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Revision 0

Evaluation of Chloroform and Trichloroethene Concentration Data for the Remedial Investigation/Feasibility Study for the 100-BC-1, 100-BC-2, and 100-BC-5 Operable Units

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

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

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Evaluation of Chloroform and Trichloroethene Concentration Data for the Remedial Investigation/Feasibility Study for the 100-BC-1, 100-BC-2, and 100-BC-5 Operable Units

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Terms

CHPRC	CH2M HILL Plateau Remediation Company
COPC	contaminant of potential concern
Cr(VI)	hexavalent chromium
HISI	Hanford Information Systems Inventory
OU	operable unit
SSP&A	S.S. Papadopulos and Associates, Inc.
TCE	trichloroethene

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1 Purpose

The purpose of this environmental calculation brief is to present calculations for the fate of low-level trichloroethene (TCE) and chloroform concentrations in the 100-BC-5 Operable Unit (OU).
This calculation supports evaluations for the 100-BC-5 portion of the Hanford Site (DOE/RL-2010-96, *Remedial Investigation/Feasibility Study for the 100-BC-1, 100-BC-2, and 100-BC-5 Operable Units*), under the *Comprehensive Environmental Response, Compensation, and Liability Act of 1980*, which will support final remedy selection and provide the basis for a final record of decision for the 100-BC-5 OU.

2 Background

Chloroform and TCE concentrations in several wells were greater than the 2007 WAC 173-340-720, "Model Toxics Control Act—Cleanup," "Groundwater Cleanup Standards," which are based on a 1×10^{-6} target risk level for individual contaminants. In most cases, the well-specific risk assessment (Chapter 6, DOE/RL-2010-96) determined that the cumulative risk level was less than the WAC 173-340-708, "Human Health Risk Assessment Procedures," risk threshold of 1×10^{-5}. However, three wells screened at the bottom of the aquifer (199-B3-51, 199-B5-5, and 199-B5-6) exceeded the cumulative risk threshold, based on the combined concentrations of chloroform and TCE.

Figure 1 shows a plot of measured chloroform and TCE concentrations at monitoring wells screened at the bottom of the aquifer.

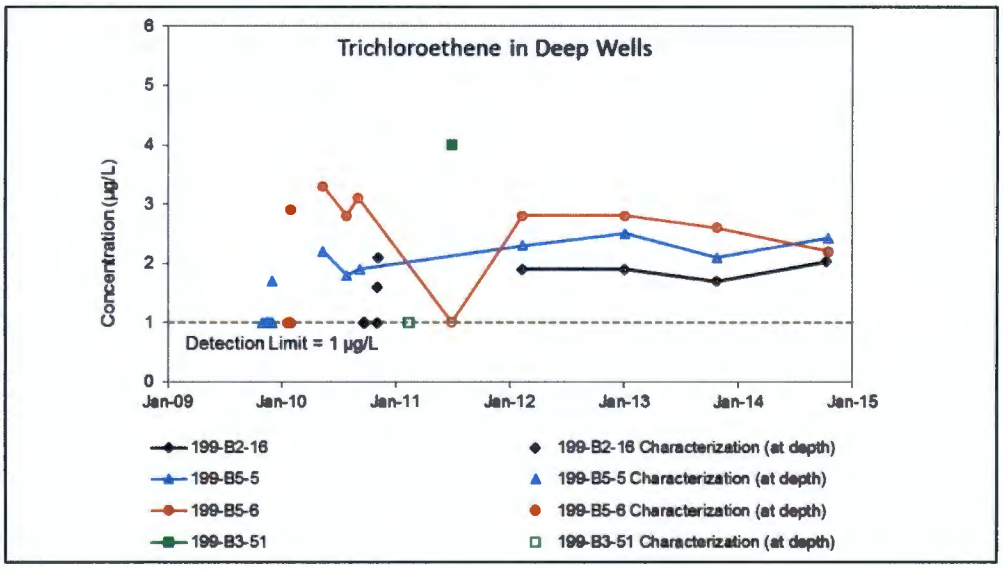

Figure 1. Chloroform and TCE Concentrations at Monitoring Wells Screened at the Bottom of the Aquifer

The relative location of the three wells of interest is depicted in Figure 2.

Chloroform and TCE are identified as contaminants of potential concern (COPCs) that warrant evaluation of remedial alternatives for wells 199-B3-51, 199-B5-5, and 199-B5-6. An approach developed for evaluating the fate of these COPCs and the corresponding calculations are presented in the following chapters.

