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Revision 0

Evaluating Adequacy of One-Dimensional Transport Calculation in the Saturated Zone of the Far-Field Portion of the 200-PO-1 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

CH2MHILL
Plateau Remediation Company

P.O. Box 1600
Richland, Washington 99352

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CH2M HILL Plateau Remediation Company

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Environmental Calculation Cover Page

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Calculation Title & Description: Evaluating adequacy of one-dimensional transport calculation in the saturated zone of the far-field portion of the 200-PO-1 Operable Unit

Preparer: Sunil Mehta	**Basis of Qualification:** Education and Experience
Checker: Amena Mayenna	**Basis of Qualification:** Education and Experience
Senior Reviewer: Will Nichols	**Basis of Qualification:** Education and Experience

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SIGNATURE 1 Sep 10 DATE

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Terms

CHPRC	CH2M Hill Plateau Remediation Company
HEIS	Environmental Information System (database of environmental data)
HISI	Hanford Information Systems Inventory (database of software)
OU	operable unit

1 Purpose

The purpose of this report is to evaluate the adequacy of one-dimensional (1-D) transport of contaminants in the saturated zone of the far-field portion of the 200-PO-1 Groundwater Operable Unit (OU). This evaluation is conducted as part of the graded approach, where the simplest calculation tool that is deemed suitable for performing baseline risk assessment is chosen. Under the graded approach, a 1-D analytical solution to the mass transport calculation is deemed to be the simplest approach for evaluating concentrations in the far-field portion of the 200-PO-1 OU for baseline risk assessment.

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2 Methodology

To determine adequacy of this approach a calculation is conducted along a representative stream tube, where the time varying tritium concentration from a long-term monitoring well is introduced at the upstream boundary while the downstream concentrations are calculated and compared with those observed in the monitoring wells located along the inferred flow path.

The location of the stream tube is shown in Figure 1, which is chosen along an inferred flow path in the far-field portion of 200-PO-1 OU, based on the water table conditions for calendar year 2008. The location of the stream tube pathway is chosen based on: (a) its relative position compared to the historic migration pathway of the tritium plume and (b) location of the monitoring wells in near vicinity for which long-term tritium concentration records are available.

The southern flow path shown in Figure 1 presents the hydraulic gradient variation in the far-field portion of the 200-PO-1 OU. Under the present conditions, hydraulic gradient is approximately 2×10^{-4} in the west (closer to the Central Plateau) and increases by about an order of magnitude to 2×10^{-3} towards the east. Based on the well hydrograph comparisons presented in Figure 2 [dataset taken from the Hanford Environmental Information System (HEIS) database] the hydraulic gradients are calculated among the upgradient-downgradient well pairs at every quarter of a year time interval (Figure 3). The long-term trend indicates that hydraulic gradients have changed little over the past 40 years, although in certain time intervals the gradients have fluctuated by over a factor of two resulting from operational discharges. From upgradient to downgradient direction along the inferred flow path, the wells are numbered as 699-31-31, 699-32-22A, 699-35-9, and 699-37-E4.

As shown in Figure 4, long term tritium records are available for the selected wells (data taken from the HEIS database); all except one well has monitoring record greater than 40 years. Comparing the calculation results to the observed dataset over this long period that includes the Hanford Site's operational period provides the necessary information to evaluate whether or not the 1-D transport calculation methodology is adequate to the needs of a baseline risk assessment. The total transport length along the identified flow path is about 11 km.

