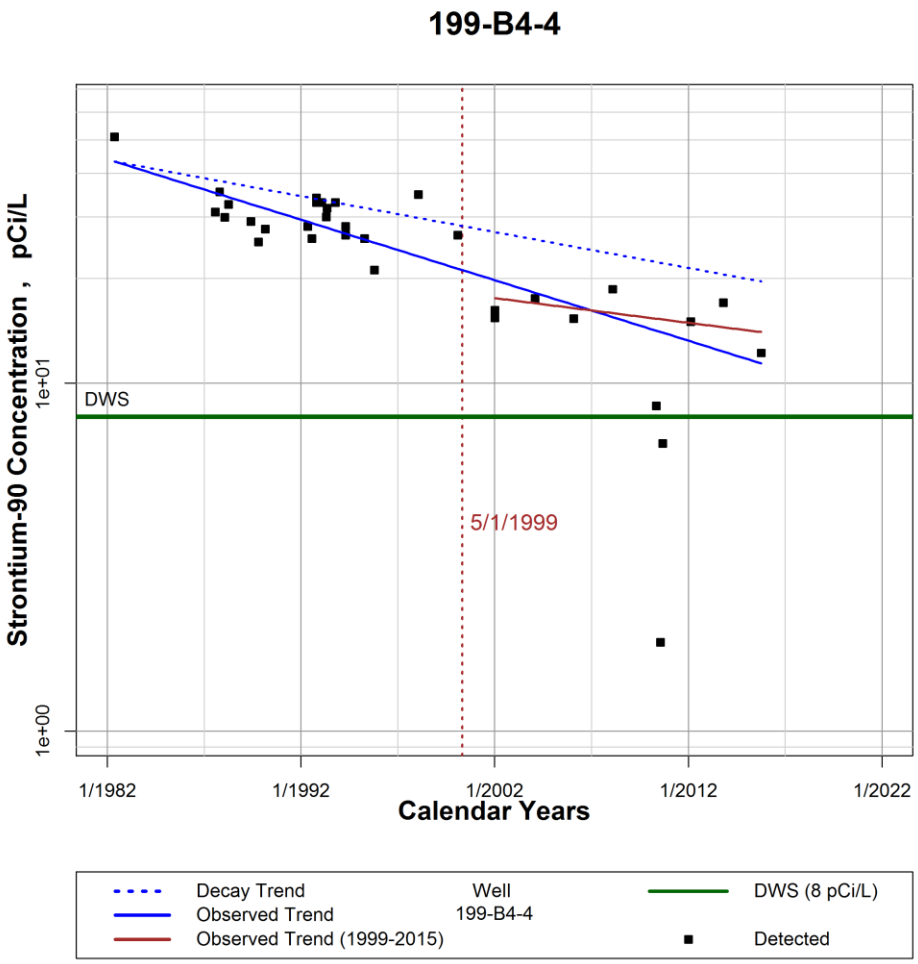

Figure 4-6. Observed Trend Analysis Plot for Well 199-B4-4

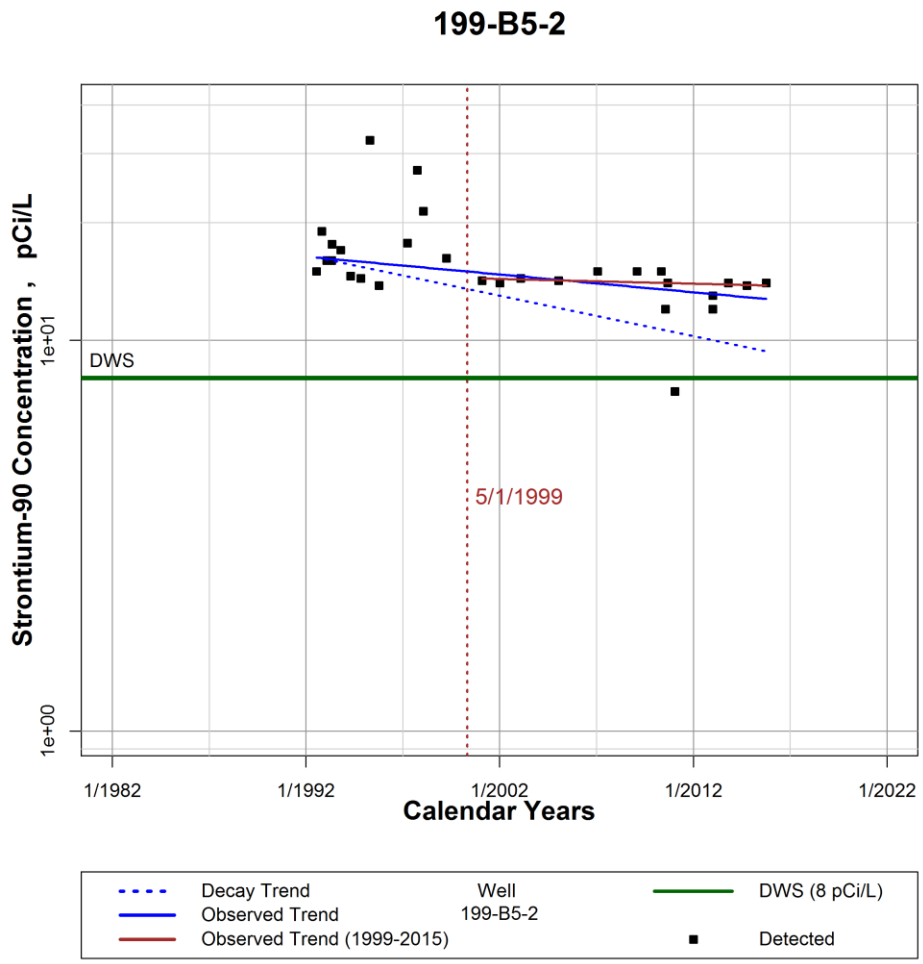

Figure 4-7. Observed Trend Analysis Plot for Well 199-B5-2

4.4 Simulation Period

The 1-D STOMP model setup uses two sequential STOMP simulations similar to ECF-Hanford-15-0129. The first stage, historic pre-2000 simulation, modeled flow through the representative columns for a 2000-year period prior to the commencement of predictive modeling. The purpose of this arbitrarily long simulation period is merely to achieve equilibrium (steady state) in the flow conditions in the model domain. Review of the first-stage matric potential and volumetric water content values over the last 100 years revealed that they had reached equilibrium prior to the end of the simulation. The second stage, predictive post-2000 simulation, modeled flow and transport for a 1000-year period commencing in calendar year 2000.

Predictive simulation of 100-BC GWFTM starts in calendar year 2015 and continues for 125 years. Calibration setup uses simulated concentrations from calendar year 2015 to 2020 to perform trend analysis. This range (2015-2020) was selected so that observed trend analysis (1999-2015) and simulated trend analysis has similar flow conditions (recharge changes from 63 mm/yr to 8 mm/yr in calendar year 2021).

4.5 Uncertainties, Assumptions, and Conservatism

Potential sources of model uncertainties, assumptions, and conservatism for 1-D STOMP simulation and MODFLOW/MT3D based flow and transport model are discussed in section 3.6 of ECF-Hanford-15-0129 and in section 4.2 of SGW-59365, respectively. Some key uncertainties, assumptions, and conservatisms for deriving a continuing source term are as follows:

1. Strontium-90 flux (i.e., the characteristic breakthrough curve) was obtained by assuming a uniformly distributed concentration throughout the soil column. However, in reality, strontium-90 concentration in the vadose zone varies in space.
2. It is known that strontium-90 sources have been contributing to the aquifer for a long time. As a result, it is uncertain which point of the characteristic breakthrough curve represents current time period (i.e., calendar year 2015)
3. Vadose zone 1-D STOMP modeling in the 100 area uses a distribution coefficient of 25 mL/g for strontium-90 but this calculation uses a more conservative value of 15 mL/g which is also consistent with the 100-BC GWFTM.

The requirement to match observed data ameliorates much of these issues.

5 Software Applications

STOMP, MODFLOW-2000-MST, MT3D-MST, Excel®, PEST, R, and Groundwater Vistas™[2] software programs were used for this calculation. These are CH2M Hill Plateau Remediation Company (CHPRC) approved software, managed and used in compliance with the requirements of PRC-PRO-IRM-309, *Controlled Software Management*. STOMP, MODFLOW-2000-MST and MT3D-MST are approved calculation software and Excel®, PEST, and Groundwater Vistas™ are approved support software (CHPRC-00258).

MODFLOW-2000-MST, MT3D-MST, and PEST were executed on the Green Linux® Cluster. The details regarding the cluster is presented below. A copy of the *Software Installation and Checkout Form* for the MODFLOW-2000 and MT3D-MST installation used for this calculation is provided in Attachment A to this ECF.

All the STOMP, MODFLOW-2000-MST, MT3D-MST, and PEST simulations were executed on the INTERA Richland Green Linux cluster that is owned and managed by INTERA, Inc., a pre-selected subcontractor to CHPRC. The computer property tag identifier for the front-end node is #469 at INTERA's Richland, Washington office. This node is a Dell® PowerEdge® R510 with two six-core Intel® Xeon® X5660 processors @ 2.80GHz and 48 GB of RAM. As given by the command "uname –a", the operating system details are:

```
Linux green 2.6.32-32-server #62-Ubuntu SMP Wed Apr 20 22:07:43
UTC 2011 x86_64 GNU/Linux (gcc version Ubuntu 4.4.3-4ubuntu5
4.4.3)
```

[2] Groundwater Vistas™ is a trademark of Environmental Simulations, Inc.

