2003 Initial Assessments of Closure for the C Tank Farm: Numerical Simulations

Z. F. Zhang V. L. Freedman M. D. White

July 2003

Pacific Northwest National Laboratory Richland, WA 99352

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY operated by BATTELLE for the UNITED STATES DEPARTMENT OF ENERGY under Contract DE-ACO6-76RLO1830

Printed in the United States of America

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831-0062; ph: (865) 576-8401 fax: (865) 576-5728 email: reports@adonis.osti.gov

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161 ph: (800) 553-6847 fax: (703) 605-6900 email: orders@ntis.fedworld.gov online ordering: http://www.ntis.gov/ordering.htm



2003 Initial Assessments of Closure for the C Tank Farm: Numerical Simulations

Z. F. Zhang V. L. Freedman M. D. White

July 2003

Prepared for the U.S. Department of Energy under Contract DE-AC06-76RL01830

Pacific Northwest National Laboratory Richland, WA 99352

Summary

In support of CH2M HILL Hanford Group, Inc.'s (CHG) preparation of a Field Investigative Report (FIR) for the closure of the Hanford Site Single-Shell Tank (SST) Waste Management Area (WMA) tank farms, a set of numerical simulations of flow and solute transport was executed to investigate different potential contaminant source scenarios that may pose long-term risks to groundwater from the closure of the C Tank Farm. This report documents the simulation of 14 cases (plus two verification and five sensitivity cases) involving two-dimensional cross sections through the C Tank Farm (Tanks C-103–C-112). Using a unit release scenario at Tank C-112, four different types of leaks were simulated. These simulations assessed the effect of past leaks and leaks during retrieval as well as residual wastes and ancillary equipment after closure. Two transported solutes were considered: uranium-238 (U-238) and technetium-99 (Tc-99). To evaluate the effect of sorption on contaminant transport, six different sorption coefficients were simulated for U-238. Overall, simulations results for the C Tank Farm showed that only a small fraction (<1.2%) of the U-238 with sorption coefficients greater than 0.6 mL/g migrated from the vadose zone in all of the cases. For the conservative solute, Tc-99, results showed that the simulations investigating leaks during retrieval demonstrated the highest peak concentrations and the earliest arrival times due to the high infiltration rate before water was added and surface barriers installed. Simulations investigating past leaks showed peaks and arrival times similar to the retrieval cases. Several different release rates were used to investigate contaminant transport from residual tank wastes. All showed similar peak concentrations and arrival times, except for the lowest initial release rate, which was 1,000 times slower than the highest release rate. Past leaks were also investigated with different release rate models, including advection-dominated, diffusion-dominated, and saltcake release models. Of the three models, peak concentrations were lowest and arrival times later for the saltcake model due to the low solubility (and hence lower release rate) of the residual tank waste solids. For the tank ancillary equipment leak case, the diffusion-dominated release rate model yielded peak concentrations and late arrival times that were similar to the majority of the past leak cases for residual tank wastes. For all source types, the peak concentrations and arrival times were sensitive to the estimated saturated hydraulic conductivity of the unconfined aquifer. When the saturated hydraulic conductivity was increased by a factor of 10, peak concentrations at the first compliance point, the fence line boundary, were decreased by approximately the same magnitude. Peak arrival times also occurred earlier with the higher estimate of hydraulic conductivity.