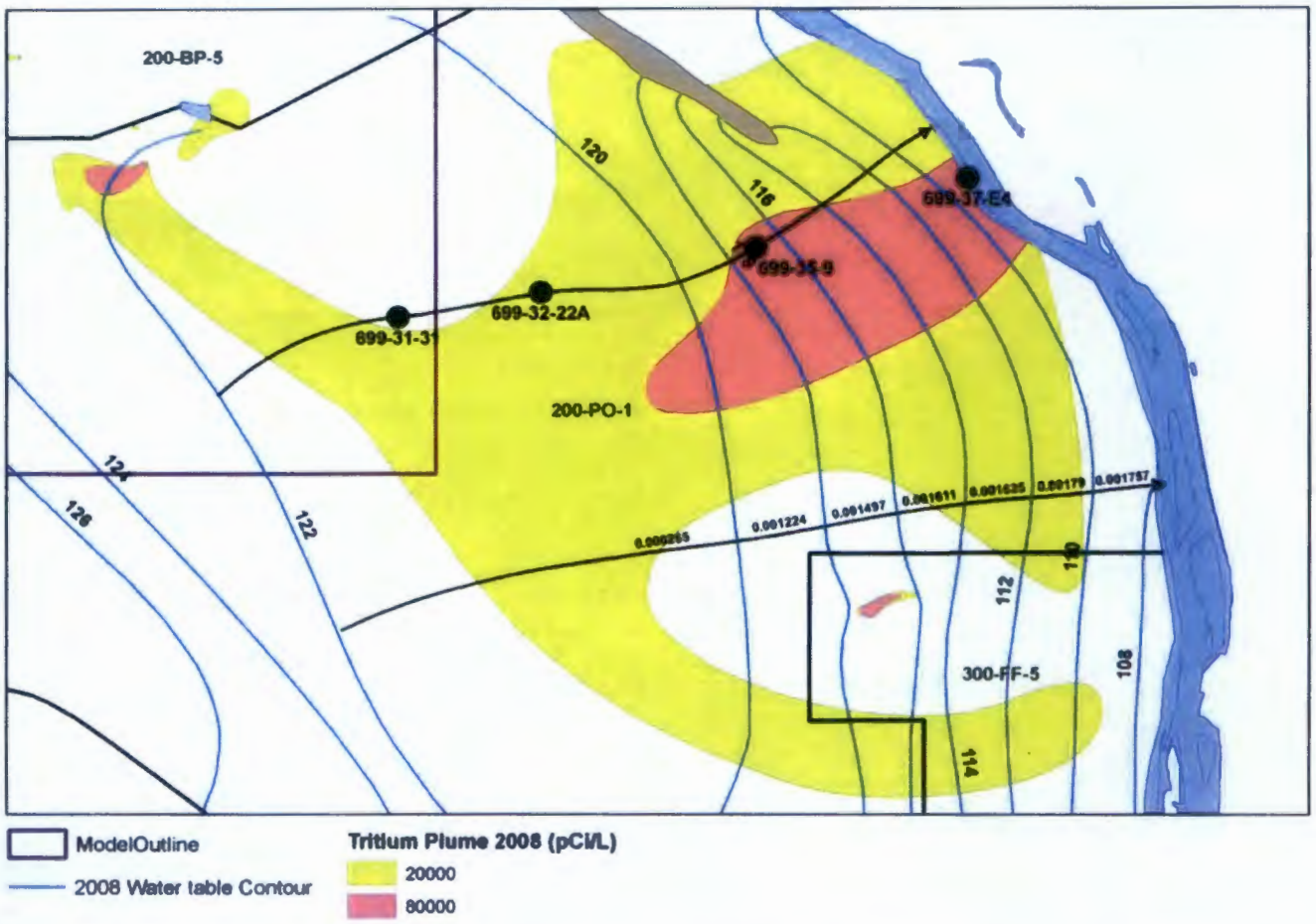

Figure 1. Far Field Portion of the 200-PO-1 OU showing the inferred flow paths for the CY 2008 Water Table along with the tritium plume concentration distribution. The stream tube is chosen to be the flow path that has co-located monitoring wells. The four monitoring wells that are shown are chosen for comparing the stream tube results.

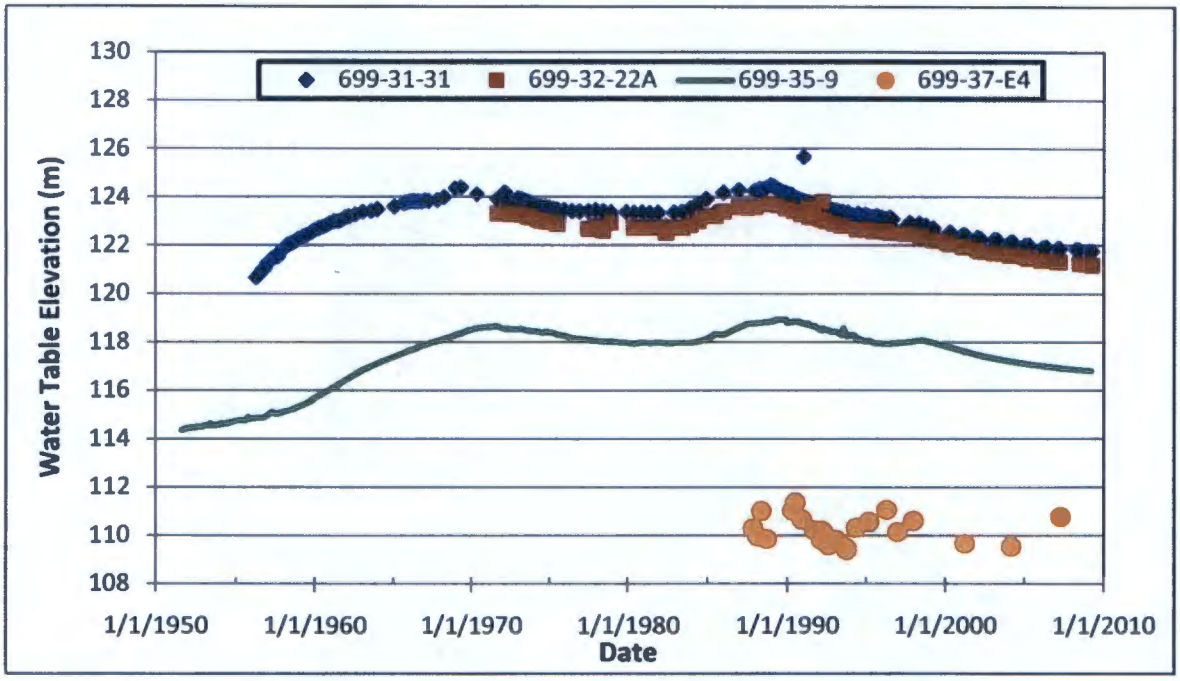

Figure 2. Well hydrographs for the four monitoring wells presented in Figure 1.