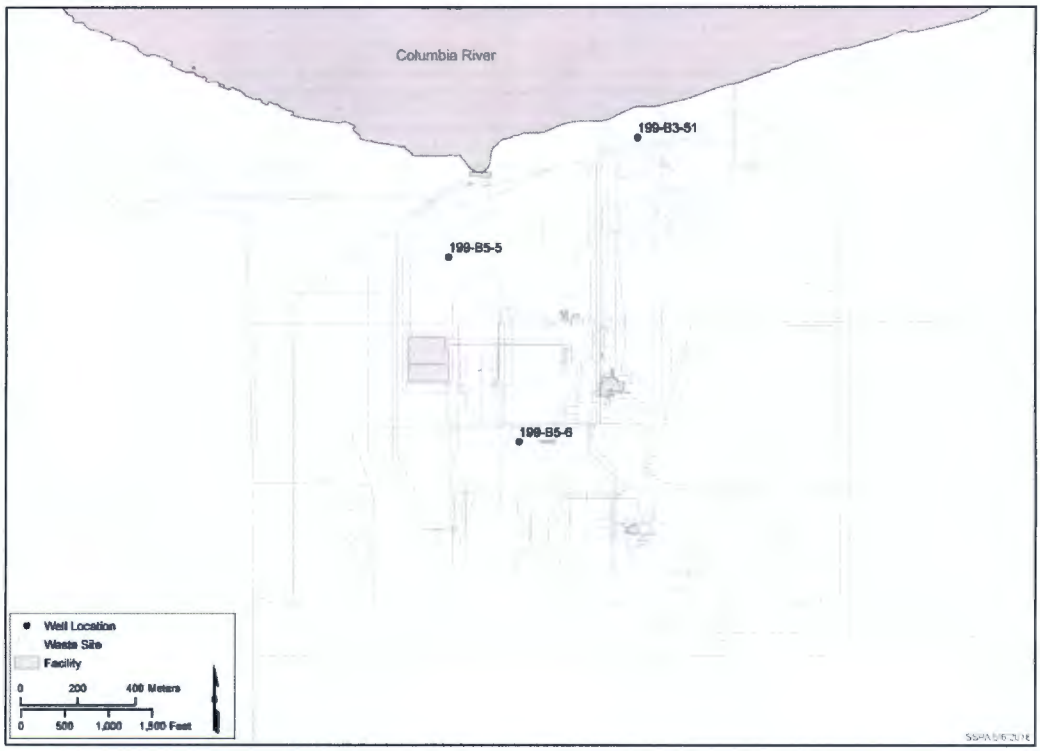

Figure 2. Location of Monitoring Wells 199-B3-51, 199-B5-5, and 199-B5-6

3 Calculation Methods

A simple approach was developed to evaluate the fate of chloroform and TCE at wells 199-B3-51, 199-B5-5, and 199-B5-6, given that (1) there are only three monitoring locations in the deep zone of the unconfined aquifer with concentrations above the detection limit, and (2) concentration levels at those wells are within a very narrow range (less than 3 µg/L). At such low concentration levels and short timeframe of available data, it is not possible to calculate a meaningful trend and project cleanup timeframes under ambient flow conditions. In addition, the lack of distributed concentration data and narrow range of measured concentrations did not warrant the deployment of the three-dimensional 100-BC flow and transport model. Instead, the proposed methodology employs one-dimensional flow and transport calculations assuming uniform, mean flow conditions representative of the flow conditions in the deep zone of the unconfined aquifer and a normalized concentration profile for calculating and evaluating relative changes to concentrations over time.

The proposed methodology was based on the following procedure:

1. The flow field calculated by the predictive, three-dimensional 100-BC groundwater flow model, assuming ambient flow conditions, was used for conducting particle tracking to estimate an approximate mean groundwater velocity in the deep zone of the unconfined aquifer.
2. One-dimensional flow modeling was performed with uniform hydraulic parameters and boundary conditions to simulate mean groundwater flow conditions estimated during Step 1.
3. One-dimensional advection-dispersion transport modeling was performed to (a) develop an initial concentration distribution assuming a unit source inland of the three wells; and (b) calculate breakthrough curves at distances downgradient, to develop concentration time series.

4. Relative changes to concentrations over time were calculated to estimate approximate timeframes resulting in lowering the cumulative risk threshold below 1×10^{-5}.

A discussion of each step of the procedure outlined above is provided in the following sections.

3.1 Groundwater Flow and Particle Tracking

Simulations of groundwater flow and particle tracking were conducted using the numerical model developed by Intera specifically for the 100-BC-5 OU, as detailed in SGW-59365, *100-BC Scale-Appropriate Fate and Transport Model* (Draft A).