Contents

1.0 Intr	oduction	1.1
1.1	Modeling Approach	1.2
1.2	Model Application	1.2
2.0 Cas	e Descriptions	2.1
2.1	Retrieval Leak (8,000 gallons)	2.3
2.2	Retrieval Leak (20,000 gallons)	2.3
2.3	Past Leak	2.3
2.4	Past Leak from Ancillary Equipment	2.3
2.5	Residual Tank Waste (release rate R ₀)	2.3
2.6	Residual Tank Waste (release rate R ₁)	2.4
2.7	Residual Tank Waste (release rate R ₂)	2.4
2.8	Residual Tank Waste (release rate R ₃)	2.4
2.9	Residual Tank Waste (release rate R ₄)	2.4
2.10	Residual Tank Waste (advection dominated)	.2.4
2.11	Residual Tank Waste (diffusion dominated)	.2.5
2.12	Residual Tank Waste (saltcake)	2.5
2.13	Residual Ancillary Equipment Waste (diffusion dominated)	2.5
2.14	Residual Tank Waste (diffusion dominated)	2.5
3.0 Tec	hnical Approach	3.1
3.1	Overview	3.1
3.2	Modeling Data Package	3.2
3.2	2.1 Recharge Estimates	3.3
3.2	2.2 Vadose Zone Flow and Transport Properties	3.4
3.2	2.3 Stochastic Model for Macroscopic Anisotropy	3.4
3.2	2.4 Bulk Density and Sorption Coefficient	3.6
3 2 '	2.5 DIFFUSIVITY	3.1
33	Input File Generation	3.8
3	3.1 Input File	3.8
3.3	3.2 Zonation File	3.8
3.4	Implemented Features	3.9
3.4	4.1 Advection-Dominated Release Model	3.10
3.4	4.2 Diffusion-Dominated Release Model.	3.11
3.4	4.3 Saltcake Release Model	3.12
3.5	Source 1 erms	5.13
3.6	STOMP Execution	3.14
3.7	Result Translation	3.14
3.8	Analytical Groundwater Transport Modeling	3.15

4.0 Sin	nulat	ion Results	
4.1	Sur	nmary Description of the Simulations	
4.2	Sec	tion Organization	
4.3	Init	ial Conditions and Saturation Distributions	4.3
44	Ret	rieval Leaks	43
1.1	7 1	$C_{ase} \rightarrow 8000$ Gellons at C 112	
4.4 4 '	2.1	Case 1 (HiK): 8000 Gallons at C-112 C-109 C-106 and C-103	
4	2.2	Case 1v ⁻ 8000 Gallons at C-112, C-109, C-106 and C-103	4 5
4.2	2.4	Case 2: 20000 Gallons at C-112.	4.6
4.2	2.5	Leak Volume Effects: Comparison of Cases 1 and 2	
4.3	Pas	t Leaks	
4.3	3.1	Case 3: Past Leak	
4.3	3.2	Case 3 (Hi K): Past Leak	
4.3	3.3	Case 4: Past Leak	
4.	3.4	Case 4 (HiK): Past Leak	
4.	3.5	Inventory Depth Effects: Comparison of Cases 3 and 4	
4.4	Res	sidual Tank Wastes with Rate-Controlled Releases	
4.4	4.1	Case 5: Release Rate R0 at C-112	
4.4	4.2	Case 5v: Release Rate R ₀ at C-112, C-109, C-106, and C-103	
4.4	4.2	Case 6: Release Rate R1 at C-112	
4.4	4.3	Case 7: Release Rate R2 at C-112	
4.4	4.4	Case 8: Release Rate R3 at C-112	
4.4	4.5	Case 9: Release Rate R4 at C-112	
4.4	4.7	Release Rate Effects: Comparison of Cases 5–9	
4.5	Res	sidual Tank Wastes with Different Controlling Processes	
4.:	5.1	Case 10: Advection-Dominated Release	
4.:	5.2	Case 10 (HiK): Advection-Dominated Release	
4.:	5.3	Case 11: Diffusion-Dominated Release	
4.:	5.4	Case 11 (HiK): Diffusion-Dominated Release	
4.:	5.5	Case 14: Diffusion-Dominated Release	
4.:	5.6	Diffusion Coefficient Effects: Comparison of Cases 11 and 14	
4.:	5./ D	Case 12: Saltcake Release	
4.6	Res	sidual Ancillary Equipment Wastes	
4.0	6.1	Case 13: Diffusion-Dominated Release	
4.7	Pea	k Concentrations and Arrival Times at Compliance Points	
4.′	7.1	Average Travel Time to Compliance Points	
4.′	7.2	Peak Concentrations at Compliance Points	
4.	7.3	Effect of K_d on Peaks and Arrival Times	
4.8	Sol	ute Mass Balance	
5.0 Ele	ectroi	nic Files	
5.1	Soi	irce Coding	
5.2	Gee	ology	
5.3	Init	ial Inventory	