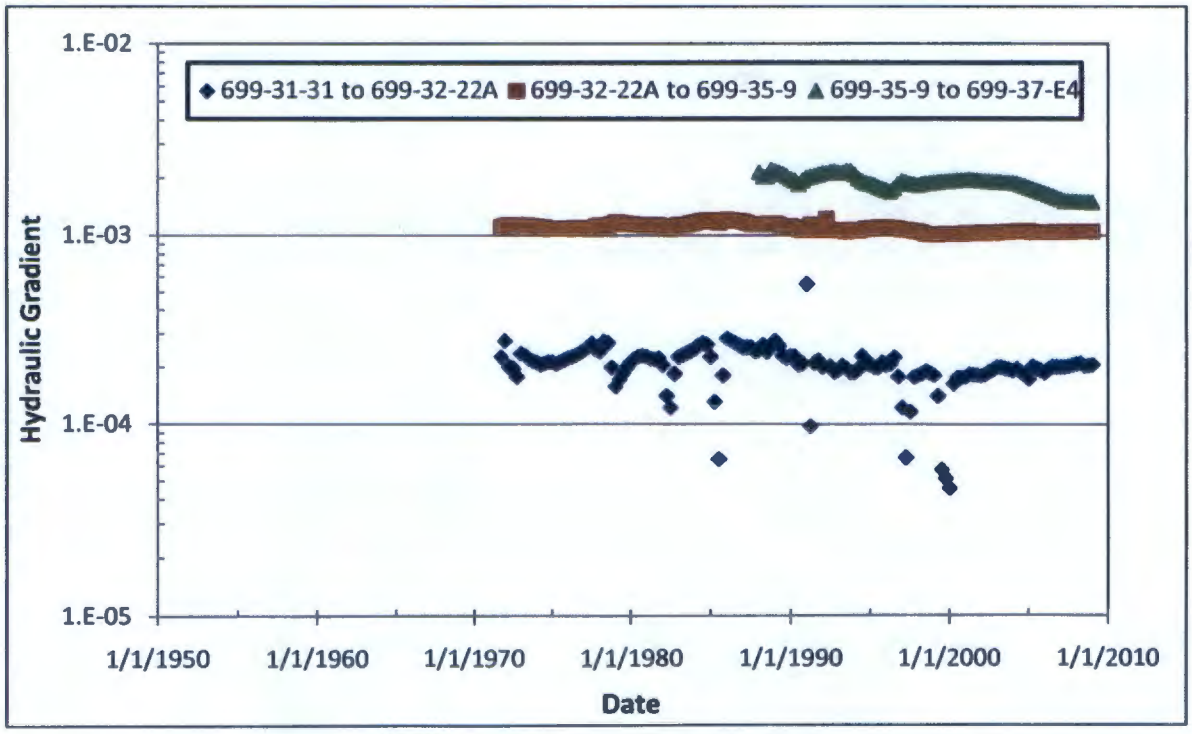

Figure 3. Hydraulic Gradient between monitoring wells presented in Figure 1.

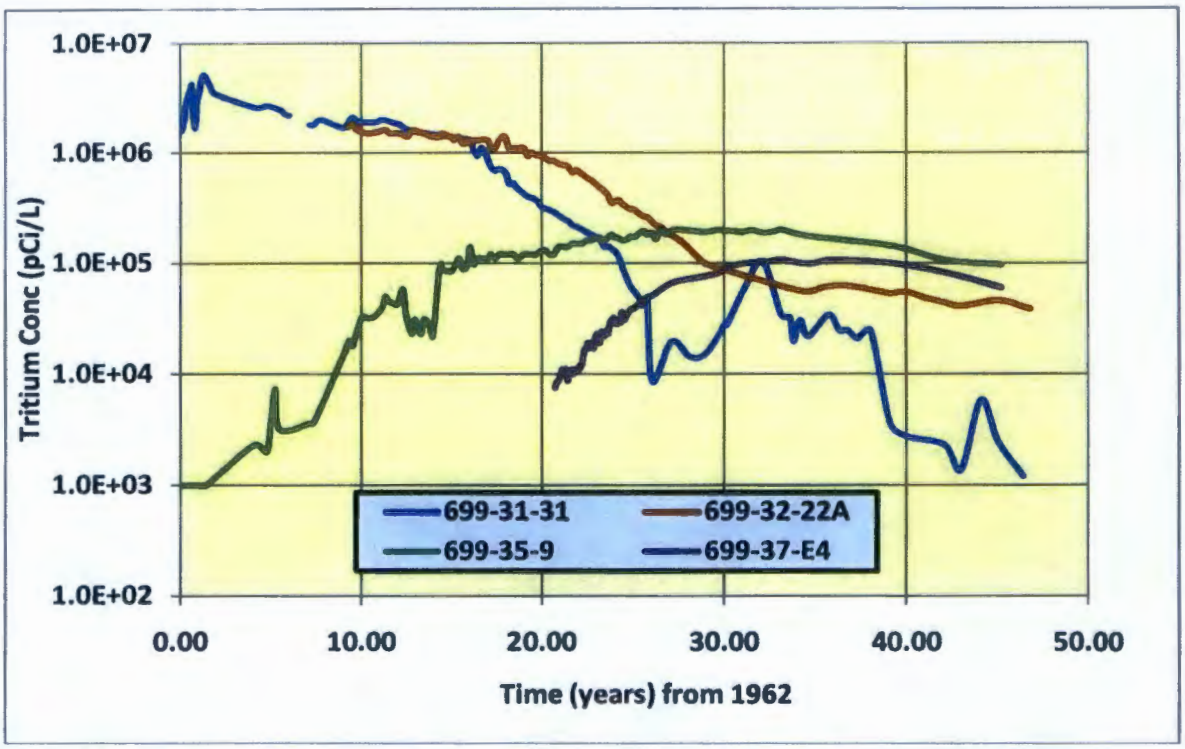

Figure 4. Tritium concentration history for the four monitoring wells presented in Figure 1.

Analytical solutions for transport in the stream tube that solves the 1-D advection-dispersion equation are available and can be easily applied for conditions where a constant concentration is applied at the upstream boundary over a period of time. But when the concentration at the upstream boundary is changing over time then the calculations need to be discretized in time so that constant concentrations can be applied over each time step and contribution from each time step can be tracked to be added later. Since upstream boundary concentration (monitoring well 699-31-31 in Figure 4) varies over orders of magnitude, a semi analytical solution is preferred.

