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Effect of Waste Depth on Barrier Effectiveness

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

Project Hanford Management Contractor for the
U.S. Department of Energy under Contract DE-AC06-96RL13200

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ABSTRACT

Barriers are being considered at many underground contaminated sites for mitigating potential groundwater impact from vadose-zone contamination. Improved groundwater quality results from the barrier reducing the amount of infiltrating water into the soil (which causes slower water movement and contaminant transport through the vadose zone and into the groundwater) thereby reducing the contaminant concentration in the groundwater. The primary purpose of this analysis is to examine the potential effectiveness of a surface barrier over contamination at different depths in the vadose zone. Other purposes are to explain barrier performance and function, and to provide a screening methodology for determining potential waste sites at Hanford worthy of more study for barrier emplacement. In addition to waste depth, other parameters considered were the vadose zone thickness, historical recharge rate, soil anisotropy, the degree to which the barrier overlaps the buried waste, and contaminants with small absorption on the soil particles. The model results are applied to a specific waste site (BC Cribs and Trenches or similar site) at Hanford as an example application of the scoping-analysis methodology.

The potential effectiveness of a barrier to mitigate groundwater impact from the vadose-zone contamination can be estimated from the depth of the pre-barrier waste zone and the historical recharge value. The waste zone has to be located more than half way toward the aquifer before barrier effectiveness is markedly diminished, with some barrier effectiveness still predicted at a waste zone location that is 90-m below ground surface in a 104-m vadose zone. A barrier that limits the water recharge into the vadose zone to 0.5 mm/yr over the long-term can be effective by more than a factor of thirty in reducing the groundwater contaminant concentration for fully-mobile contaminants. Barriers are more effective for contaminants with some adsorption on the soil, especially for deeper wastes. Barrier edge effects and assumed soil anisotropy are not as important as other parameters examined in this analysis.

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Details of individual review comments and their dispositions are documented separately in report SGW-35380 (*Peer Review Package for SGW-34059, "Effect of Waste Depth on Barrier Effectiveness"*).

EXECUTIVE SUMMARY

Barrier effectiveness is determined by reducing the historical recharge from 25 mm/yr and 5 mm/yr values to a 0.5 mm/yr value, corresponding to the design goal for the Hanford Barrier. Liquid waste with fully mobile contaminants is assumed to have been collected in an underground discrete 120 m long by 3 m thick zone at the time of barrier emplacement, resulting in an additional 4% moisture content above that available from historical recharge. The concentration of the waste in the waste zone moisture is set to 1.0, and set to 0.0 in moisture outside of the waste zone. This yields 12.7% moisture in the waste zone with high recharge and 10.9% in the waste zone with lower recharge. The extra 4% moisture increases the initial downward water velocity in the waste zone. The additional moisture content in the waste zone decreases over time and distance as the water flows downward, moving excess water both laterally and vertically, causing the downward water velocity to eventually slow down to 0.5 mm/yr, the percolation rate through the barrier.

Contaminant concentrations are modeled as a function of time downward through the vadose zone into the 6-m thick aquifer and the 6-m screen of the monitoring well. Several waste depths are assumed, from 30 to 100 m at 10-m increments. Two performance metrics of barrier effectiveness are used to compare behavior with and without the barrier; the time delay factor, and the concentration reduction factor. The time delay factor is calculated by dividing the arrival time of peak concentration with a barrier by the corresponding arrival time without a barrier. The concentration reduction factor is calculated by dividing the peak groundwater contaminant concentration without a barrier by the corresponding peak concentration with a barrier.

The base case modeled for barrier effectiveness has the following assumptions:

- Two-dimensional (2D) domain,
- Infinite horizontal dimension of barrier,
- Single 104-m deep vadose zone soil type and single aquifer soil type,
- Isotropic soil properties,
- Waste zone size 120 m long and 3 m thick,
- Waste zone moisture content 4% above background moisture,
- Historic recharge values 25 and 5 mm/yr; barrier recharge value 0.5 mm/yr,
- Initial waste concentration 1.0 within the waste zone, 0.0 outside the zone, and
- No contaminant retardation or absorption.