The flow field developed by the groundwater flow simulation for 125 years under the "no further action" alternative presented in ECF-100BC5-16-0059, *2016 Modeling of RI/FS Design Alternatives for 100-BC-5*, was used for performing particle tracking. Particles were released from cells in Layer 6 of the groundwater model, corresponding to the locations of the three wells. The resulting pathlines reflect the tortuous migration pathways toward the river and therefore, the total length of the pathlines and travel times to discharge to the river provide the basis for determining mean groundwater flow conditions at the bottom of the unconfined aquifer.

The pathline length and migration timing of each particle were recorded, and a mean groundwater velocity was calculated.

3.2 One-Dimensional Modeling

A one-dimensional groundwater flow and transport model was developed to simulate migration in the deep zone of the aquifer under mean groundwater flow conditions calculated as described in Section 3.1. A uniform hydraulic conductivity was assigned to all model cells, corresponding to the approximate mean hydraulic conductivity of Layer 6 of the 100-BC model, calculated along the pathline emanating from the most inland well, 199-B5-6.

A unit source, placed in a cell corresponding to a distance of 250 m inland of well 199-B5-6, was used for generating initial conditions along the column. The simulation ceased when a concentration profile was developed, with a concentration of 1.0 at the location corresponding to well 199-B5-6 and 0.7 at a distance downgradient corresponding to the location of well 199-B5-5. This is consistent with the approximate ratio of maximum concentrations measured at these wells.

A steady-state simulation was then performed, with this concentration profile used as initial condition and migrating in the column under ambient flow conditions (i.e., mean groundwater velocity). It is assumed that the maximum concentration measured at well 199-B5-6 is the maximum concentration in the deep zone of the aquifer and, therefore, it is expected to migrate downgradient in the future. Projected concentration time series in the aquifer were calculated at a scale representing a mean separation distance among the wells of interest and other wells in the deep zone of the unconfined aquifer. This distance also corresponds to the location of well 199-B5-5 from well 199-B5-6. Concentrations were recorded at each time step, and breakthrough curves were developed. These breakthrough curves provide the basis for evaluating relative changes of concentration over time, so that health risk assessment can be performed and estimate approximate timeframes for lowering the cumulative risk threshold below 1×10^{-5}.

3.3 Model Structure

The spatial and temporal discretization of the models used for performing the calculations described in this calculation brief are briefly discussed below.

3.3.1 100-BC Model

The numerical groundwater flow and transport model of the 100-BC-5 OU area (100-BC model) was developed by Intera for use by the CH2M HILL Plateau Remediation Company (CHPRC) in support of remedy design evaluation. A detailed discussion of the numerical model is presented in SGW-59365.

The model was developed to simulate conditions for the period of 2006 to 2015, with stress periods ranging from 5 to 30 days. The model was calibrated to data from the period of 2012 to 2014 and a predictive flow and transport model was then developed, repeating the 2006 to 2015 conditions for 125 years.

3.3.2 One-Dimensional Model

The one-dimensional model has 1 column and 253 rows. The cell size is 5 by 5 m squared. Flow and transport simulations were performed under steady-state conditions. A schematic of the model structure is depicted in Figure 3.

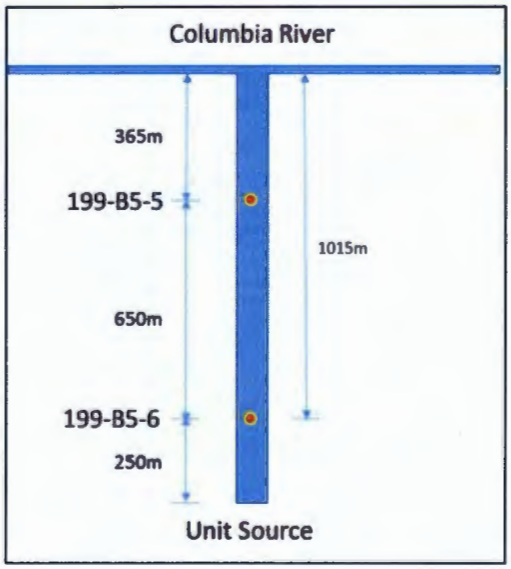

Figure 3. Schematic Structure of the One-Dimensional Flow and Transport Model

4 Assumptions and Inputs

Assumptions, limitations, and inputs to the calculations presented in this brief are discussed below.

4.1 Model Assumptions and Limitations

Conceptual and parameter uncertainties associated with the groundwater flow and contaminant transport model are presented in SGW-59365.