[2] Linux® is the registered trademark of Linus Torvalds in the U.S. and other countries

[3] Intel® and Xeon® are registered trademarks of Intel, Incorporated in the United States and other countries.

[4] Dell® and PowerEdge® are registered trademarks of Dell Inc.

Microsoft Excel® spreadsheets were used to tabulate mass inventory, and chart modeling results produced by STOMP, MODFLOW-2000, MT3D-MST and PEST. Groundwater Vistas™ was used in pre-processing some input. These calculations and analysis were performed on a laptop computer with INTERA ID PSC-Lithium.

5.1 Approved Software

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

5.1.1 Description

- Workstation type and property number (from which software is run): STOMP, MODFLOW, and MT3D were executed on the INTERA Richland GREEN Linux®[3] Cluster that is owned and managed by INTERA, Inc., a pre-selected subcontractor to CHPRC. The computer property tag for the front-end node is #469 at INTERA's office in Richland, Washington. This node is a Dell® PowerEdge® R510 with two 6-core Intel®[4] Xeon X5660 processors @ 2.80GHz and 48 GB of RAM. As given by the command "uname –a", the operating system details are

  ```
  Linux green 3.2.0-54-generic #82-Ubuntu SMP Tue Sep 10 20:08:42 UTC
  2013 x86_64 GNU/Linux
  ```

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

STOMP

- Software Title: STOMP
- Software Version: CHPRC Build 4
- HISI Identification Number: 2471

MODFLOW

- Software Title: MODFLOW-2000-MST
- Software Version: CHPRC Build 7 (executable "mf2k-mst-0007dpl.x"), double precision compilation

[3] Linux® is the registered trademark of Linus Torvalds in the U.S. and other countries.

[4] Intel® is a registered trademark of Intel Corporation.

- Hanford Information System Inventory (HISI) Identification Number: 2517 (Safety Software, Level C)

MT3D-MST

- Software Title: MT3D-MST
- Software Version: CHPRC Build 7 (executable name “mt3d-mst-0007dpl.x”) , double precision compilation
- HISI Identification Number: 2518 [Support Software; CHPRC-00258]

R

- Version 3.2.3

The R programming environment, a language and environment for statistical computing and graphics, (R: A Language and Environment for Statistical Computing, by R Core Team, R Foundation for Statistical Computing, Vienna, Austria, 2012. ISBN 3-900051-07-0, http://www.R-project.org.; R: A Language for Data Analysis and Graphics, Journal of Computational and Graphical Statistics, 5, 299–314, Ihaka & Gentleman, 1996) was used to perform the trend analysis calculations listed in Section 6. The following R packages were also used:

- R: package **tis** is a set of functions and S3 classes for time indexes and time indexed series.
- R: package **date** is set of functions to manipulate objects of classes "POSIXlt" and "POSIXct" representing calendar dates and times.

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 CHPRC. Because MODFLOW 2000-MST and MT3D-MST are graded as 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 Number 2517 and 2518.

6 Calculation

A 1-D STOMP model was created and run using the processes (i.e., model parameters, initial and boundary conditions) described in ECF-Hanford-15-0129 and chapter 4 in this document. A surface at the water table was defined to calculate strontium-90 flux entering the saturated zone. Figure 6-1 shows strontium-90 flux entering the saturated zone over time, which is known as characteristic breakthrough curve. For all four representative columns, STOMP simulated similar characteristic solute breakthrough curves. Any of these four characteristic breakthrough curves could be used to determine the temporal distribution of strontium-90 activity for the source/sink mixing package. However, results from representative column 6 were used as this column represents source area closest to the river. It is important to define the starting point from the characteristic curve that represents current condition (i.e.,

calendar year 2015). The initial concentration in the 1-D STOMP column is assumed to be uniformly distributed throughout the soil column except clean backfill at top and 0.5 m of clean soil just above water table. Moreover, the vadose zone transport simulation was initiated at the beginning of calendar year 2000. It is known that waste sites within the strontium-90 plume have been leaking for a long time and contaminated vadose zone source has already reached water table. That means the front segment of the breakthrough curve (i.e., a few years from the start of the simulation) is already gone. Simulation year 2015 when strontium-90 flux is reasonably high enough is assumed to be representing the current condition. As described in section 3, the release rate to the saturated zone from the vadose zone is scaled and converted to source/sink mixing package for the 100-BC GWFTM.

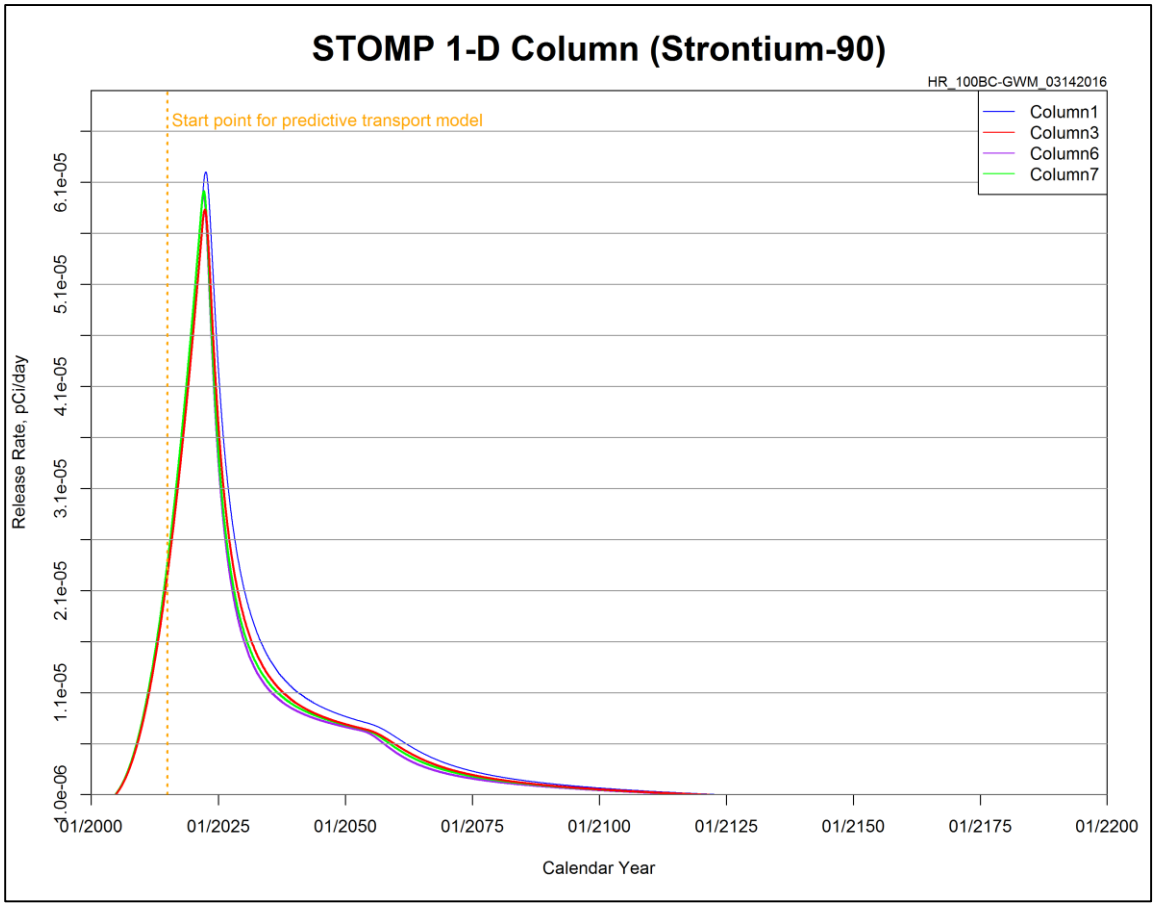

Figure 6-1. Strontium-90 Flux for the Stratigraphic Representative Column in the 100-BC Operable Unit

MT3D-MST based 100-BC transport model for strontium-90 was simulated under PEST framework for deriving a calibrated source/sink mixing package. PEST estimates the pilot point based soil concentration in the soil column above each uppermost active groundwater model cell within the source area required to match the trend from May 1999 onward. This period was chosen instead of the complete record because it uniformly shows much less decline, and is thus more conservative. The soil concentration is then converted to total activity available in the vadose zone using equation 3.

$$M = \sum_{n=1}^{t} \rho_d * C_n * V_n \tag{3}$$

Where, M is the total mass (M) in the vadose zone, ρ_d is bulk density (M/L^3) of soil, C_n is the calibrated soil concentration (M/M), V_n is vadose zone volume above groundwater cell (L^3), and t is the total number of grid cells in Layer 1 of the groundwater model.

The overall calibration process was as follows:

- Run the PEST software
- Review estimated model parameters and model fit to data for reasonableness and agreement
- Identify potential conceptual or parameter issues to be resolved and an approach for fixing
- Implement parameter, model setup, or other change
- Repeat

PEST provides several outputs of the process, including a file listing the residual (.res) between simulated and observed. This data was used to review goodness of fit. No absolute value of goodness of fit was set as a stopping criteria; an overall weight of evidence was considered including goodness of fit and plausibility of estimated parameters.