Additional cases were run to test sensitivity of parameters and assumptions. These parameters and assumptions were the following:

- Finite barrier over anisotropic soil with different size overlaps,
- Thinner vadose zone (74 m vs. 104 m in base case),
- Contaminant adsorption to soil, and
- Example application to a waste site.

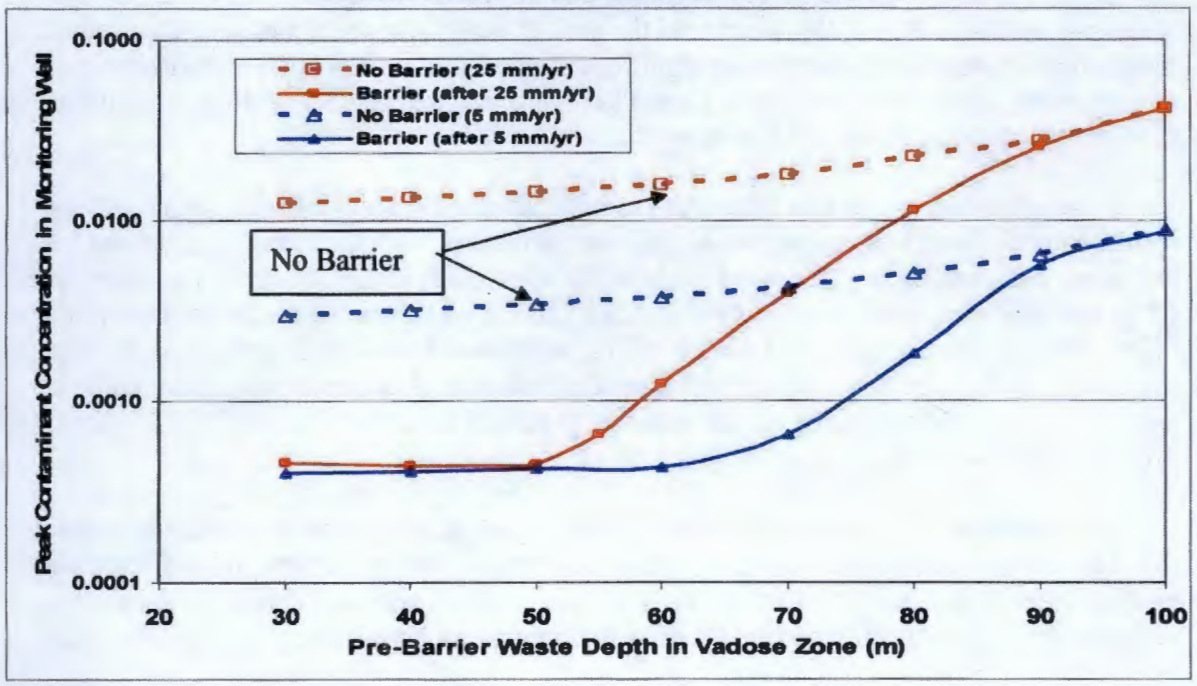
The last case used the modeled reduction of contaminant concentration to illustrate potential barrier performance at an actual waste site with a peak Tc99 concentration of 1.4×10^6 pCi/L in the waste zone moisture.

BASE-CASE BARRIER EFFECTIVENESS

The results of the base case are shown in Figure ES-1 and the details are given in Section 3.1. The peak contaminant concentration in the monitoring well is plotted as a function of the depth, for results from each of the specific waste zones depths modeled, from 30 to 100 m deep. Concentration plots for no-barrier cases for the 25 mm/yr and 5 mm/yr historic recharge are given, with corresponding plots showing the effect on peak concentration for each historic recharge after the construction of a barrier. The peak concentration with no barrier increases somewhat with depth, as there is less opportunity for mixing and spreading with downward flow for deeper waste zones. The peak concentration is also higher with the higher recharge, as the larger moisture content causes a higher downward velocity and a larger contaminant flux rate into the aquifer.