Chloroform and TCE are assumed to be migrating in the aquifer under ambient flow conditions with mechanical dispersion being the only mechanism for concentration reduction during particle migration and ultimate discharge to the river. Also, no continuing sources are considered, as there is no evidence of presence of such sources in the sediments of the vadose zone or the saturated zone. The available data are under evaluation and further monitoring is planned to ensure that potential changes in concentrations are recorded and investigated.

Flow and transport conditions simulated by the one-dimensional flow and transport model represents an approximation of the mean flow and transport conditions in the deeper zone of the aquifer. It does not represent the variability of hydraulic properties in the aquifer. It linearly approximates the relatively tortuous migration pathways expected to be observed in the aquifer. Finally, it provides a simple tool for evaluating mean migration patterns for constituent distributions that cannot be accurately delineated.

Consistent with recommendations made throughout the remedy design process, simulated COPC concentrations in the future should be interpreted as relative estimates and not as absolute predictions of actual plume migration patterns. Numerical transport modeling over long timeframes should be used principally for qualitative assessments of long-term plume migration patterns, rather than accurately calculating such long-term predictions of point concentrations.

Upon implementation of any remedy design, monitoring data should be compiled and analyzed to improve estimation of the parameters associated with the simulation of the fate and transport of the COPCs and performance of the implemented remedies. The model should be updated to provide improving estimates of remedy performance.

4.2 Model Inputs

Inputs to the models used in the calculation presented in this brief are documented below.

4.2.1 100-BC Model

Particles are released in Layer 6 of the three-dimensional model at the cells listed in Table 1.

Table 1. Model Cells for Particle Starting Locations

Row	Column	Layer
114	282	6
65	154	6
196	73	6

4.2.2 One-Dimensional Flow Model

A hydraulic conductivity of 18 m/d and porosity of 18 percent are uniformly assigned to all cells of the model. Constant-head boundaries at the two edges of the column develop a hydraulic gradient of 4.98×10^{-4}, resulting in a mean groundwater velocity of 0.05 m/d.

Transport simulations were performed assuming a conservative contaminant, that is, no degradation or decay are incorporated in the model. Consistent with the flow and transport simulations performed for hexavalent chromium using the 100-BC model, a longitudinal dispersivity of 10 m was applied.

A unit source was applied 250 m upgradient of the cell corresponding to the location of well 199-B5-6.

5 Software Applications, Descriptions, Installation and Checkout, and Statements of Validity

Software use for this calculation was in accordance with PRC-PRO-IRM-309, *Controlled Software Management*.

5.1 Approved Software

The following software, approved and compliant with PRC-PRO-IRM-309, was used to perform the calculations. The software is managed under the following documents consistent with PRC-PRO-IRM-309:

- CHPRC-00257, Rev. 1, *MODFLOW and Related Codes Functional Requirements Document*
- CHPRC-00258, Rev. 4, *MODFLOW and Related Codes Software Management Plan*
- CHPRC-00259, Rev. 3, *MODFLOW and Related Codes Software Test Plan*
- CHPRC-00260, Rev. 8, *MODFLOW and Related Codes Requirements Traceability Matrix CHPRC Build 8*
- CHPRC-00261, Rev. 8, *MODFLOW and Related Codes Acceptance Test Report CHPRC Build 8*

CHPRC-00258 distinguishes between safety software and support software based on whether the software managed calculates reportable results or provides run support, visualization, or other similar functions. Brief descriptions of the software are provided in the following sections.

5.2 Descriptions

5.2.1 MODFLOW (Controlled Calculation Software)

- Software Title: MODFLOW-2000 – Solves transient groundwater flow equations using the finite-difference discretization technique (Harbaugh et al., 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model—User Guide to Modularization Concepts and the Ground-Water Flow Process*)
- Software Version: Version 1.19.01 modified by S.S. Papadopulos and Associates, Inc. (SSP&A) to address dry cell issues and to use the Orthomin solver; approved as CHPRC Build 8 using the executable "mf2k-mst-chprc08dpv.exe" compiled to default double precision for real variables and optimized for speed
- Hanford Information Systems Inventory (HISI) Identification Number: 2517 (safety software, graded Level C)
- Workstation type and property number (from which software is run): SSP&A, FE407

5.2.2 MT3DMS (Controlled Calculation Software)

- Software Title: 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*; Zheng, 2010, *MT3DMS v5.3 Supplemental User's Guide*)
- Software Version: Version 5.3 modified by SSP&A to address dry cell issues; approved as CHPRC Build 8 using executable "mt3d-mst-chprc08dpv.exe" compiled to default double precision for real variables and optimized for speed
- HISI Identification Number: 2518 (safety software, graded Level C)
- Workstation type and property number (from which software is run): SSP&A, FE407