7 Results/Conclusions

PEST was run for several iterations to obtain good fits of the simulated trends with the observed trends. Figure 7-1 shows the pilot point locations used in the PEST simulation and the sampling well locations where post May 1999 trends that were fitted. Figure 7-2 through Figure 7-7 show the results of the trend analysis. The slopes derived from data trend analyses for these locations are listed in Table 7-1. The spatial distribution of strontium-90 soil concentrations as estimated by PEST calibration within the assumed vadose source zones are displayed in Figure 7-1. PEST estimated a soil concentration between 0.8 and 0.96 pCi/g near well 199-B4-4 to fit the observed groundwater concentration trend. No observed soil concentration data (Table 7-1) were available to verify the possible ranges of soil concentration at well 199-B4-4. However, estimated observed soil concentration at well 199-B4-15 (Table 7-1) range from 0.40 to 5.8 pCi/g which is very close to well 199-B4-4. Therefore, it is possible that actual soil concentrations are higher near 199-B4-4. No source zone was applied at 199-B4-15 because the well does not have any Sr-90 groundwater data for trend evaluation. PEST estimated soil concentrations in other areas are similar to the estimated values in Table 7-1.

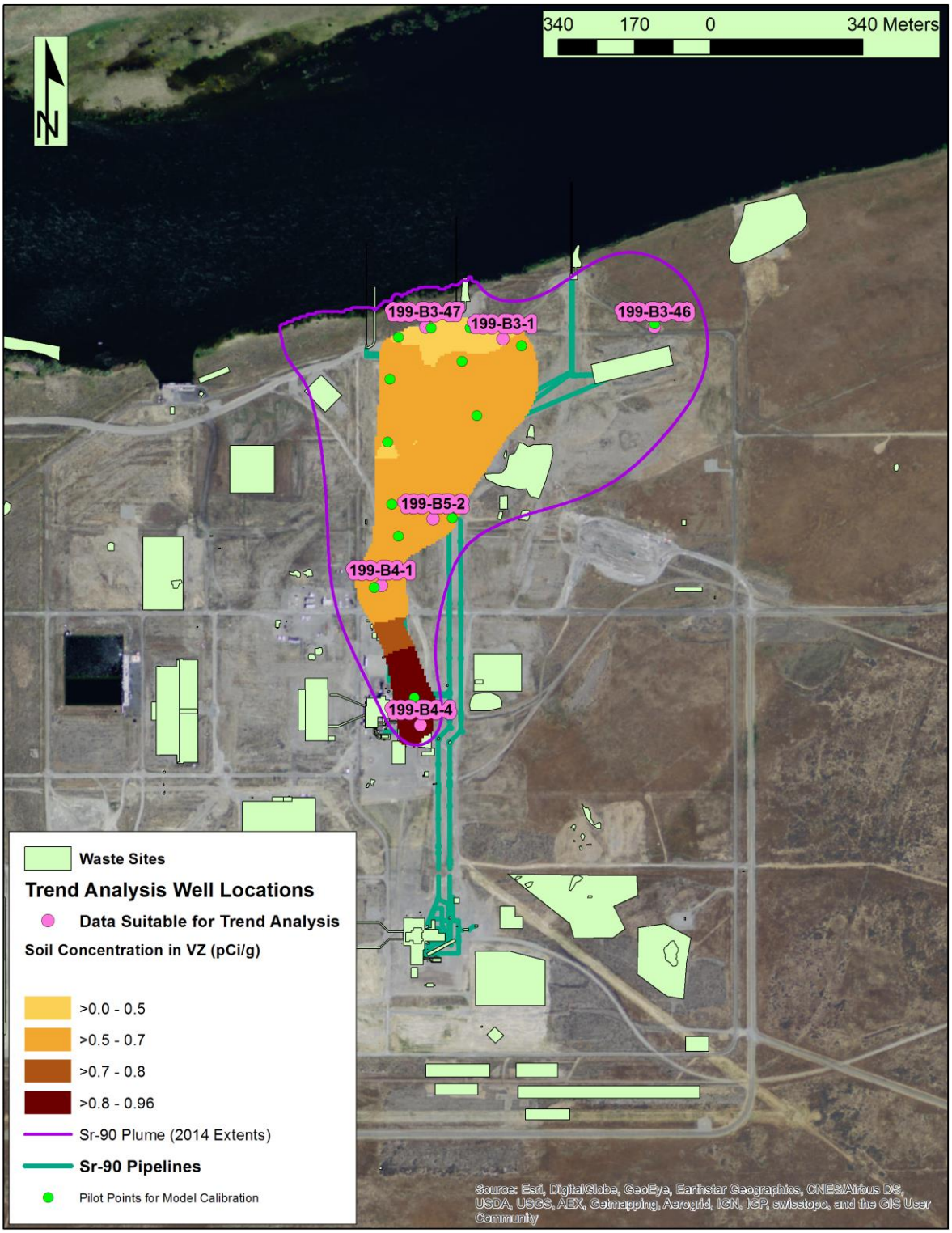

Figure 7-1. PEST Calibrated Soil Concentration in the Vadose Zone

Table 7-1. Strontium-90 Concentration Trend at Selected Monitoring Wells

Well Name	Observed Slope	Simulated Slope	Residual
199-B3-1	-5.92E-03	-6.02E-03	9.43E-05
199-B3-46	-8.03E-03	-4.91E-03	-3.12E-03
199-B3-47	-5.17E-03	-2.15E-03	-3.02E-03
199-B4-1	-7.18E-04	-4.11E-04	-3.07E-04
199-B4-4	-6.46E-03	-8.30E-03	1.84E-03
199-B5-2	-1.21E-03	-1.23E-03	1.87E-05

The 100-BC transport model was used to simulate conditions for both continuing and non-continuing sources present in order to observe the impact on the simulated trend. Figure 7-2 though Figure 7-7 show the comparison between model results with continuing and non-continuing sources. In all cases except 199-B3-46, the no source results show a faster rate of decline than radioactive decay, indicating that the high groundwater velocity is advecting strontium away from the well. Figure 7-3 shows that observed trend fits well with model results without a source being present. Thus, no source was applied in the vicinity of 199-B3-46 and model results with and without a continuing source overlap. The results with the estimated vadose zone source match the general observed trend. These observations, coupled with the general agreement with decayed soil concentrations in Table 7-1, suggest that the source is plausible.

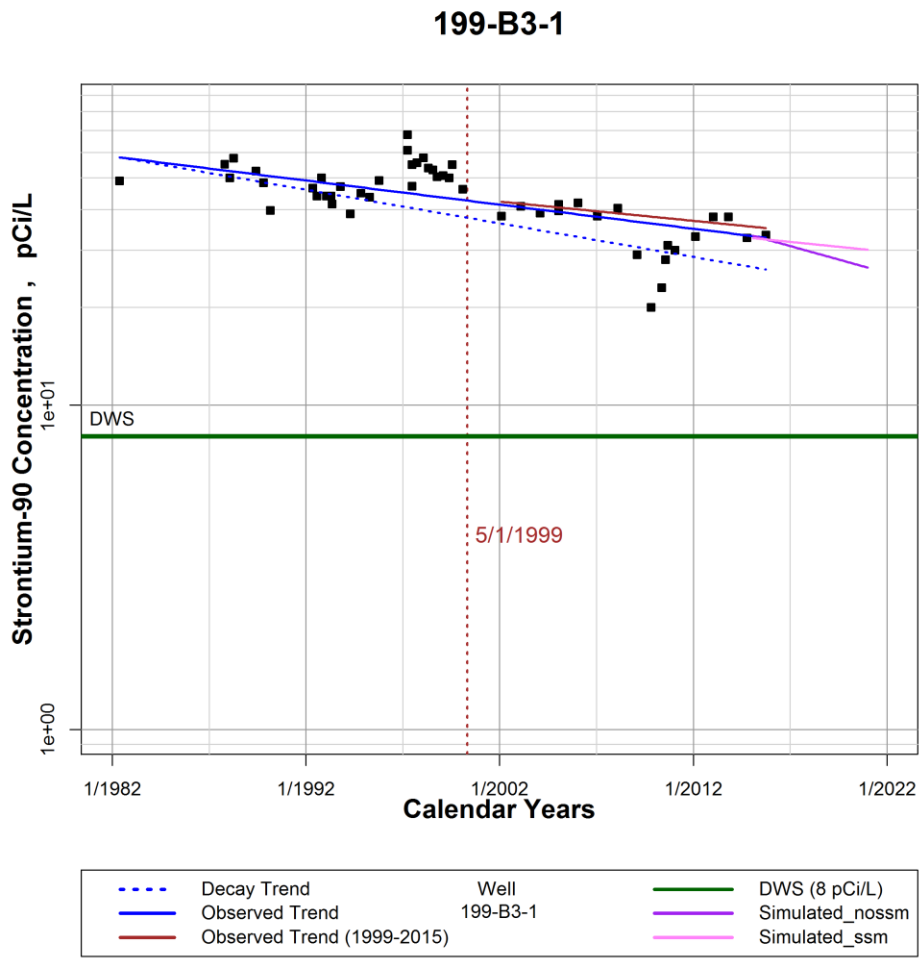

Figure 7-2. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and without Continuing Source for Well 199-B3-1