The barrier produces a dramatic effect on groundwater peak contaminant concentration as shown in Figure ES-1, particularly for waste zone depths of 30, 40, or 50 m. Reductions in concentrations up to a factor of 33 were achieved with a barrier, compared to the no-barrier case. The lowered moisture content above the waste zone from barrier emplacement yields much slower downward water velocities. There is little difference in concentration at 30 to 50 m depths, as there is a limit on impact to mixing from the slower downward water velocity, which is the barrier's percolation rate of 0.5 mm/yr. Below 50 m, the antecedent water causes an increase in contaminant flux to the aquifer and the eventual peak concentration at the monitoring well. There is significant benefit (a concentration reduction factor of 2) in terms of reduced peak concentration even at the 80-m depth for both historical recharges for fully-mobile contaminants.

Figure ES-1. Effects of Waste Depth and Historical Recharge on Peak Groundwater Contaminant Concentration



ADDITIONAL SENSITIVITY CASES

The results of the additional sensitivity cases are briefly summarized. Details for the additional cases are given in Sections 3.2 through 3.6.

Finite Barrier and Soil Anisotropy: Soil anisotropy with a ratio of 10 to 1 for the horizontal to vertical hydraulic conductivity was modeled. Anisotropy causes more lateral movement of water and waste. Little impact of either anisotropy or finite barrier overlap was observed for pre-barrier waste depths of 70 m or deeper. Finite barrier overlap generally had a rather slight positive impact (reducing peak groundwater concentration) for shallow wastes of 30-40 m in depth with both isotropic and anisotropic soils. This is caused from water curling under the barrier to intersect the outermost areas of the waste zone, and hasten its transport to the aquifer relative to the bulk mass that causes the eventually peak concentration in the aquifer. A large barrier overlap of 60 m resulted in very similar peak concentrations as the infinite barrier case, for the bounding 50-m waste-zone depth with anisotropic soil. Mid-range soil depths of 50-60 m showed smaller barrier effectiveness with a finite barrier for anisotropic soils than for the infinite barrier, particularly for high recharge and an overlap size of 30 m or less. This also resulted from increased recharge curling underneath the barrier, intersecting a large portion of the outer waste zone and causing more rapid downward contaminant transport for these contaminants.

Thinner Vadose Zone: A 74-m thick vadose zone was analyzed with an infinite barrier and 25 mm/yr recharge. Trends were similar to the 104 m vadose zone, with the highest barrier effectiveness occurring for waste zones located midway in the vadose zone. However, the barrier effectiveness factors are slightly smaller for the top half of the thinner vadose zone.

Contaminant Adsorption: Distribution coefficients (K_d) of 0.1 and 1.0 mL/g were used to model solid phase adsorption, for no-barrier and infinite barrier cases with the 25-mm/yr historical recharge. Adsorption decreased the peak groundwater contaminant concentration for all pre-barrier waste depths, including significant reduction at depths of 70 m or deeper. Concentration reduction factors were almost as high as 40, which is higher than those from fully-mobile contaminants at any pre-barrier waste zone depth.

Application to a Waste Site: An example calculation, showing how the modeling results can be related to an actual waste site, was performed, with the infinite barrier and both historical recharge values. A cross-section of the waste zone in the 216-B-26 Trench in the BC Cribs and Trenches Area is similar in size to the 120 m by 3 m waste zone in this report. Its peak ^{99}Tc porewater concentration of 1.4×10^6 pCi/L, which was located at a depth of 31 m, was multiplied by the relative concentrations from the base case. If a barrier were installed, eventual peak ^{99}Tc concentrations in the groundwater are predicted to be less than 900 pCi/L, which is the drinking water standard.