5.2.3 MODPATH (Controlled Calculation Software)

- Software Title: MODPATH – A particle-tracking post-processor developed for use with the MODFLOW codes; used to evaluate the approximate directions and rates of groundwater flow and the approximate extent of hydraulic capture developed by proposed pump and treat well configurations (Pollock, 1994, *User's Guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model*)
- Software Version: Version 8 modified by SSP&A to address dry cell issues; approved as CHPRC Build 6 using executable "modpath-mst-chprc08.exe"
- Workstation type and property number (from which software is run): SSP&A, FE407

5.3 Support Software

The following programs are classified as support software.

5.3.1 MODFLOW Suite Support Software

- **Groundwater Vistas** Provided graphical tools used for model quality assurance and model input/output review (Rumbaugh and Rumbaugh, 2011, *Guide to Using Groundwater Vistas*)
- **ArcGIS™:** Provided visualization tool for assessing simulated plume distributions, identifying extraction/injection well coordinates, and mapping auxiliary data (Mitchell, 1999, *The ESRI Guide to GIS Analysis Volume 1: Geographic Patterns & Relationships*)

5.4 Software Installation and Checkout

Safety software is checked out in accordance with procedures specified in CHPRC-00258. Executables are obtained from the CHPRC software owner who maintains the configuration-managed copies in MKS Integrity; performs the installation tests identified in CHPRC-00259 and confirms successful installation; and completes the required software installation and checkout forms and obtains approvals for installations used to perform model runs. Approved users are registered in HISI for safety software. Copies of the software installation and checkout forms are provided in Appendix A.

5.4.1 Statement of Valid Software Application

- The software identified above was used consistent with intended use for CHPRC as identified in CHPRC-00257 and is a valid use of this software for the problem addressed in this application.
- The software was used within its limitations as identified in CHPRC-00257.
- R and Python languages have not been identified in CHPRC-00258, but are scheduled by the software owner to be included as support software in the next revision to that document. They are publically available, open-source freeware.

™ ArcGIS is a trademark of Esri in the United States, the European community, or other jurisdictions.

6 Calculation

6.1 Particle Tracking

Particle tracking was performed by releasing particles in Layer 6 of the three-dimensional 100-BC model, at cells corresponding to the location of wells 199-B3-51, 199-B5-5, and 199-B5-6. Particle pathlines were recorded by the program and reported in the output file *pathline*. The output file was post-processed to calculate pathline lengths and time of travel. The longest pathline, emanating from the cell corresponding to the location of well 199-B5-6, was selected for calculating the mean groundwater velocity in the deep zone of the unconfined aquifer, representing the most conservative migration pathway.

6.2 One-Dimensional Flow and Transport Modeling

The one-dimensional flow and transport model was run under steady-state conditions in two phases. In Phase 1, the flow simulation was used for developing a concentration profile along the column, caused by a unit source placed 250 m upgradient of the cell corresponding to the location of well 199-B5-6. The resulting concentration profile was developed such that a concentration of 1.0 was calculated at the location of well 199-B5-6 and a concentration of about 0.7 was calculated at a distance of 900 m from the source or 650 m from well 199-B5-6, corresponding to the location of well 199-B5-5. This is consistent with the approximate ratio of maximum concentrations measured at these wells.

Once the concentration profile was developed, the simulation was terminated. Phase 2 of the simulation incorporated the concentration profile developed in Phase 1 as initial conditions, without the presence of the constant source. Phase 2 simulated contaminant migration under ambient flow conditions and breakthrough curves at distance were developed. These breakthrough curves provide the basis for evaluating concentration changes over time, so that health risk assessment can be performed.

7 Results and Conclusions

7.1 Particle Tracking using the 100-BC Model

Figure 4 depicts a plan view of the pathlines calculated using the 100-BC model for particles released from cells corresponding to wells 199-B3-51, 199-B5-5, and 199-B5-6. Particles migrate horizontally until the reach the area by the shoreline at which point they migrate vertically and through the river bottom, discharging to the river.

Particle locations were recorded until each particle discharged to the river. The corresponding pathline lengths and travel times were tabulated in Table 2.

The longest pathline, emanating from well 199-B5-6, was selected for groundwater velocity calculations. Based on the pathline length and travel time, a mean groundwater velocity of 0.05 m/d was calculated.