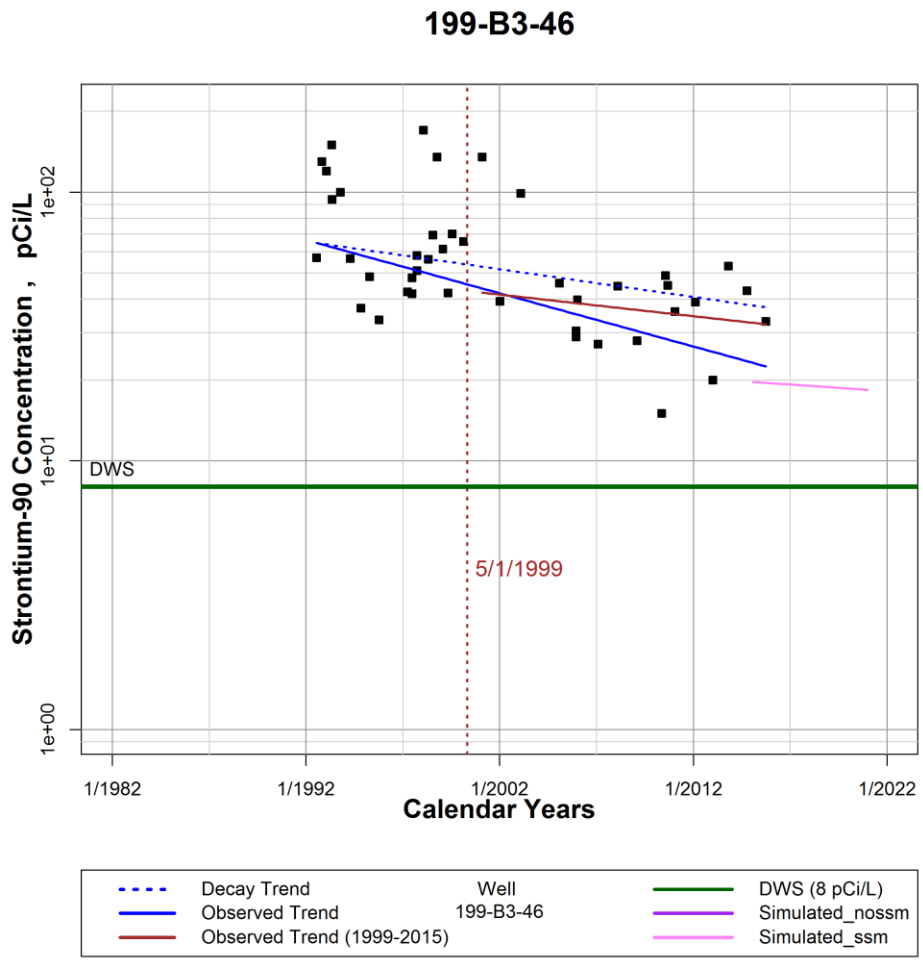

Figure 7-3. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and Without Continuing Source for Well 199-B3-46

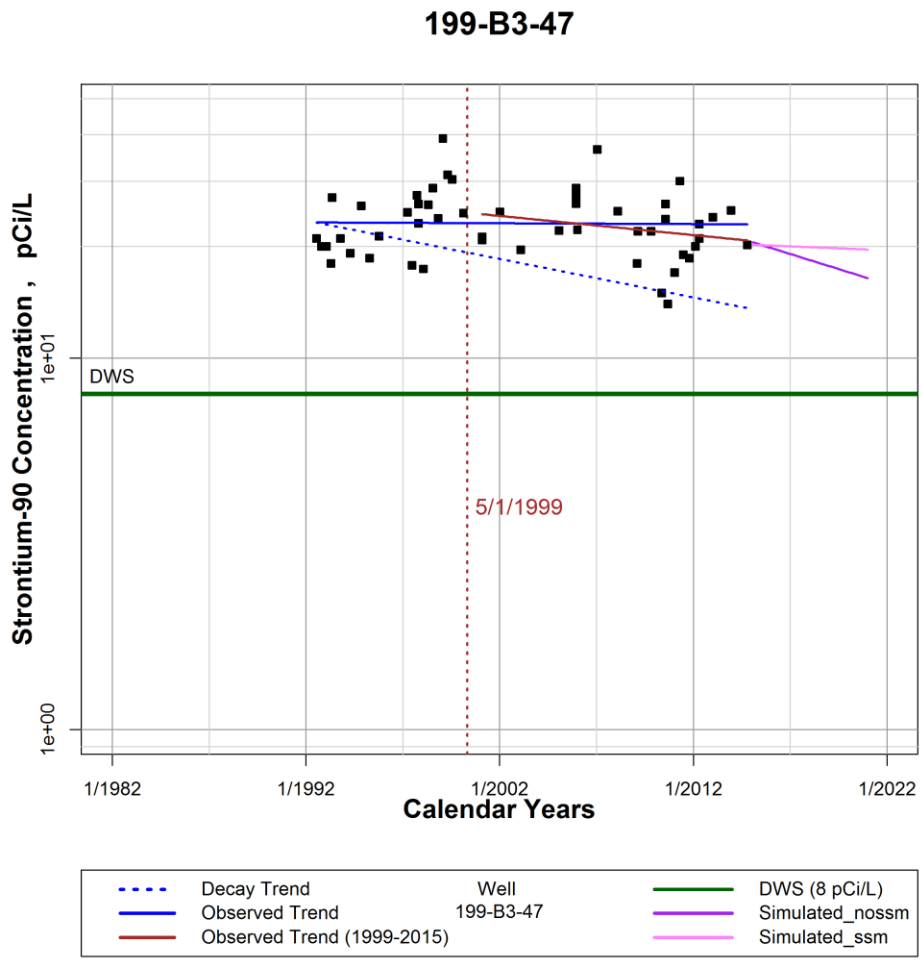

Figure 7-4. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and Without Continuing Source for Well 199-B3-47

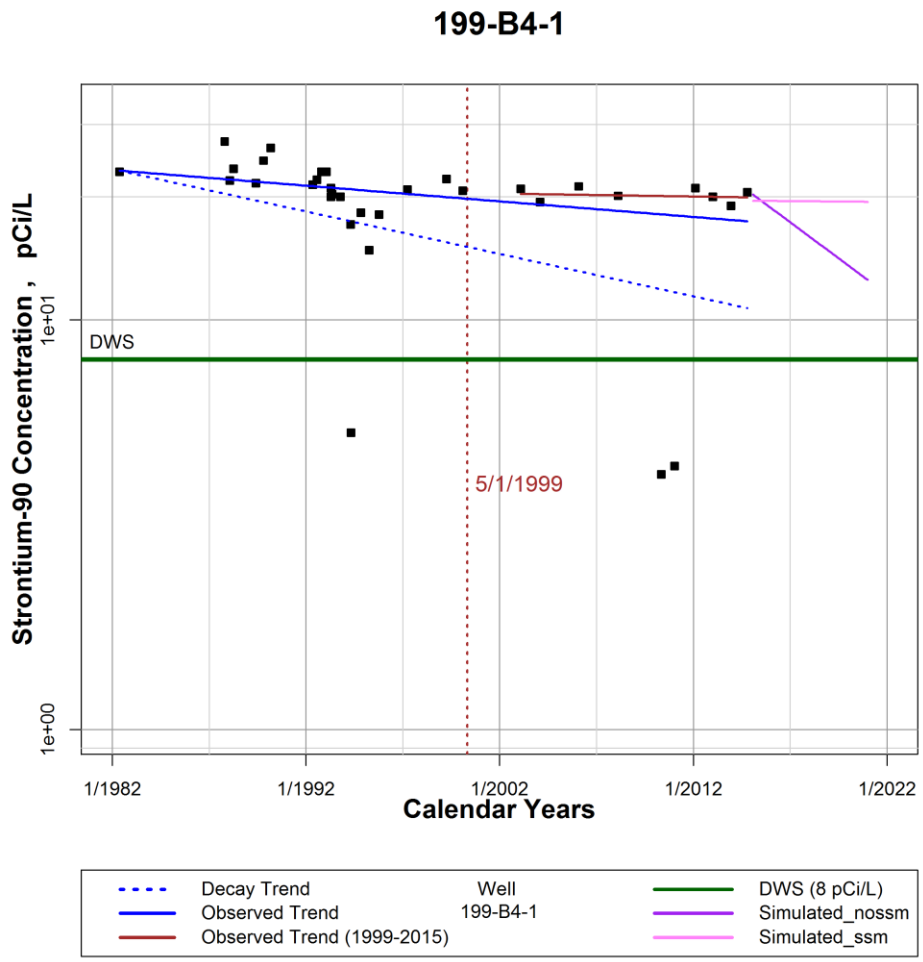

Figure 7-5. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and Without Continuing Source for Well 199-B4-1