Summary: The results of modeling using a general, simplified approach show clearly that a barrier can be effective in reducing peak contaminant concentrations in the groundwater, even at waste depths down to 80 m for fully-mobile contaminants, and deeper for less-mobile contaminants. Site-specific barrier design would require modeling using site-specific detail.

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List of Acronyms

DOE	U.S. Department of Energy
GW	Groundwater
PNNL	Pacific Northwest National Laboratory
STOMP-W	Subsurface Transfer Over Multiple Phases, Water mode, computer code
VZ	Vadose Zone

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1.0 INTRODUCTION

Barriers are being considered at many underground contaminated sites for mitigating potential groundwater impact from vadose zone contamination. Barriers achieve their effectiveness by limiting the water recharge from precipitation to reduce the driving force for contaminant transport to the groundwater. The primary purpose of this analysis is to define and examine the potential effectiveness of a surface barrier over contamination at different depths in the vadose zone. Another purpose is to explain the phenomena that cause a surface barrier to mitigate contaminant concentrations in the groundwater. Also, this study provides a screening methodology for determining potential candidate sites for barrier emplacement at Hanford, and to justify more or less investigation for sites. Site specific detail would of course be required to decide on any individual site.

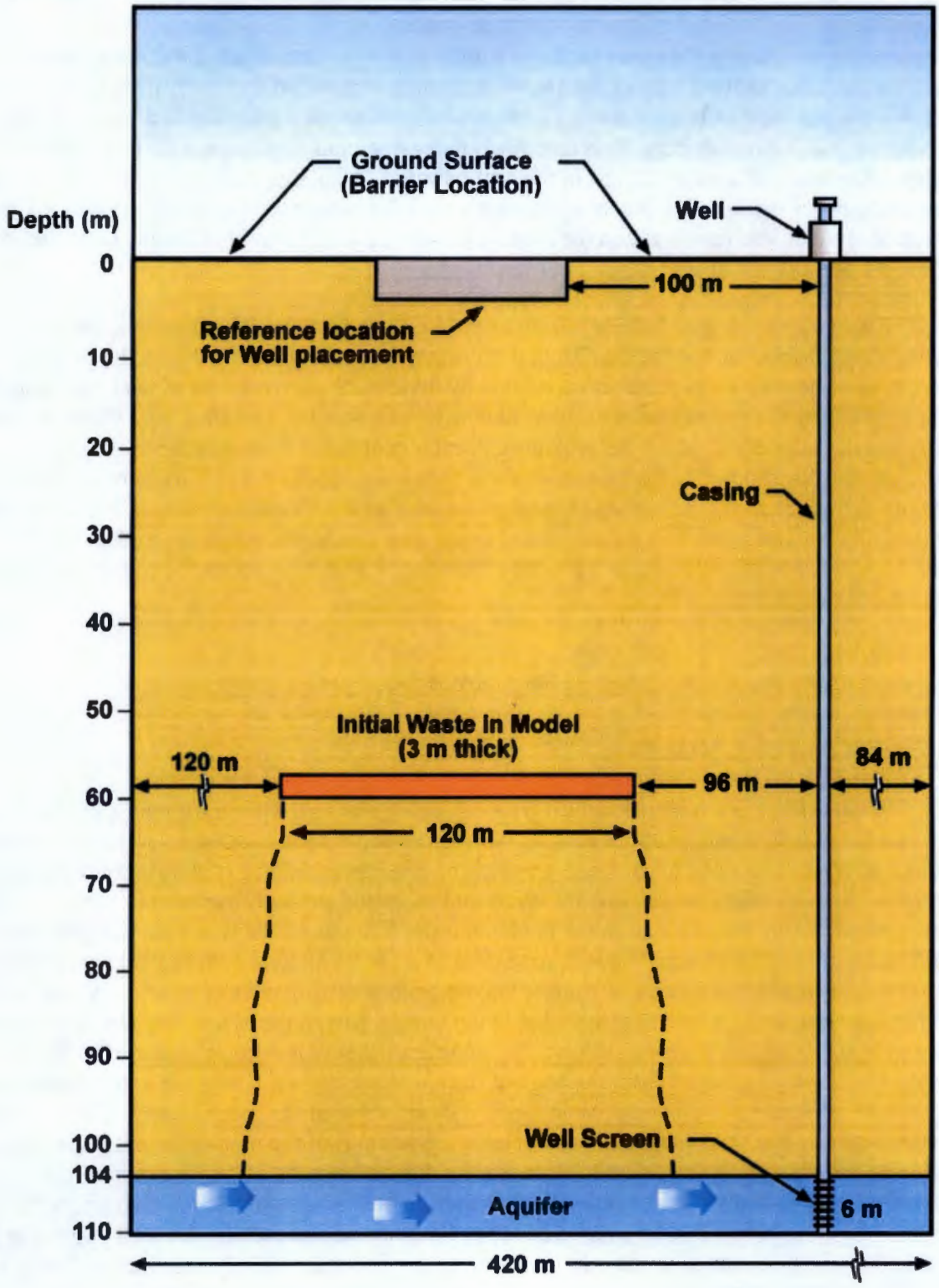
This analysis defines barrier effectiveness with two performance measures, time delay and concentration reduction factors. Both performance measures are relative to the no-barrier alternative. The *time delay factor* is calculated by dividing the arrival time of peak concentration with a barrier by the corresponding arrival time without a barrier. The *concentration reduction factor* is calculated by dividing the peak groundwater contaminant concentration without a barrier by the corresponding peak concentration with a barrier. These performance measures quantify the effectiveness of barriers to protect the aquifer from contamination at various waste depths in the vadose zone, and are calculated for several conditions/scenarios in this report. Intuitively, a barrier should be more effective for waste that is high above the water table rather than near the water table.