For the purpose of solving the 1-D advection-dispersion equation, the Pipe Pathway element of GoldSim Pro 10.00 (SP2) (GoldSim Technology Group, 2009), an acquired computer software package, is used. The Pipe Pathway element in GoldSim contaminant transport module is designed to calculate rates of contaminant transport along pathways that behave as stream tubes or fluid conduits. Pipe Pathways use a Laplace transform approach to provide analytical solutions to a broad range of advective-dominated mass transport systems involving one-dimensional advection, longitudinal dispersion, retardation, decay and ingrowth, and exchanges with immobile storage zones. The geometry of the pathway is defined by specifying length, a cross-sectional area, and a perimeter. Mass enters at one end of a Pipe (or along some specified length of Pipe), advects through (with dispersion, sorption, and diffusion within) the mobile zone of the Pipe, and then exits at the other end.

Figure 5 shows the geologic cross-section along a line approximately parallel to the axis of the tritium plume. The upper part of the unconfined aquifer is primarily located in the undifferentiated Cold Creek/Pre-Missoula unit. This information is used to develop the attributes of the far-field representation, such that the porosity and bulk density of the aquifer are consistent with the sandy-gravel sediment type description of the Cold-Creek unit.

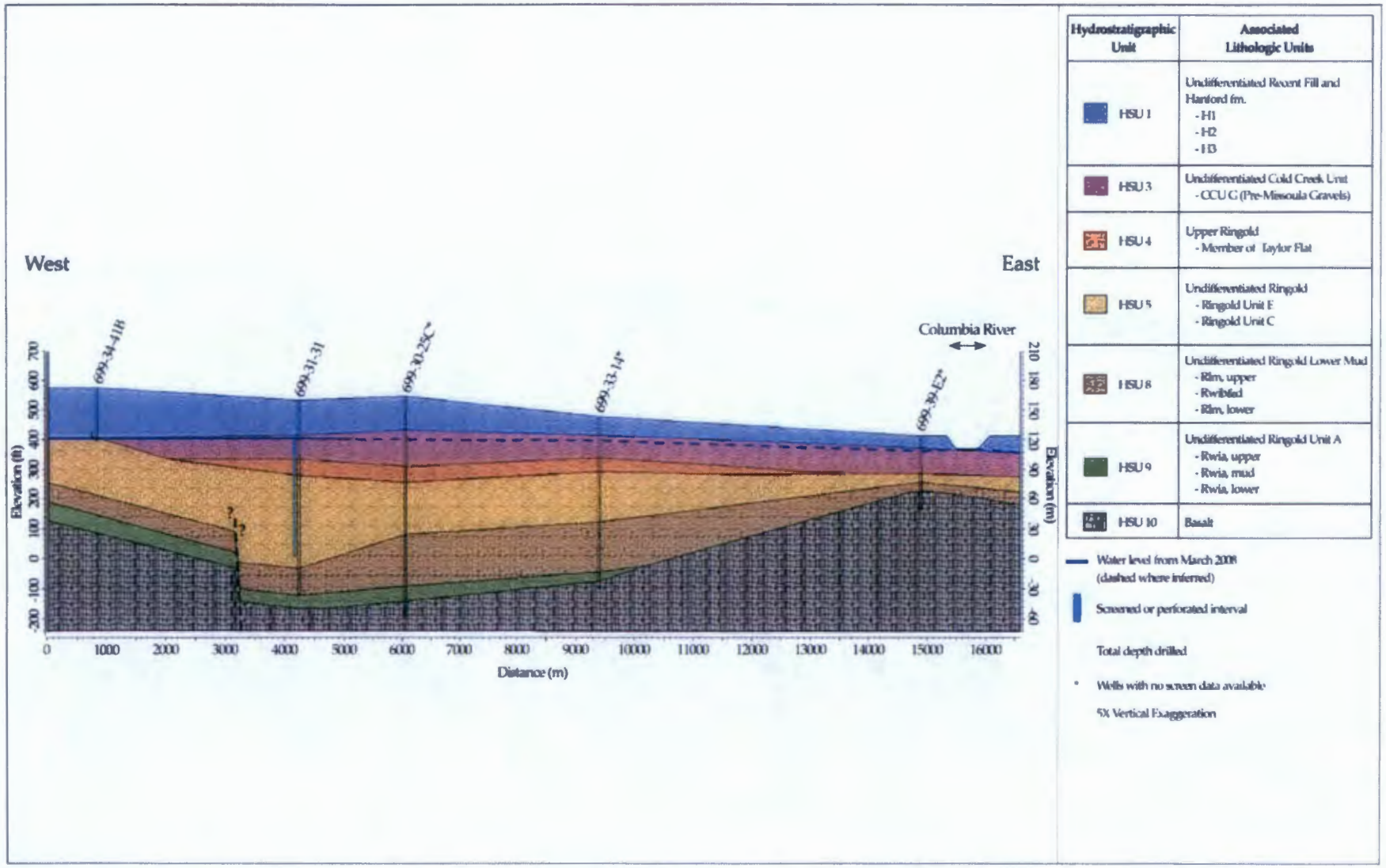

Figure 5. Geologic cross-section along a line (see inset) that approximately parallels the axis of the tritium plume in the far-field portion of the 200-PO-1 OU.

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3 Assumptions and Inputs

3.1 Domain

The stream tube is modeled by three segments of the Pipe Pathway that corresponds to the flow line with co-located monitoring wells shown in Figure 6. The first segment of the Pipe Pathway connects monitoring wells 699-31-31 and 699-32-22A (path length of 2,740 m); the second segment connects between wells 699-32-22A and 699-35-9 (path length of 4,210 m); and the third segment is between wells 699-35-9 and edge of Columbia River (path length of 4,060 m). The results of third segment are compared to the nearby monitoring well 699-37-E4.