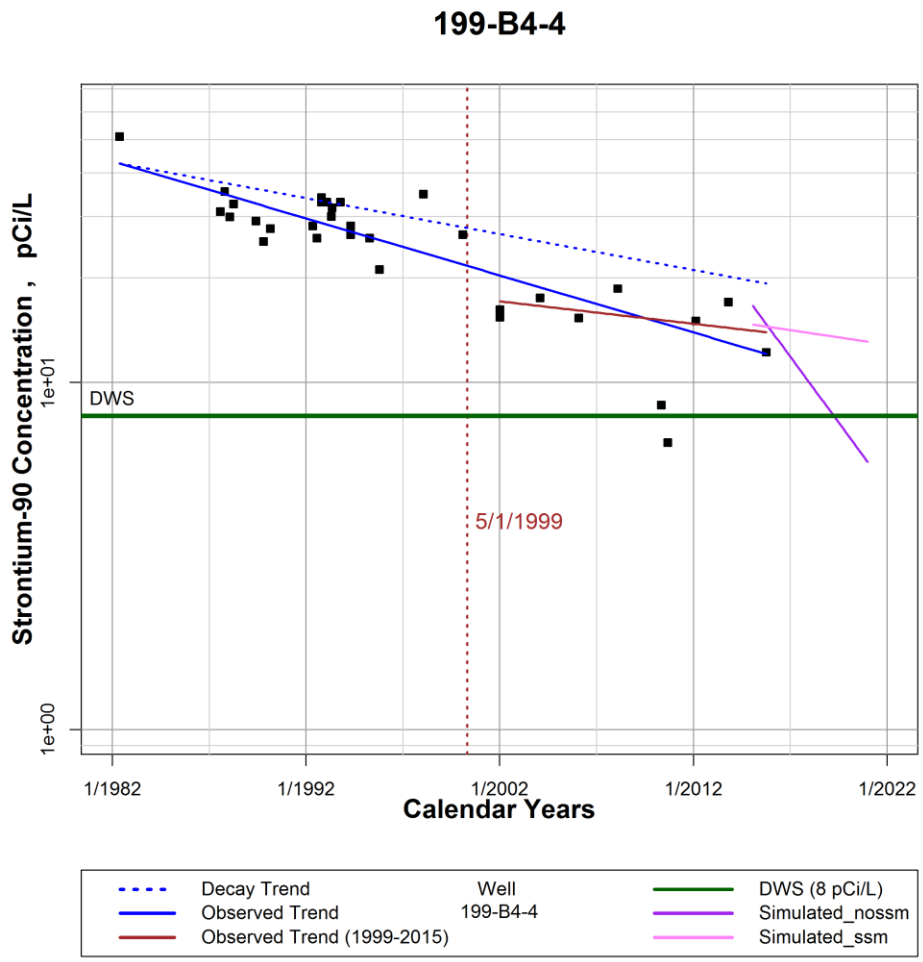

Figure 7-6. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and without Continuing Source for Well 199-B4-4

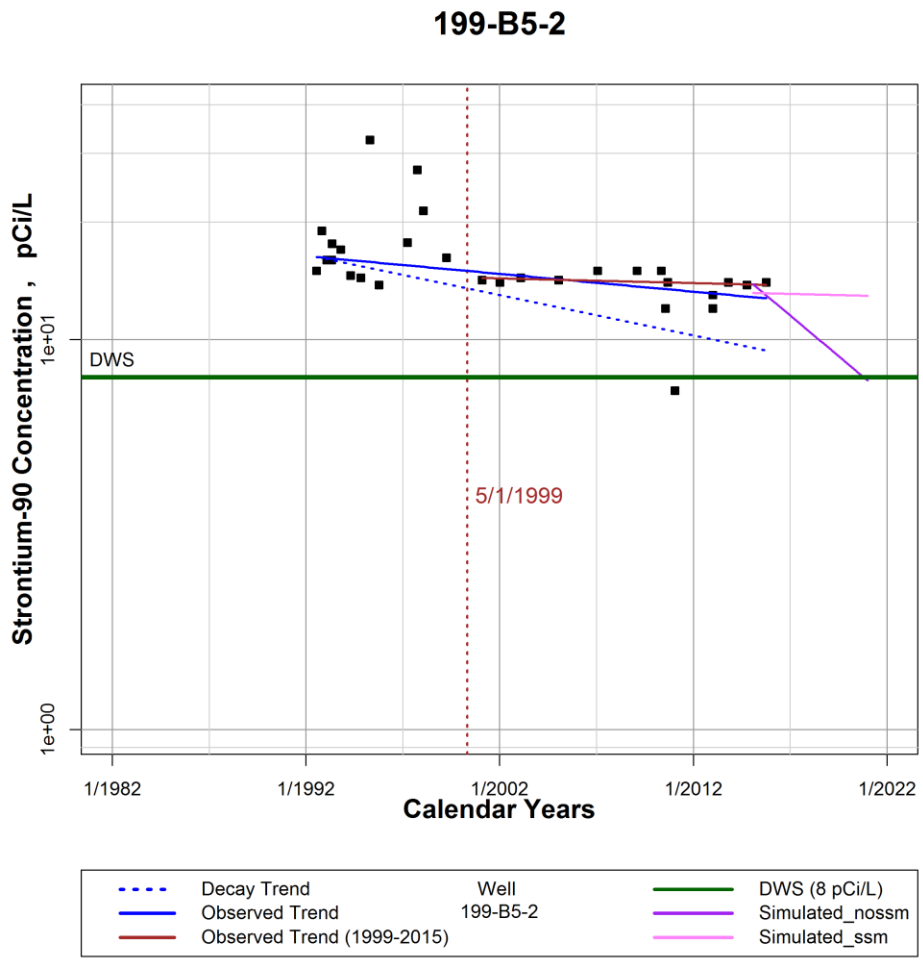

Figure 7-7. Comparison of Strontium-90 Concentration Trends between Model Results with Continuing Source and Without Continuing Source for Well 199-B5-2

The 100-BC RI/FS considered several remedial alternatives to keep Cr(VI) and strontium-90 concentrations below MCL. The estimated SSM concentrations would be impacted at the source locations where remedial alternatives were implemented. For example, one of the remedial alternatives at waste site 116-B-11 considered in-situ reduction in June, 2019 for Cr(VI) mass reduction. The remedial action would result in approximately 1.75E-02 m/d areal recharge for the corresponding month. Therefore, recharge based SSM concentrations for strontium-90 at waste site 116-B-11 will be diluted for the high recharge on June 2019. In addition, it was assumed that the high recharge would not affect the strontium-90 mass loading rate at the waste site 116-B-11 because it is applied only for 1 month.

The forecasted strontium-90 groundwater concentrations in model layer 1 are presented for calendar years 2035 and 2065 in Figure 7-8 and Figure 7-9, respectively. Because the source location is conceptualized as within the vadose zone, the strontium-90 concentrations are highest in model layer 1, which incorporates the water table. The maximum aquifer concentration drops below the drinking water standard of 8.0 pCi/L after about 65 years (calendar year 2080).