2.0 MODEL

2.1 CONCEPTUAL MODEL

A simplified two-dimensional (2D) model, using Hanford Site stratigraphy, is assumed as the basis for potential barrier applications. The entire vadose zone is assumed to simply consist of one soil type, comprised of sand and gravel, which is representative of the Hanford Formation sequence. Site-specific features like silt layers and other soil property variations (heterogeneities) are excluded from the model in order to focus on the waste zone depths without additional site-specific effects. Vadose zone thickness is 104 m, as shown in Figure 1, which illustrates the conceptual model. A thinner vadose zone is considered as a sensitivity case in Section 3.4. The aquifer, which is included in the bottom part of the model domain, is a different soil type and has mainly horizontal flow. The aquifer thickness is 6 m. A monitoring well, located 100 m down gradient from the edge of the assumed original waste site at the surface, is the point of interest for evaluating contaminant concentration in the groundwater. The hypothetical original waste site and waste release are not part of the model; the assumed original waste site is only used as the reference location for determining the 100-m down-gradient monitoring well as shown in Figure 1. The monitoring well is assumed to have no effect on groundwater flow because of its small amount of water extraction making the well passive in the model. All of the contaminant mass in the groundwater is conservatively assumed to flow through the monitoring well location.

Figure 1. Conceptual Model for Barrier Effectiveness as a Function of Waste Depth



The conceptual model is intended to be bounding, but selected parameter values are best-estimate or mean values, in order not to be overly conservative. A 2D model is expected to be more conservative than a 3D model where contaminants can flow in another dimension, resulting in more contaminant spreading and lower concentrations. The model's simplified stratigraphy without silt layers is also expected to be conservative. The barrier is assumed to have infinite horizontal dimensions to allow easier focus on barrier potential for different waste depths. However, the more complicating effects of a finite barrier are also considered in sensitivity cases. Various waste depths are assumed at the time the surface barrier is installed.