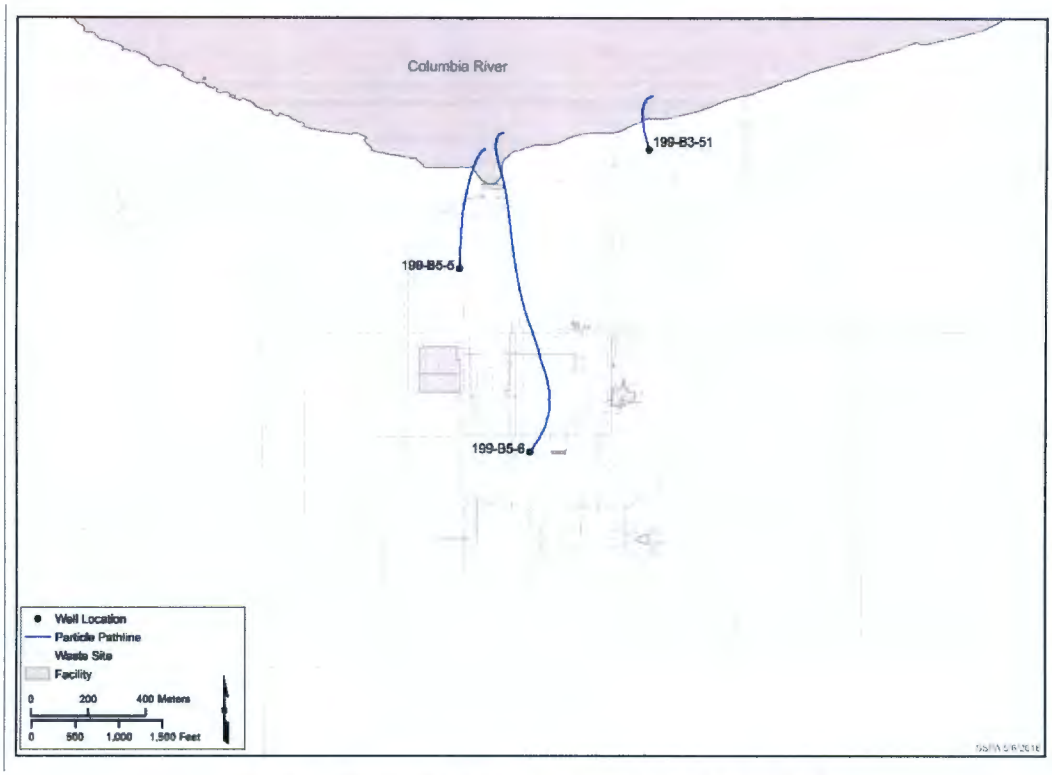

Figure 4. Pathlines Calculated Using the 100-BC Model

Table 2. Pathline Lengths, Travel Times, and Calculated Mean Groundwater Velocity

Well Name	Pathline Length (m)	Travel Time (days)	Travel Time (yr)	Mean Groundwater Velocity (m/day)
199-B3-51	110	620	1.7	0.18
199-B5-5	353	3,550	9.7	0.10
199-B5-6	1,015	20,855	57.1	0.05

7.2 One-Dimensional Flow and Transport Modeling

7.2.1 Phase 1: Development of Initial Conditions

The one-dimensional flow and transport model was used for developing initial conditions for the predictive simulation. Applying a unit source upgradient of well 199-B5-6, a concentration profile was developed, as depicted in Figure 5. The X-axis represent the distance from the river. The Y-axis shows concentration levels, calculated by the model given the operation of a constant source with a unit concentration. The relative location of wells 199-B5-5 and 199-B5-6 are also depicted.