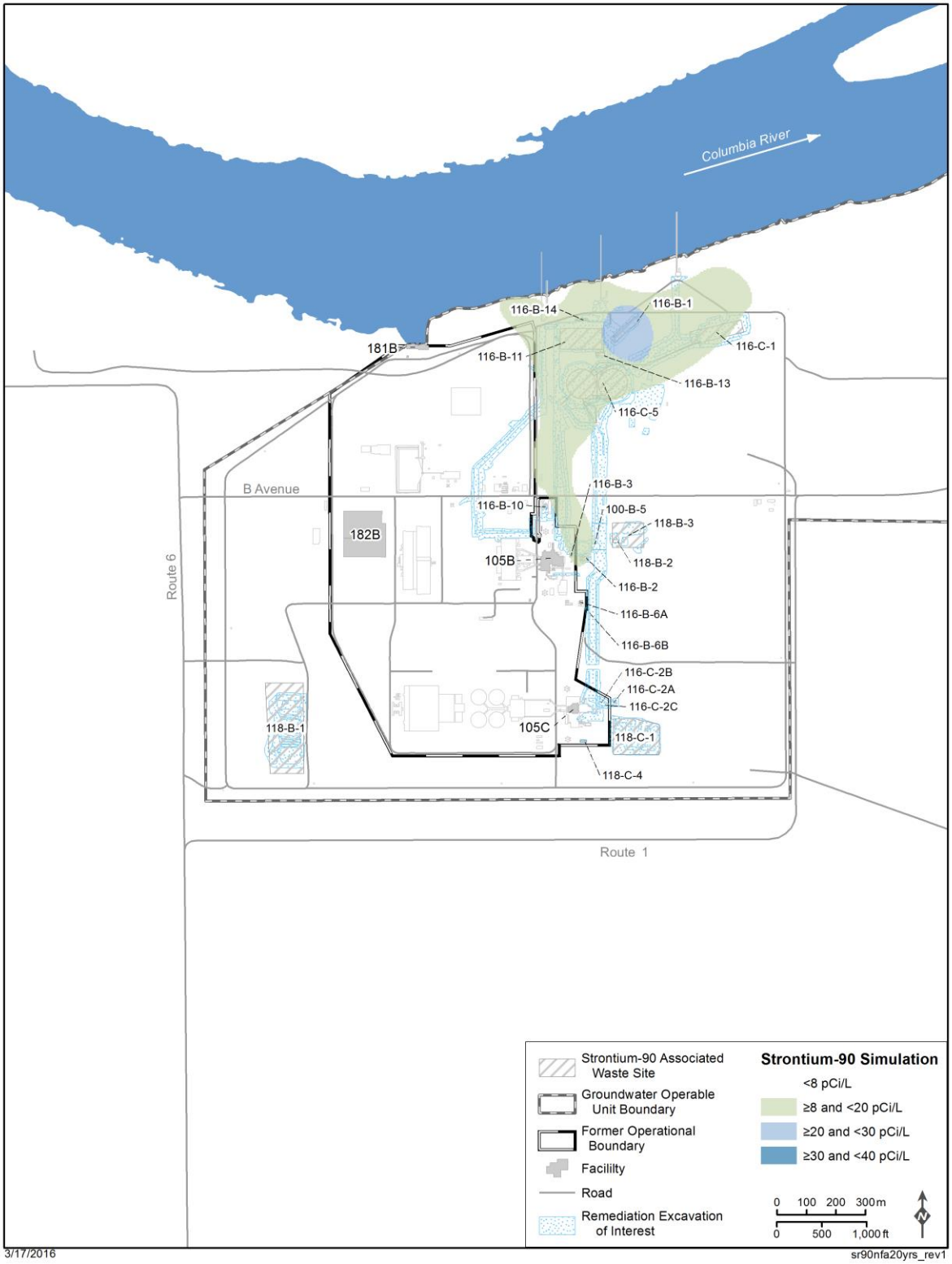

Figure 7-8. Simulated 2035 Strontium-90 Plume Extents in Model Layer 1 - No Further Action Case

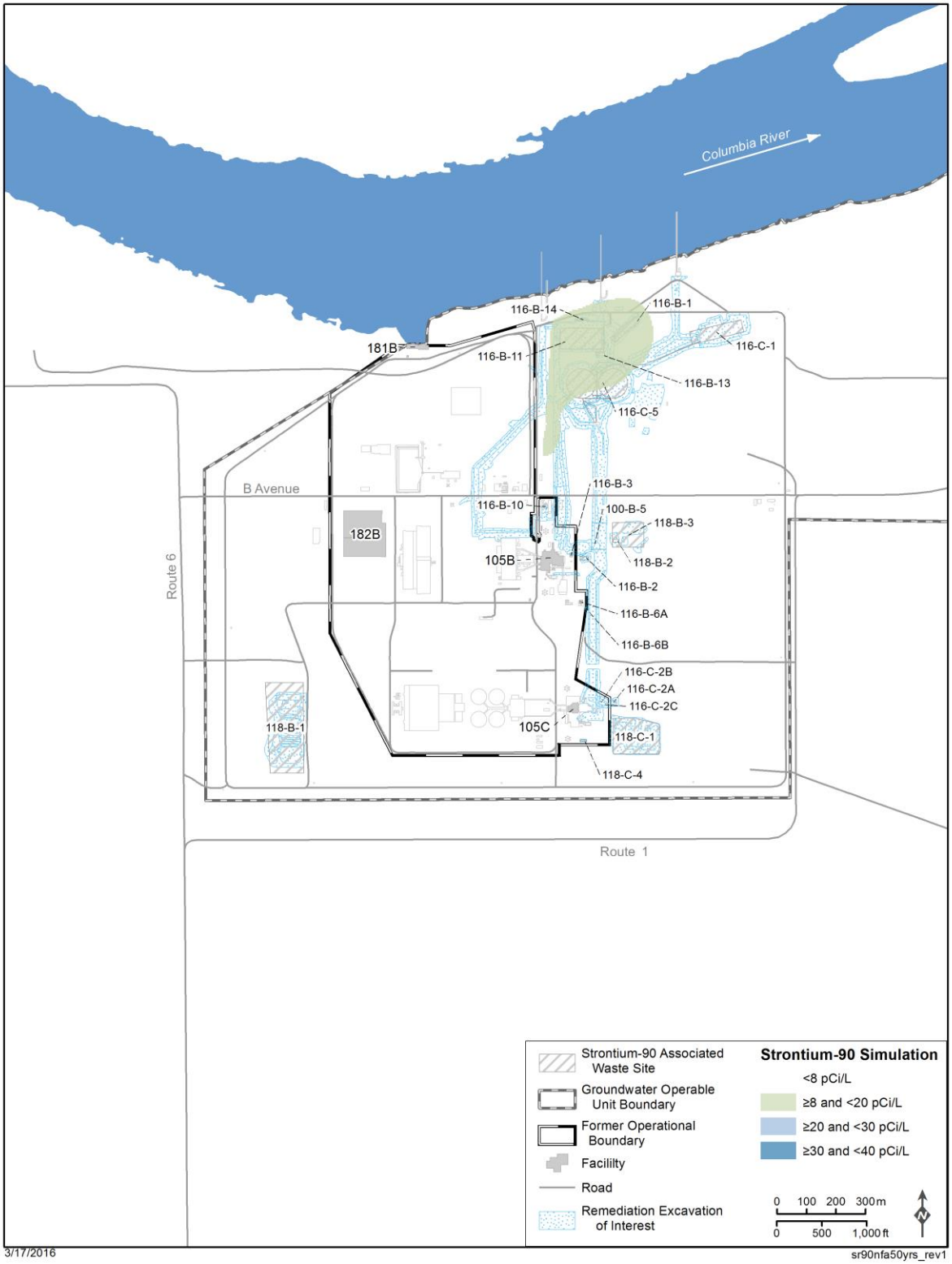

Figure 7-9. Simulated 2065 Strontium-90 Plume Extents in Model Layer 1 - No Further Action Case

8 References

CHPRC-00176, 2011, *STOMP Software Management Plan*, Rev. 2, CH2M Hill Plateau Remediation Company, Richland, Washington.

CHPRC-00211, 2011, *STOMP Software Test Plan*, Rev. 1, CH2M Hill Plateau Remediation Company, Richland, Washington.

CHPRC-00222, 2011, *STOMP Functional Requirements Document*, Rev. 1, CH2M Hill Plateau Remediation Company, Richland, Washington.

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.

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Attachment A

Software Installation and Checkout Form for STOMP and MODFLOW and Related Codes

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: STOMP (Subsurface Transport Over Multiple Phases) Software Version No.: Bld 4

EXECUTABLE INFORMATION:

2. Executable Name (include path):

All executable files installed in directory [redacted]/bin

MD5 File Signature	Executable File Name
6536b8e12d8c5b83dca76f2c947b6153	stomp-wae-bcg-chprc04i.x
e0cdf04bc1a2f6c55c5a1b499939f663	stomp-wae-bcg-chprc04l.x
6e72340bb39f6056e232fe5ff241c4d4	stomp-wae-bd-chprc04i.x
3f837a0fb8d9f47dbcada686f542d7fc	stomp-wae-bd-chprc04l.x
7e5b4cc36a8991b3d5a8ea2ed155ce47	stomp-wae-cgsq-chprc04i.x
00a898c0c3ec06817485781ad1c9ec46	stomp-wae-cgsq-chprc04l.x
f18ff5ab5667065d8ab12657344fb6a0	stomp-wae-cgst-chprc04i.x
061af86cf21ad8435b046d0efabe971b	stomp-wae-cgst-chprc04l.x
3c8111a9855dc0e430bf3c8a7abcf37e	stomp-w-bcg-chprc04i.x
20436d615a94955a2ce8eecdb8cba546	stomp-w-bcg-chprc04l.x
8b3df29df21d040189c3e2a50ef823bb	stomp-w-bd-chprc04i.x
066a289a75aedb933eb2536da5d7d1ff	stomp-w-bd-chprc04l.x
c8e62ad7a0d9b6fca39d8a8952ef5d8e	stomp-w-cgsq-chprc04i.x
28ad16806e1307aca51fd7bf89793e75	stomp-w-cgsq-chprc04l.x
6c25051016db2fe1f883a7caaaab1e97	stomp-w-cgst-chprc04i.x
ff9ff6f29b3469419ffaece87d7e772b	stomp-w-cgst-chprc04l.x
0c3e3fba40f5b93e71bcf9586432fd27	stomp-w-r-bcg-chprc04i.x
78492aee80a8c2d0a4e82aabf4a9c213	stomp-w-r-bcg-chprc04l.x
84b129786aba9c4be884e15e45a67389	stomp-w-r-bd-chprc04i.x
e990f1566c8099a8d54508de3da9cd88	stomp-w-r-bd-chprc04l.x
18a589a2b55aab2db290efea19b39351	stomp-w-r-cgsq-chprc04i.x
6569959476772a137df35ce874821889	stomp-w-r-cgsq-chprc04l.x

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

COMPILATION INFORMATION:

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

Tellus Subsurface Modeling Platform

5. Operating System (include version number):

Linux tellusmgmt.rl.gov 2.6.18-308.4.1.el5 #1 SMP Tue Apr 17 17:08:00 EDT 2012 x86_64 x86 64 x86 64 GNU/Linux

INSTALLATION AND CHECKOUT INFORMATION:

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

Green Linux Cluster

7. Operating System (include version number):

Linux green 3.2.0-35-generic #55-Ubuntu SMP Wed Dec 5 17:42:16 UTC 2012 x86_64 x86_64 x86 64 GNU/Linux

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CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: STOMP (Subsurface Transport Over Multiple Phases) Software Version No.: Bld 4

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

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]/itc

10. Procedure(s):

CHPRC-00211 Rev 1, STOMP Software Test Plan

11. Libraries:

N/A (static linking)

12. Input Files:

Input files for ITC-STOMP-1, ITC-STOMP-2, and ITC-STOMP-2
(Baseline for comparison are results files from ATC-STOMP-1, ATC-STOMP-2, and ATC-STOMP-3 prepared on Tellus during acceptance testing)

13. Output Files:

plot.* files produced by STOMP in testing

14. Test Cases:

ITC-STOMP-1, ITC-STOMP-2, and ITC-STOMP-3

15. Test Case Results:

Pass for all executable files listed above.