The waste zone for each depth is simply assumed to have the same dimensions (120 m long and 3 m thick) and the same initial contaminant concentration (1.0, unit-less) in its pore water at the time of barrier installation. Waste is assumed to be all liquid rather than solid, therefore, release is not an issue. The model excludes initial contamination outside of the waste zone (120 m x 3 m) as shown in Figure 1. The high concentration in such a wide zone can be caused by capillary breaks such as a fine silt loam layer over coarse sand, but the causes of highly concentrated waste zones are not a subject for this report, and are simply assumed to exist. By assuming no hydro-geologic layers in the model, the pore water will initially travel downward much faster than if there were a capillary break, making the model more conservative than reality in this aspect. Several waste depths, from 30 to 100 m with 10-m increments, are simulated with only the 60-m waste depths depicted in Figure 1. This study focuses on fully mobile contaminants, so pre-barrier waste depths shallower than 30 m were not analyzed.

2.2 KEY ASSUMPTIONS

The key assumptions, some of which were discussed in previous section, are presented in this section. More detailed assumptions and soil properties are provided in Appendix A, and several input files for the computer code are shown in Appendix B. Appendix C contains additional information and concentrations for the finite barrier with anisotropic soil cases. The key assumptions and parameters used in the model are grouped into the following areas and are summarized in the following sections:

1) Vadose Zone and Contaminant Transport,

2) Barrier and Recharge, and

3) Aquifer and Monitoring Well.

2.2.1 Vadose Zone and Contaminant Transport Assumptions

1) **Two-dimensional (2D) Model Domain (Figure 1):** 420 m by 110 m (104-m thick vadose zone, 6-m thick aquifer).

2) **No Soil Layers or Heterogeneities**: The vadose zone in the model simply consists of one Hanford soil type, and another soil type for the aquifer (see Appendix A for elucidation of all soil properties).

3) **Isotropic Soil Properties:** This results in less lateral spreading of moisture and contamination, resulting in higher contaminant concentrations in the vadose zone and

aquifer. However, anisotropic soil properties are examined with sensitivity cases along with finite, instead of infinite, barriers in Section 3.2 and Appendix C.

4) **Waste Zone Size is 120 m Long and 3 m Thick:** Initial contaminant concentration in the waste zone is uniform and set to 1.0, and outside of the waste zone is set to 0.0. The moisture content of waste zone is enhanced by 4 vol% (see more discussion in 4th assumption in following Section 2.2.2). Larger waste zones have more contaminant mass, which causes larger contaminant concentrations in the aquifer, but are not expected to affect barrier effectiveness very much. Barrier effectiveness is expected to be insensitive to waste-zone size because the no-barrier and barrier cases have the same waste size.

5) **No Contaminant Retardation or Adsorption:** Fully-mobile contaminants with no retardation by adsorption to the soils are assumed in the base case. Also, no solubility limits are used in the model, which, along with no adsorption, maximizes contaminant transport rates in the vadose zone and to the groundwater, causing shorter travel times and higher concentrations in the groundwater. In effect, instantaneous solubilization is assumed. However, small adsorption effects are examined with sensitivity cases in Section 3.5.

2.2.2 Barrier and Recharge Assumptions

1) **Horizontal Dimension of Barrier is Infinite:** This simplifying assumption eliminates the potential for infiltrating water to run around the edges of the simulated barrier. However, finite barrier effects are examined with sensitivity cases along with anisotropic soils.

2) **Recharge through the Barrier is 0.5 mm/yr:** This barrier recharge value or percolation rate is an average value over many years and was kept constant in the model. The 0.5-mm/yr recharge was the design goal for the Hanford Barrier (*Recharge Data Package for the 2005 Integrated Disposal Facility Performance Assessment*, PNNL-14744). No barrier degradation over time is included in the model for simplification purposes, and no short-term temporal changes of the percolation rate were considered. The recharge is the Darcy velocity, which is a bulk water velocity divided by the cross-sectional flow area. The word 'recharge' is used in a general sense in this report to mean downward water velocity in the vadose zone and percolation rate through the barrier.