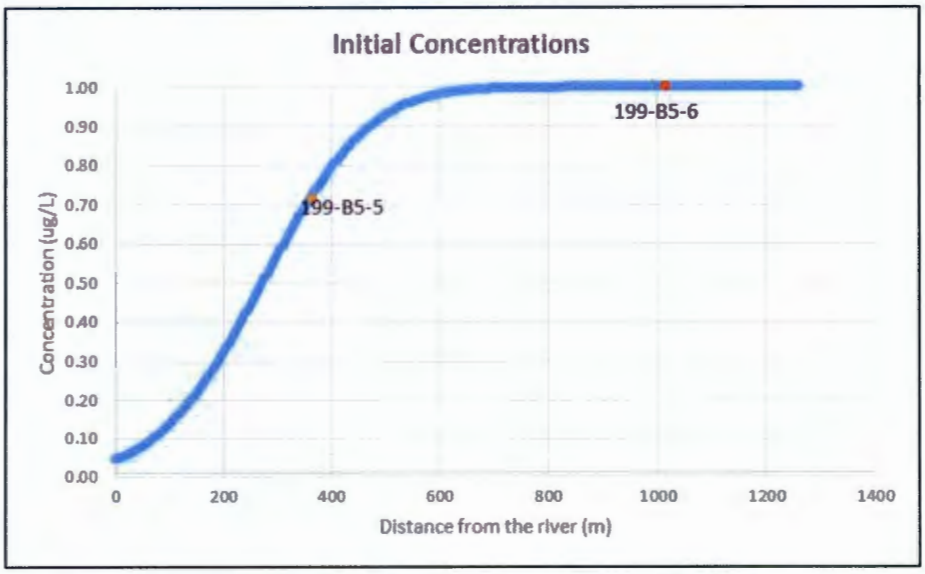

Figure 5. Concentration Profile for Initial Condition in Predictive Simulation

7.2.2 Phase 2: Predictive Calculations

The calculated concentration breakthrough curve at a distance of 650 m from well 199-B5-6 is depicted in Figure 6.

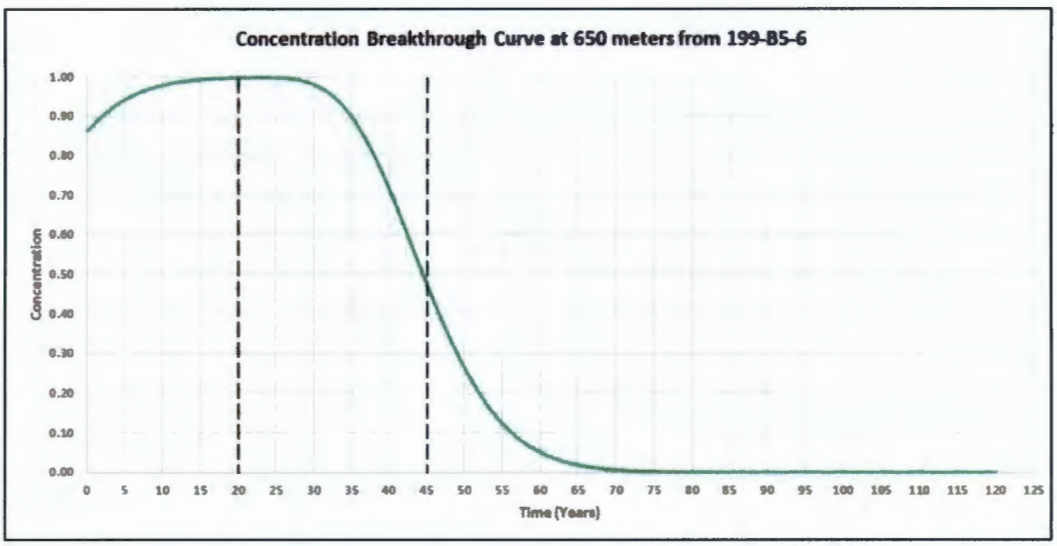

Figure 6. Concentration Breakthrough Curve at 650 m from Well 199-B5-6

7.3 Conclusions

Figure 6 illustrates the change in concentration over time at the location of interest. The calculation results suggest that, on average, a conservative estimate of the expected timeframe for peak chloroform or TCE concentrations to be lowered by 50 percent or more, under ambient flow conditions, is about 25 years. This estimate relies on the assumption that the concentration distribution at the bottom of the aquifer does not exceed the maximum measured chloroform or TCE concentration to date.

These results are also compared to the simulated changes in hexavalent chromium (Cr(VI)) concentration at the bottom of the unconfined aquifer, as presented in ECF-100BC5-16-0059, *2016 Modeling of RI/FS Design Alternatives for 100-BC-5*. Figure 7 depicts snapshots of the Cr(VI) plume in Layer 6 after 20, 40, 60, and 80 years, as simulated using the 100-BC model under "no further action" conditions. The relative location of the three wells of interest are shown in these snapshots. The model results for this simulation suggest that chromium concentrations in the vicinity of well 199-B5-6 reduce at a rate of about 50 percent over a period of 20 years, which is comparable to the calculated timeframe of 25 years for chloroform or TCE concentrations to be lowered by 50 percent or more.