16. Test Performed By: WE Nichols

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

18. Disposition (include HISI update):

Accepted; Installation noted in HISI for users TJ Budge, N Hasan, A Mayenna, WJ McMahon, WE Nichols, S Mehta, H Rashid.

Prepared By:

19. Software Owner (Signature)	WE Nichols Print	25 APRIL 2013 Date

20. Test Personnel:

Sign	WE Nichols Print	25 APRIL 2013 Date
Sign	Print	Date
Sign	Print	Date

Approved By:

21. Software SME (Signature)	N/R (per CHPRC-00211 Rev 1) Print	Date

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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 and Related Codes Software Version No.: Bld 7

EXECUTABLE INFORMATION:

2. Executable Name (include path):

```
Following executable files installed and tested:

MD5 Signature (unique ID)         Executable File Name   Code
--------------------------------  ---------------------  --------------------------
8b0b28c5e102e63df95de542d83d013b  mf2k-chprc07spl.x      MODFLOW-2000 single precision
2fade33e27978063a9a70ff8605e4c0c  mf2k-chprc07dpl.x      MODFLOW-2000 double precision
d879defafdc5ad25be51a484d73ea65d  mf2k-mst-chprc07spl.x  MODFLOW-2000-MST single prec.
80d670658425653bf5bcbb97ad2a2730  mf2k-mst-chprc07dpl.x  MODFLOW-2000-MST double prec.
d879defafdc5ad25be51a484d73ea65d  mt3d-chprc07spl.x      MT3DMS single precision
80d670658425653bf5bcbb97ad2a2730  mf3d-chprc07dpl.x      MT3DMS double precision
400023b180f265b0341a6ea1f75f19c3  mt3d-mst-chprc07spl.x  MT3DMS-MST single precision
d3ea3cf04938fcba54eea87cf1eb4ab0  mt3d-mst-chprc07dpl.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):

Tellus Subsurface Modeling Platform (Linux(R) cluster)

5. Operating System (include version number):

Redhat Linux 5.8
2.6.18-308.4.1.el5 #1 SMP Tue Apr 17 17:08:00 EDT 2012 x86 64 x86 64 x86 64 GNU/Linux

INSTALLATION AND CHECKOUT INFORMATION:

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

INTERA's Green Linux(R) cluster

7. Operating System (include version number):

Linux green 3.2.0-65-generic #98-Ubuntu SMP Wed Jun 11 20:27:07 UTC 2014 x86_64 x86_64 x86 64 GNU/Linux

8. Open Problem Report? ◉ No ○ Yes PR/CR No.

TEST CASE INFORMATION:

9. Directory/Path:

[redacted]/modflow-build-7/

10. Procedure(s):

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

11. Libraries:

N/A (static linking)

12. Input Files:

Per CHPRC-00259 Rev. 3

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: MODFLOW and Related Codes Software Version No.: Bld 7

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 tests passed

16. Test Performed By: WE Nichols

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

18. Disposition (include HISI update):

Installation added to HISI Entry 2517 (MODFLOW) and 2518 (MT3DMS)

Prepared By:

19. William E. Nichols — Digitally signed by William E. Nichols DN: cn=William E. Nichols, o=CHPRC, ou=Risk & Modeling Integration, email=william_e_nichols@pnl.gov, c=US... Date: 2015.03.31 11:23:02 -07'00' — Software SME (Signature) | WE Nichols (Print) | Date

20. Test Personnel:

Sign	Print	Date
	WE Nichols	

Approved By:

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

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Attachment B

R Scripts for Trend Analysis and Plot Generation

MakeHydroPlots_SR90_model_new.R

```
library("tis")
library("date")
source("TheilSen.R")

#Remove previous results
unlink("./plots",recursive=TRUE)
file.remove("stats_1999-2015.csv")
file.remove("stats_all.csv")
file.remove("stats_simulated.csv")

#
dir.create("./plots")
DWS=8
basetime<-as.numeric(mdy.date(1,1,1982))/365.25

#Read in observed results to display on the charts
wellnames<-read.table("welllist.txt",header=TRUE,sep=",")

wells<-unique(wellnames$WELLID)

obs<-read.table("Sr90_100BC_GW_Data.txt",header=TRUE,sep=",")
obs_sorted<-obs[order(obs$SAMP_SITE_NAME,as.Date(obs$SAMP_DATE_TIME,
format="%m/%d/%Y")),]
obs_sorted$STD_VALUE_RPTD<-obs_sorted$STD_VALUE_RPTD
tmpDate<-paste(substr(obs_sorted$SAMP_DATE_TIME,7,10),"-
",substr(obs_sorted$SAMP_DATE_TIME,1,2),"-",substr(obs_sorted$SAMP_DATE_TIME,4,5),sep="")
obsJULTIME<-(as.numeric(mdy.date(month(tmpDate),day(tmpDate),year(tmpDate)))/365.25)-basetime


# Read in model results

basetime_sim<-as.numeric(mdy.date(1,1,1982))/365.25

mods<-read.delim("simulated_Sr90_output.dat",header=FALSE,sep="")
mods$V4<-mods$V4/1000
tmpDate_mods<-paste(substr(mods$V2,7,10),"-",substr(mods$V2,1,2),"-",substr(mods$V2,4,5),sep="")
modsJULTIME<-
(as.numeric(mdy.date(month(tmpDate_mods),day(tmpDate_mods),year(tmpDate_mods)))/365.25)-
basetime_sim


for (i in 1:length(wells)) {

well_min<-min(which(obs_sorted$SAMP_SITE_NAME == as.character(wells[i])))
well_max<-max(which(obs_sorted$SAMP_SITE_NAME == as.character(wells[i])))

range_min<-min(which(obsJULTIME[well_min:well_max] > 18.33))+well_min-1
```

```
range_max<-max(which(obsJULTIME[well_min:well_max] > 18.33))+well_min-1
obs_index<-range_min:range_max

# Selecting model results for each well
mods_index<-which(as.character(mods$V1) == as.character(wells[i]))

# Extracting data to plot all the detects as point
range_min_pts<-min(which(obsJULTIME[well_min:well_max] > 0))+well_min-1
range_max_pts<-max(which(obsJULTIME[well_min:well_max] > 0))+well_min-1
obs_index_pts<-range_min_pts:range_max_pts
well_name=as.character(wellnames$WELLID[i])

#Create a plot for the main aquifer
png(paste("./plots/",wells[i],".png",sep=""),width=3294,height=2580,res=300)

#Build plot
layout(matrix(c(1,2), 2, 1, byrow=TRUE),heights=c(0.9,0.1), respect=TRUE)
y_length =
1.2*max(obs_sorted$STD_VALUE_RPTD[range_min_pts:range_max_pts],(DWS),na.rm=TRUE)
y_min = DWS/2
y_min = 10^round(log10(y_min)-0.5,0)
par(ylog=FALSE)
plot(obsJULTIME[range_min:range_max],obs_sorted$STD_VALUE_RPTD[range_min:range_max]
    ,xlab=" ",ylab="
",type="l",log="y",xaxt="n",yaxt="n",xlim=c(0,40),ylim=c(y_min,y_length),lwd=3,col="white")

#draw axis
x_major<-seq(0,40,na.rm=TRUE,10)
x_minor<-seq(0,40,na.rm=TRUE,5)
y_major<-c(0.1,1.0,10,100,1000,10000,100000)
y_minor<-
c(seq(0.1,1,0.1),seq(10,100,10),seq(100,1000,100),seq(1000,10000,1000),seq(10000,100000,10000),seq(
100000,1000000,100000))
axis(2,at=y_major)

#convert Julian dates to m/d/yr
x_julian<-as.numeric(x_major*365.25 + as.numeric(mdy.date(1,1,1982,nineteen=FALSE)))
x_datetext<-date.mdy(x_julian)
x_Labels<-paste(x_datetext$month,x_datetext$year,sep="/")
axis(side=1,at=x_major,labels=x_Labels)

#draw gridlines
abline(h=y_minor,col="lightgray")
abline(h=y_major,col="gray60")
abline(v=x_minor,col="lightgray")
abline(v=x_major,col="gray60")

#Line and text for May, 1999
abline(v=18.33,,lty=3,col="brown",lwd=2)
text(21,y_min+3,labels="5/1/1999",offset=1.5,col="brown",cex=1.2)
```