The saturated thickness for all segments of the Pipe Pathway is chosen to be 10 m, which represents the upper part of the unconfined aquifer. Since tritium is a highly mobile contaminant, it is expected to be present at highest concentrations near the water table and thus modeling upper part of the Cold Creek/Pre-Missoula hydrostratigraphic unit is deemed adequate. A unit width (1-m) of the Pipe Pathway is chosen to represent the third dimension for the purpose of calculating volumetric fluxes.

3.2 Groundwater Velocities

The groundwater flow velocities in each of the three pipe segments are computed separately. These are based on the observed concentration of tritium at monitoring wells shown in Figure 4, since tritium is transported without any retardation. For the purpose of estimating flow rates the observed concentrations

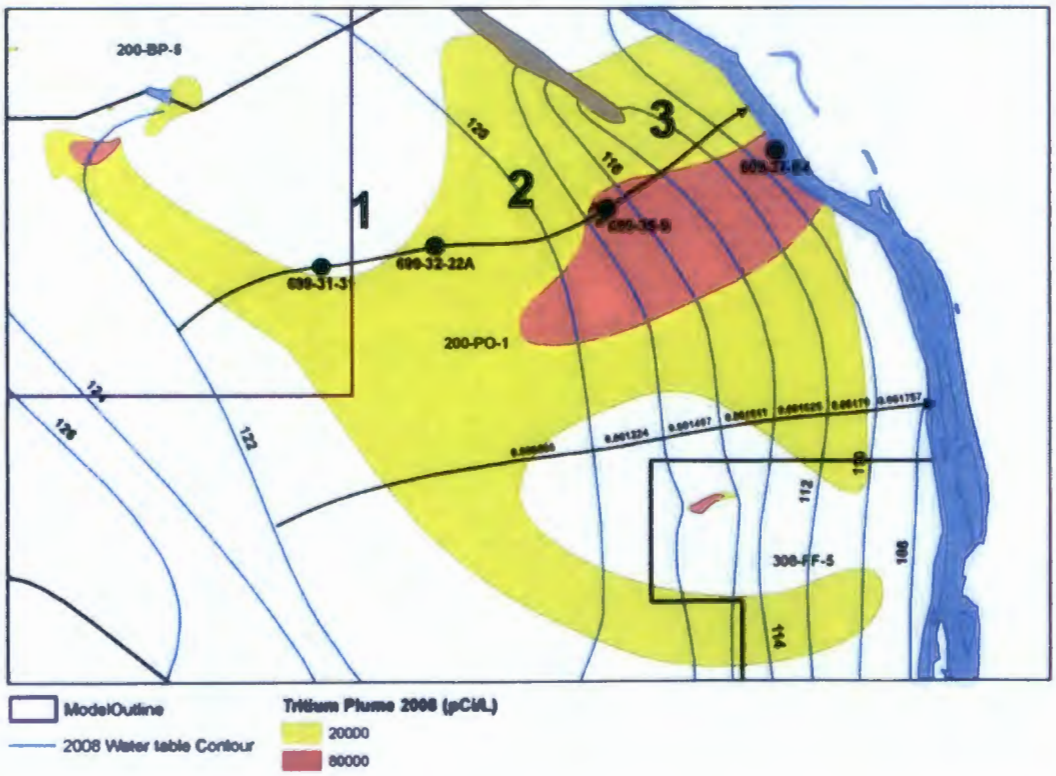

Figure 6. The three segments of the Pipe Pathway are shown along with the inferred flow path. Results from the four monitoring wells are used for comparing the modeling results.

were first adjusted for radioactive decay. Because the first available data point at the upstream monitoring well 699-31-31 is from January 1962 (reported tritium concentration is 1.7×10^6 pCi/L) the remaining concentration dataset for all the monitoring wells were decay corrected to this date for the purpose of comparison. Next the concentrations were normalized. For this purpose the maximum concentration for well 699-31-31 was considered. Because the maximum concentration (of 5.2×10^6 pCi/L) occurs about 1.27 years after January 1962, this concentration was decay adjusted (by 1.27 years), resulting in the theoretical maximum reference concentration of 5.6×10^6 pCi/L. All of the concentrations were normalized to this value, as shown in Figure 7. The normalization process helps identify the relative concentration changes and thereby can be used to estimate the lag times between upstream and downstream wells for calculating flow velocity. By this means, the average lag time in Segment 1 (between monitoring wells 699-31-31 and 699-32-22A) is estimated to be about 17 years while in Segment 2 (between wells 699-32-22A and 699-35-9) is estimated to be about 15 years. Based on the path lengths among segments (calculated above) the average flow velocity for Segment 1 is estimated to be about 164 m/yr while that for Segment 2 is estimated to be about 277 m/yr. The flow velocity in Segment 3 could not be calculated from Figure 7, but is expected to be similar to that for Segment 2 (based on the similarities between these segments in terms of flow gradient and aquifer properties). It should be noted that these velocity estimates are approximate and can vary by over a factor of two in certain time periods due to changes in hydraulic gradients imposed by operational discharges (Figure 3). The flow velocities are changed into volumetric fluxes for model input by multiplying with the porosity and cross-sectional area of the Pipe Pathway.

3.3 Dispersivity

The longitudinal dispersivity for each Pipe segment is based on the actual measurements of tritium concentrations in wells located along the flow path. The reason for choosing tritium is that it is considered a conservative tracer because it is non-sorbing and because long-term measurements exist along these wells for a period extending over 20 years.