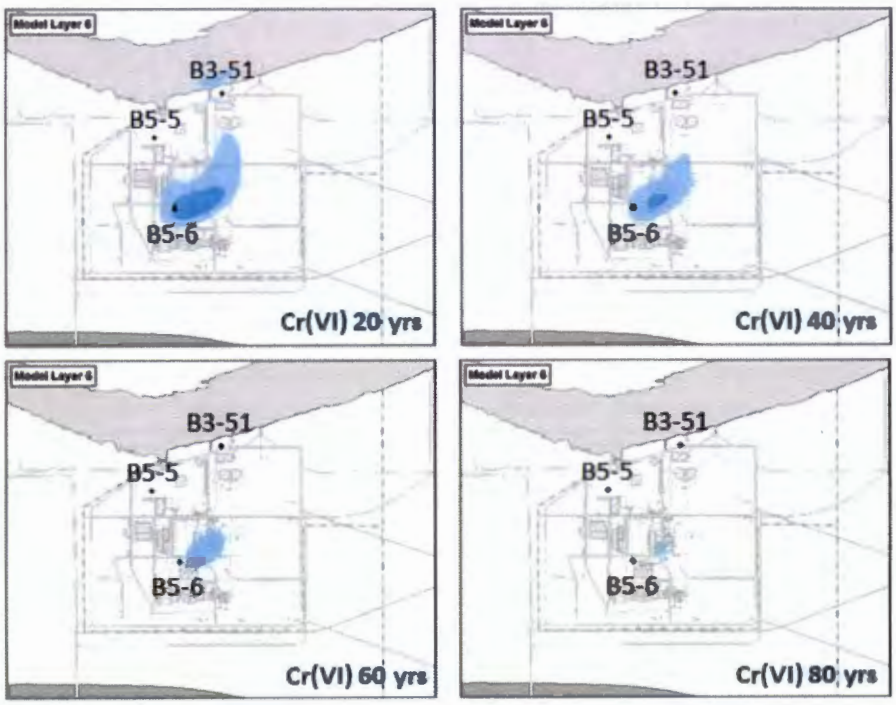

Figure 7. Simulated Predicted Cr(VI) Concentration Distributions under No Further Action Conditions

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Appendix A

Software Installation and Checkout Forms

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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 8

EXECUTABLE INFORMATION:

2. Executable Name (include path):

Following executable files in directory: _____

MD5 Signature (unique ID)	Executable File Name	
919F74196F5FB5BF0364FC373011B507	mf2k-chprc08dpl.exe	MODFLOW-2000 double precision
EAF037703ADD2C62CDD9CBC47468D2F6	mf2k-chprc08spl.exe	MODFLOW-2000 single precision
4E7F29DD5496D2CBA7144ADACB13DAAD	mf2k-mst-chprc08dpv.exe	MODFLOW-2000-MST single prec
CEB80288C616E0552E4CE5A2D4719387	mf2k-mst-chprc08spv.exe	MODFLOW-2000-MST double prec
ECA9828530B68D2D7C34078C019D5D0C	mt3d-chprc08dpl.exe	MT3DMS double precision
0920CC235862665D9400A3FC80F682DD	mt3d-chprc08spl.exe	MT3DMS single precision
5C61432D2C898E83DDFE242C52A755AB	mt3d-mst-chprc08dpv.exe	MT3DMS-MST double precision
68F89DAF2E6913D2578DE53CBD34FBA0	mt3d-mst-chprc08spv.exe	MT3DMS-MST single precision

3. Executable Size (bytes): MD5 signatures listed above uniquely identify executable files

COMPILATION INFORMATION:

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

Vendor Provided (SSP&A)

5. Operating System (include version number):

Vendor Provided (SSP&A)

INSTALLATION AND CHECKOUT INFORMATION:

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

FE 407

7. Operating System (include version number):

MS Windows 10 Pro

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

TEST CASE INFORMATION:

9. Directory/Path:

_____\test-windows

10. Procedure(s):

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

11. Libraries:

N/A (static linking)

12. Input Files:

MF-ITC-1 and MT-ITC-1 inputs

13. Output Files:

MF-ITC-1 and MT-ITC-1 outputs

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

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

14. Test Cases:

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

15. Test Case Results:

```
MODFLOW, MODFLOW-MST, and MT3DMS-MST Installation Testing Log
Eight instances of /FC: no differences encountered/ in log below indicates
that all installation tests were successful.
Alex_2
Wed 05/04/2016
03:33 PM

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG

---------- TESTRESULTS.LOG
```

16. Test Performed By:

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

18. Disposition (include HISI update): Installation added to HISI entries 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, Date: 2016.05.18 11:42:57 -07'00')	Software Owner (Signature)	WE Nichols	Print		Date
20. A Spiliotopoulos	Sign	Alex Spiliotopoulos	Print	2/15/2016	Date
	Sign		Print		Date
	Sign		Print		Date

Approved By:

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