```
#draw observed results results
obs_dt_index_pts =
obs_index_pts[which(grepl("U",as.character(obs_sorted$LAB_QUALIFIER[obs_index_pts]))==FALSE)
]
obs_nd_index_pts =
obs_index_pts[which(grepl("U",as.character(obs_sorted$LAB_QUALIFIER[obs_index_pts]))==TRUE)]


if (length(obs_dt_index_pts) > 0) {

points(obsJULTIME[obs_dt_index_pts],obs_sorted$STD_VALUE_RPTD[obs_dt_index_pts],pch=22,bg
="black",col="black")
}

if (length(obs_dt_index_pts) > 7) {

# Historic Trend Line
tband_all<-
theil_ucl_lines(obsJULTIME[obs_dt_index_pts],log10(obs_sorted$STD_VALUE_RPTD[obs_dt_index_
pts]))
yt_all= tband_all$ths0$coef[1] + tband_all$ths0$coef[2]*tband_all$xcut
yt_all<-10^yt_all
write(c(as.character(wells[i]),tband_all$ths0$coef[1],tband_all$ths0$coef[2]),
file="stats_all.csv",ncolumns=3,sep=",",append=TRUE)
lines(yt_all~tband_all$xcut,type='l',col="blue",lwd=2)

# Historic Radioactive Decay
init=yt_all[1]
final=init*(exp(-2.380313E-2*(tband_all$xcut[length(tband_all$xcut)]-tband_all$xcut[1])))
lines(c(tband_all$xcut[1],tband_all$xcut[length(tband_all$xcut)]),c(init,final),type='l',col="blue",lwd=2,
lty=3)
}

# Historic Trend for years after May, 1999
obs_dt_index =
obs_index[which(grepl("U",as.character(obs_sorted$LAB_QUALIFIER[obs_index]))==FALSE)]
if (length(obsJULTIME[obs_dt_index]) > 7) {

# Historic Trend Line
tband<-
theil_ucl_lines(obsJULTIME[obs_dt_index],log10(obs_sorted$STD_VALUE_RPTD[obs_dt_index]))
yt= tband$ths0$coef[1] + tband$ths0$coef[2]*tband$xcut
yt<-10^yt
write(c(as.character(wells[i]),tband$ths0$coef[1],tband$ths0$coef[2]), file="stats_1999-
2015.csv",ncolumns=3,sep=",",append=TRUE)
lines(yt~tband$xcut,type='l',col="brown",lwd=2)
}

# Model Plot Line (plots model results as a line)
tband_mods<-theil_ucl_lines(modsJULTIME[mods_index],log10(mods$V4[mods_index]))
yt_mods= tband_mods$ths0$coef[1] + tband_mods$ths0$coef[2]*tband_mods$xcut
```

```
yt_mods<-10^yt_mods
write(c(as.character(wells[i]),tband_mods$ths0$coef[1],tband_mods$ths0$coef[2]),
file="stats_simulated.csv",ncolumns=3,sep=",",append=TRUE)
lines(yt_mods~tband_mods$xcut,type='l',col="orchid1",lwd=2)

abline(h=DWS,col="darkgreen",lwd=4)
text(x=0,y=DWS,"DWS",pos=3,offset=0.5)

#add the axis labels
mtext(text="Calendar Years",side=1,font=2,cex=1.4,line=2)
mtext(text=well_name,side=3,font=2,cex=1.7,line=2)
mtext(text=paste("Strontium-90 Concentration",",  ", "pCi/L"),side=2,font=2,cex=1.4,line=2)

op<-par("mar")  # Record the current margins
par(mar=c(0.5,op[2],0.0,op[4]))  # Set up new margins

# Create the legend
legX<-c(0,1)
legY<-c(0,1)
plot(legX,legY,,xlab=" ",ylab=" ",type="l",xaxt="n",yaxt="n",col="white")

text(0.5,1,paste("Well ",as.character(wells[i]),sep="\n"),pos=1)
text(0.82,0.5,"Simulated",pos=4)
lines(x=c(0.7,0.8),y=c(0.5,0.5),lwd=3,col="orchid1")
text(0.1,0.5, "Observed Trend",pos=4)
lines(x=c(0.01,0.08),y=c(0.5,0.5),lwd=3,col="blue")
text(0.1,0.8, "Decay Trend",pos=4)
lines(x=c(0.01,0.08),y=c(0.8,0.8),lwd=3,lty=3,col="blue")
text(0.82,0.8, "DWS (8 pCi/L)",pos=4)
lines(x=c(0.7,0.8),y=c(0.8,0.8),lwd=3,col="darkgreen")
text(0.82,0.2,"Detected",pos=4)
points(x=c(0.75),y=c(0.2),pch=22,bg="black",col="black")
text(0.1,0.2, "Observed Trend (1999-2015)",pos=4)
lines(x=c(0.01,0.08),y=c(0.2,0.2),lwd=3,col="brown")

par(mar=c(op[1],op[2],op[3],op[4]))
dev.off()
}
```

TheilSen.R

```
# R script for Theil-Sen Confidence band
# Compute bootstrapped confidence band around Theil-Sen trend line
# user inputs: list of x-values, list of y-values, desired confidence level
# Note: replace numbers in parentheses below with specific x and y values
# corresponding to data-specific ordered pairs
# x-values should be numeric values representing sampling dates or events
# y-values should be concentration values corresponding to these dates or events
# Script produces a plot of the Theil-Sen trend line, the confidence band around the trend,
# and an overlay of the actual data values
##########################################################################################
#
#           CODE FOR CREATING ELIMINATING MISSING DATA
#                TAKEN FROM EPA 540 R-09-007
##########################################################################################
elimna= function(m){
#
# remove any rows of data having missing values
m= as.matrix(m)
ikeep= c(1:nrow(m))
for(i in 1:nrow(m)) if (sum(is.na(m[i,])>=1)) ikeep[i]= 0
elimna= m[ikeep[ikeep>=1],]
elimna
}
##########################################################################################
#
#           CODE FOR CREATING THEIL-SEN LINEAR REGRESSION
#                TAKEN FROM EPA 540 R-09-007
```

```
##########################################################################################
####
theilsen2= function(x,y){
#
# Compute the Theil-Sen regression estimator
# Do not compute residuals in this version
# Assumes missing pairs already removed
#
ord= order(x)
xs= x[ord]
ys= y[ord]
vec1= outer(ys,ys,"-")
vec2= outer(xs,xs,"-")
v1= vec1[vec2>0]
v2= vec2[vec2>0]
slope= median(v1/v2)
coef= 0
coef[1]= median(y)-slope*median(x)
coef[2]= slope
list(coef=coef)
}

##########################################################################################
###
#
#                    CODE FOR Calculating 95th percentile upper confidence limit
#
##########################################################################################
####
tdistucl95<-function (x, conf = 0.95) {
  a<-mean(x)
```

```
  s<-sd(x)
  e<-qt(conf,df=length(x)-1)*s/sqrt(length(x))
  tdistucl95<-a+e
}
#####LINEAR REGRESSION AND UCL FOR THEIL-SEN METHOD
theil_ucl_lines<-function(x,y,conf=0.95) {

nb= 1000
temp= matrix(c(x,y),ncol=2)
temp= elimna(temp) #remove any pairs with missing values
x= as.numeric(temp[,1])
y= as.numeric(temp[,2])
n= length(x)
ord= order(x)
cut= min(x) + (0:100)*(max(x)-min(x))/100 #compute 101 cut pts
t0= theilsen2(x,y) #compute trend line on original data
tmp= matrix(nrow=nb,ncol=101)
for (i in 1:nb) {
idx= sample(ord,n,rep=T)
xboot= x[idx]
yboot= y[idx]
tboot= theilsen2(xboot,yboot)
tmp[i,]= tboot$coef[1] + cut*tboot$coef[2]
}
lb= 0; ub= 0
loIQR= 0; hiIQR= 0
for (i in 1:101){
lb[i]= quantile(tmp[,i],c((1-conf)/2),na.rm=TRUE)
ub[i]= quantile(tmp[,i],c((1+conf)/2),na.rm=TRUE)
tmpIQR=as.numeric(quantile(tmp[,i],c(0.75),na.rm=TRUE))-
as.numeric(quantile(tmp[,i],c(0.25),na.rm=TRUE))
```

```
hiIQR[i]=as.numeric(quantile(tmp[,i],c(0.75),na.rm=TRUE))+(3*tmpIQR)
loIQR[i]=as.numeric(quantile(tmp[,i],c(0.25),na.rm=TRUE))-(3*tmpIQR)
}
tband= list(xcut=cut,lo=lb,hi=ub,hiIQR=hiIQR,loIQR=loIQR,ths0=t0)
return(tband)
}

####################  FUNCTION FOR SAMPLING A VECTOR

sample_vec<-function(samp_xval,xvals,values) {
  sampled<-rep(-9999,length(samptimes))
  if (length(xvals) != length(values)){
    return (sampled)
  }
  lngCount = 1
  for ( j in 1:length(samptimes)) {
    for (i in 1:(length(xvals)-1)) {
      if (samptimes[j]<=xvals[i+1] & samptimes[j]>=xvals[i] ) {
        sampled[j]<-(((samptimes[j]-times[i])/(times[i+1]-times[i]))*(values[i+1]-values[i]))+values[i]
        break
      }
    }
  }
  for ( k in 1:length(samptimes)) {
      if ( sampled[k] == -9999.0 ) {
        print ("One or all of the values sampled values was not within the bounds of the time series")
      }
  }
  return (sampled)
}
```