The relative concentrations at the wells are plotted as breakthrough curves following the radioactive decay correction and by normalizing the concentration to the maximum observed value for that well. By assuming a constant source concentration upgradient, the breakthrough curve at the observation point (well) is assumed to follow a normal distribution. Based on the methodology given in Domenico and Schwartz (*Physical and Chemical Hydrogeology*, Section 18.2), for a two-dimensional areal extent of the plume produced by a continuous point source, the breakthrough curve at any point along the middle of the plume can be constructed by plotting relative concentration as a function of time. This breakthrough curve is a cumulative normal distribution with a 2σ value (where σ denotes the standard deviation) that can be derived graphically as:

$$2\sigma_t = (t_{84} - t_{16})$$

where t_{84} and t_{16} are the breakthrough times corresponding to relative concentration of 0.84 and 0.16, respectively. The longitudinal dispersion coefficient (D_L) is calculated as:

$$D_L = v^2 \sigma_t^2$$

and the longitudinal dispersivity (α_L) is determined as:

$$\alpha_L = \frac{D_L}{v}$$

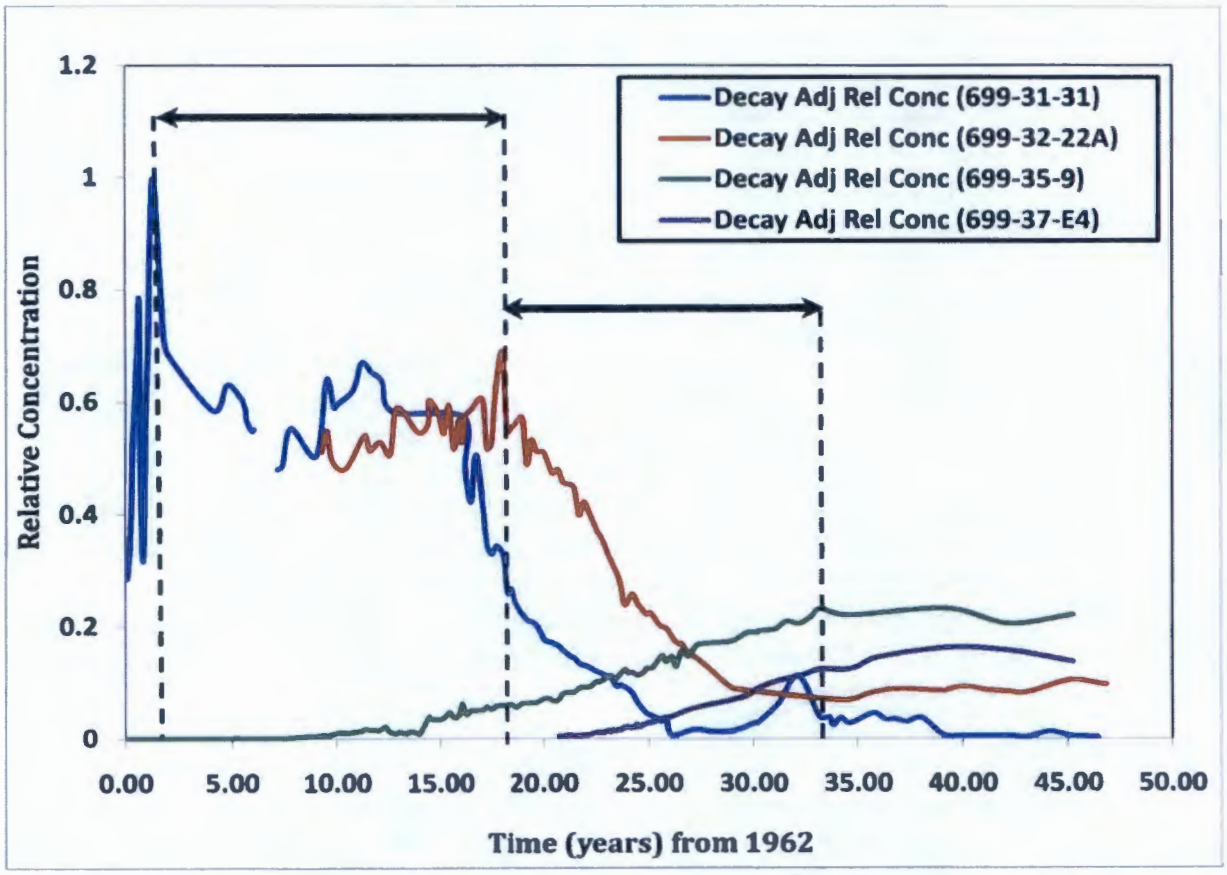

Figure 7. The relative concentration of the four monitoring wells shown in Figure 1 are presented with an estimate of average lag time to determine the flow velocity.

The longitudinal dispersivity calculated using this method varied from 120 m for first pipe segment (distance of 2,740 m); 630 m for the second pipe segment (distance 4,210 m); and 1,450 m for the third pipe segment (distance of 4,060 m). Note that these values are approximate as they are based on the flow velocity, which itself could vary significantly over the simulated timeframe.

3.4 Other Transport Parameters

The other transport relevant parameters such as the linear sorption coefficient (K_d), decay rate, effective porosity, and bulk density are taken from laboratory measurements and other modeling studies. There is no sorption modeled for tritium (that is, $K_d = 0$ ml/g). Effective porosity for the Pipe Pathways is selected to be 0.227 based on the best-estimate site-wide data presented in Table 6.4 of PNNL-18564 (*Selection and Traceability of Parameters to Support Hanford-Specific RESRAD Analyses – An FY08 Status Report*). Because there is no sorption modeled, the bulk density value for the Pipe Pathway is left at a default value of 2000 kg/m^3. The effective porosity is selected to be representative of the sandy gravel sediment from Hanford Formation due to lack of information specific to Cold Creek unit in the far-field portion of the 200-PO-1 OU. For purposes of this calculation, a single representative value is deemed adequate because of the averaging of the rock volumes over large transport distances.