Figures

3.1	Northwest–Southeast Cross Section for C Tank Farm Through Tanks C-112, C-109,	
	C-106 and C-103	3.9
3.2	Rock/Soil Zonation for the Pre- and Post-Construction Periods of the C Tank Farm	3.10

Tables

2.1	Case Descriptions	2.2
3.1	Cross-Section Aquifer Geometry and Properties	3.3
3.2	Streamtube Aquifer Geometry and Properties	3.3
3.3	Recharge Estimates	3.4
3.4	Composite van Genuchten-Mualem Parameters for Various Strata at C Tank Farm	3.4
3.5	Macroscopic Anisotropy Parameters Based on Polmann Equations for Strata at C Tank Farm	3.6
3.6	Effective Parameter Estimates for Product of Bulk Density and Retardation Coefficient	
	for U-238 at C Tank Farm	3.7
3.7	Nonreactive Macrodispersivity Estimates for Strata at the C Tank Farm	3.8
3.8	Input Parameters for the Three Release Models	3.13
3.9	Distance to Compliance Point, Groundwater Velocity, and Travel Time from C Tank Farm	3.15
3.10	Analytical Groundwater Transport Modeling Properties	3.17
4.1	Predicted Peak Concentrations and Arrival Times at Fence Line for Base Cases in Year 12000.	4.2
4.2	Predicted Peak Tc-99 Flux, Arrival Time, and Cumulative Mass at Year 12000	4.22
4.3	Predicted Peak U-238 ($K_d = 0.01$) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.23
4.4	Predicted Peak U-238 ($K_d = 0.03$) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.23
4.5	Predicted Peak U-238 ($K_d = 0.10$) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.24
4.6	Predicted Peak U-238 ($K_d = 0.30$) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.24
4.7	Predicted Peak U-238 ($K_d = 0.60$) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.25
4.8	Predicted Peak U-238 (K_d = 1.00) Flux, Arrival Time, and Cumulative Mass at Year 12000	4.25
4.9	Predicted Peak Tc-99 Aqueous Concentrations and Arrival Time Summary	4.26
4.10	Predicted Peak U-238 ($K_d = 0.01$) Aqueous Concentrations and Arrival Time Summary	4.27
4.11	Predicted Peak U-238 ($K_d = 0.03$) Aqueous and Arrival Time Summary	4.28
4.12	Predicted Peak U-238 ($K_d = 0.10$) Aqueous Concentrations and Arrival Time Summary	4.29
4.13	Predicted Peak U-238 ($K_d = 0.30$) Aqueous Concentrations and Arrival Time Summary	4.30
4.14	Predicted Peak U-238 ($K_d = 0.60$) Aqueous Concentrations and Arrival Time Summary	4.31
4.15	Predicted Peak U-238 ($K_d = 1.00$) Aqueous Concentrations and Arrival Time Summary	4.32
4.16	STOMP Mass Balance for Tc-99	4.33
4.17	STOMP Mass Balance for U-238 ($K_d = 0.01$)	4.34
4.18	STOMP Mass Balance for U-238 ($K_d = 0.03$)	4.34
4.19	STOMP Mass Balance for U-238 ($K_d = 0.10$)	4.35
4.20	STOMP Mass Balance for U-238 ($K_d = 0.30$)	4.35
4.21	STOMP Mass Balance for U-238 ($K_d = 0.60$)	4.36
4.22	STOMP Mass Balance for U-238 ($K_d = 1.00$)	4.36
5.1	Source Code Directory	5.1
5.2	Initial Inventory Distribution Files	5.2

5.3.	Steady Flow Initial Condition Files	5.2	2
5.4.	Coupled Vadose Zone and Unconfined Aquifer Modeling Files	5.3	3
5.5.	Analytical Groundwater Transport Modeling Files	5.4	4