3.5 Contaminant Initial and Boundary Conditions

The initial contaminant concentration conditions in the Pipe Pathways are set to zero. A time varying boundary concentration is applied to the upstream portion of the first segment of the Pipe Pathway based on the concentration time history observed at monitoring well 699-31-31, starting from January 1962 (Figure 4). Because the calculations are performed over time steps (chosen dynamically by GoldSim solver) that are much smaller than the boundary concentration data, the boundary concentrations are interpolated over shorter time increments to provide continuous time series data. For the purpose of applying a time varying boundary concentration, a Cell Pathway element in GoldSim is utilized. The volumetric discharge in the Cell Pathway is set equal to that applied to the first pipe segment.

Because each pipe segment has different flow velocity, the cumulative contaminant mass flux from the end of each upstream pipe segment is calculated over the time step and injected into the downstream pipe segment over the same time step so as to preserve the mass flux continuity.

4 Software Applications

Information supporting controlled use of software for this calculation is provided in this section.

4.1 Approved Software

GoldSim PRO 10.00 (SP 2) software is used for the calculations presented here. It is approved software that is managed and used in compliance with the requirements of PRC-PRO-IRM-309, *Controlled Software Management*.

4.1.1 Description

- Software Title : GoldSim Pro
- Software Version: 10.00 (SP 2)
- Hanford Information Systems Inventory (HISI) Identification Number: 2461 (Safety Software, Level C)
- Authorized Workstation type and property number: DELL PC, SUNIL-PC (INTERA Property Tag 00362)
- Authorized User: Sunil Mehta
- CH2M Hill Plateau Remediation Company (CHPRC) Software Control Documents:
    - CHPRC-00180 Rev 0, *GoldSim Pro Functional Requirements Document*
    - CHPRC-00175 Rev 1, *GoldSim Pro Software Management Plan*
    - CHPRC-00224 Rev 0, *GoldSim Pro Software Test Plan*
    - CHPRC-00256 Rev 0, *GoldSim Pro Requirements Traceability Matrix*
    - CHPRC-00262 Rev 0, *GoldSim Pro Acceptance Test Report*

4.1.2 Software Installation and Checkout

A copy of the *CHPRC Software Installation and Checkout Form* for the authorized user and the authorized workstation used for this calculation is provided below.

4.1.3 Statement of Valid Software Application

The software is appropriate for the application and used within the range of intended uses for which it was tested and accepted by CHPRC.

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:** GoldSim Pro 10.00(SP2) **Software Version No.:** 10.00

EXECUTABLE INFORMATION:

2. **Executable Name (include path):**

   C:\Program Files\GTC\GoldSim 10\GoldSim.exe

3. **Executable Size (bytes):** 1,441,000

COMPILATION INFORMATION:

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

   Compiled by vendor

5. **Operating System (include version number):**

   Windows

INSTALLATION AND CHECKOUT INFORMATION:

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

   SUNIL-PC (INTERA Property Tag 00362)

7. **Operating System (include version number):**

   Windows Vista Business SP1

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

TEST CASE INFORMATION:

9. **Directory/Path:**

   C:\Program Files\GTC\GoldSim 10\General Examples

10. **Procedure(s):**

    per CHPRC-00224 Rev 0, GoldSim Pro Software Test Plan

11. **Libraries:**

    N/A

12. **Input Files:**

    FirstModel.gsm

13. **Output Files:**

    FirstModel.gsm

14. **Test Cases:**

    GS-ITC-1

15. **Test Case Results:**

    Match expected results as presented in CHPRC-00224 Rev 0, GoldSim Pro Software Test Plan

16. **Test Performed By:** Sunil Mehta

17. **Test Results:** ◉ Satisfactory, Accepted for Use ○ Unsatisfactory

18. **Disposition (include HISI update):**

    Platform listing added to HISI entry

CHPRC SOFTWARE INSTALLATION AND CHECKOUT FORM (continued)

1. Software Name: GoldSim Pro 10.00(SP2) Software Version No.: 10.00

Prepared By:

19.	Software Owner (Signature)	W.E. Nichols (Print)	7/8/2009 (Date)

20. Test Personnel:

Sign	S. Mehta (Print)	7/8/09 (Date)
Sign	Print	Date
Sign	Print	Date

Approved By:

21.	Software SME (Signature)	C.W. Connell (Print)	7/14/09 (Date)

A-8005-149 (REV 0)

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5 Calculation

The transport calculations are performed by running the GoldSim model in a deterministic mode. The calculations are performed for the period of 47 years (from the start of calendar year 1962 to end of calendar year 2008). The contaminant transport module is run using the high solution precision setting in GoldSim with results reported at one-year time steps throughout the simulated time frame. The radioactive decay (and any ingrowth) of the contaminant mass is automatically calculated by GoldSim. Only transport of tritium is simulated. For the purpose of performing the calculations the boundary concentration units of pCi/L are converted to mg/L by dividing the concentration by the specific activity of tritium (9,672.49 Ci/g) and other unit conversions. Following the calculations, the outputs are reconverted to pCi/L for purpose of comparison.

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6 Results/Conclusions

The concentration time history results from the end of all three segments of the Pipe Pathway are presented in Figure 8 and compared to the observed concentrations from the nearby monitoring wells. As stated earlier, only the upstream time-varying boundary concentration is applied to the first pipe segment based on observed data at monitoring well 699-31-31. The concentration calculated at the end of first pipe segment (dashed red line) is compared to the observed concentration at the collocated monitoring well 699-32-32A (solid red line). The results indicate good comparison to the peak concentrations that occur in the timeframe of 10 to 20 years with similar declining trend later on. Exact matches are not expected because the imposed groundwater flow velocity (and volumetric water flux) is not varied as a function of time in the Pipe Pathway even though in reality the flow velocities changed due to operational discharges as well as natural variability in hydrologic properties.

The concentration calculated at the end of the second pipe segment (dashed green line) shows excellent comparison with the observed concentration at the collocated monitoring well 699-35-9 (solid green line). Both the peak concentrations and the declining concentration trend for the period of simulation show excellent comparison. Similarly, the concentrations calculated at the end of third pipe segment (dashed purple line) show excellent comparison with the observed concentration at the nearby monitoring well 699-37-E4 (dashed purple line), matching in both magnitude and trend.

These results indicate that the 1-D transport using simple stream tubes are adequate for modeling far-field transport in the 200-PO-1 Groundwater OU. Because the transport is advection dominated and the predominant flow paths have changed little over the simulated timeframe, it can be inferred that the spatial heterogeneity in the aquifer has not appreciably impacted the transport of contaminants. Vertical and lateral dispersion is limited. The sensitivity analysis that evaluated varying the longitudinal dispersivity within reasonable bounds (±30%) indicated limited impact on transport results. However, a reasonable estimate of longitudinal dispersivity is needed for matching the observed concentrations. Ignoring lateral dispersion of contaminants due to spatial heterogeneity and assuming Dupuit conditions in the unconfined aquifer (insignificant vertical gradients) is shown to provide a reasonable approximation for modeling transport in the far field portion of the 200-PO-1 Groundwater OU.

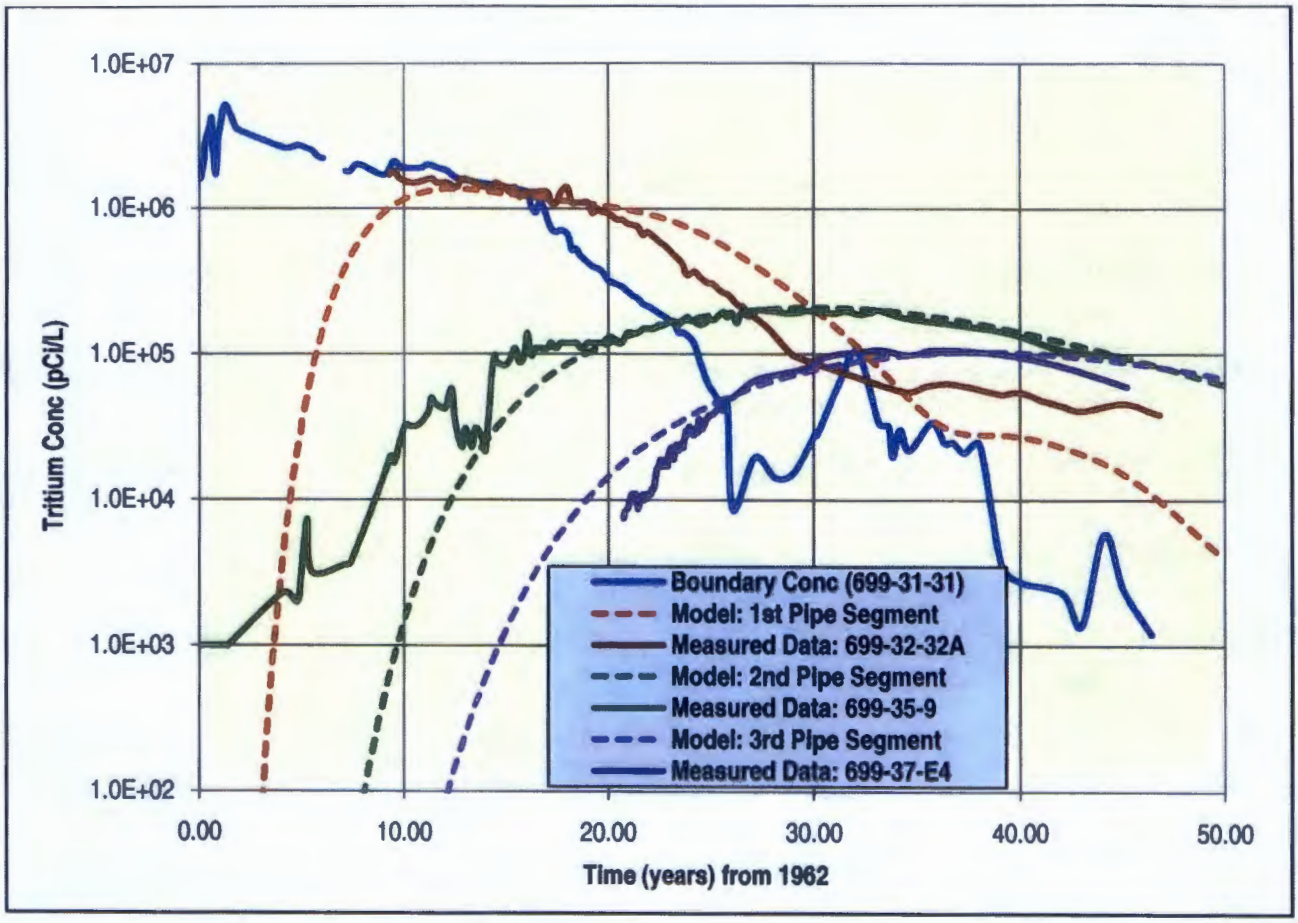

Figure 8. The relative concentration of the four monitoring wells shown in Figure 1 are presented with an estimate of average lag time to determine the flow velocity.

7 References

CHPRC-00180 Rev 0, *GoldSim Pro Functional Requirements Document,* CH2M Hill Plateau Remediation Company, Richland, Washington

CHPRC-00175 Rev 1, *GoldSim Pro Software Management Plan,* CH2M Hill Plateau Remediation Company, Richland, Washington

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