3) **Historical Recharges are 5 mm/yr and 25 mm/yr:** The 25 mm/yr recharge value corresponds to minimal vegetation and relatively coarse top soil, and the 5 mm/yr value corresponds to some grass vegetation with a finer top soil; for discussion of recharge variation at the Hanford, see PNNL-14744. The historical recharge of 5 mm/yr (25 mm/yr) results in a calculated vadose zone moisture content of 6.9 vol% (8.7 vol%) based on selected soil properties and the model. Temporal varying historical recharges were not considered.

4) **Initial Waste Moisture Content is 4.0 vol% Above the Background:** The extra moisture is associated with the liquid waste that was discharged into the assumed waste disposal site prior to barrier installation. For the low historical recharge cases, the waste zone was assumed to have an initial moisture content of 10.9 vol%, which is 4.0 vol% above the calculated background moisture content of 6.9 vol% associated with 5-mm/yr

recharge. The 10.9 vol% moisture content is 58% higher (4 %/6.9% = 0.58) than the base background moisture of 6.9 vol%. The extra 4% moisture content increases the initial downward water velocity from 5 mm/yr to about 40 mm/yr (for the model's grid size).

For the high historical recharge cases, the waste zone was also assumed to have an incremental 4 vol% moisture content above the calculated background moisture content of 8.7 vol% associated with the 25-mm/yr recharge for a total moisture content of 12.7 vol%, which is 46% higher (4 %/8.7 % = 0.46) than the background moisture. The initial extra 4 vol% moisture content increases the initial downward water velocity from 25 mm/yr to about 128 mm/yr (for the model's grid size) for the high historical recharge. The additional moisture content in the waste zone decreases over time and distance as the water flows downward, moving excess water to other locations, both laterally and vertically, thereby decreasing the downward waste-source water velocity.

The choice of 4 vol% was based on neutron probe measurements from a well at the BC Crib and Trenches Area.(RPP-20303, *Preliminary Data from 216-B-26 Borehole in BC Cribs Area*), which showed only one measurement above 12.7 vol% for depths greater than 25 m with an average moisture content of 6.5%. In effect, some of the liquid discharges into the cribs and trenches is vicariously included in the high background moisture contents of 6.9 vol% (5 mm/yr recharge) and 8.7 vol% (25 mm/yr recharge). Note that the high historical recharge cases have more contaminant mass in the waste zone than the lower historical recharge. This is because their concentrations are the same at 1.0, but the waste-zone moisture content of 12.7 vol% for the 25-mm/yr cases is higher than the moisture content of 10.9 vol% for the 5-mm/yr cases, resulting in more contaminant mass.

2.2.3 Aquifer and Monitoring Well Assumptions

1) **All Contamination in the Aquifer Passes through the Monitoring Well (6-m Screen):** The 6-m (20-ft) thick aquifer in the model allows no waste to pass underneath or above the well screen. In other words, all waste goes through the 100-m down-gradient well. This is not only conservative, but bounding.

2) **Groundwater Flow Rate (Darcy Velocity) is 0.024 m/day:** A Darcy velocity of 0.024 m/day is assumed, which is a typical velocity for the upper aquifer associated with the Hanford Site Central Plateau region (DOE/RL-2004-72, *Fiscal Year 2004 Annual Summary Report for 200-UP-1 and 200-ZP-1 Pump-and-Treat Operations*). The Darcy velocity is the average bulk volumetric water flow rate divided by the cross-sectional flow area, and is useful for estimating the contaminant concentrations in the aquifer. Note that the porewater velocity is the water velocity through the small soil pores and is useful for estimating contaminant transport times in the groundwater. The porewater velocity is calculated by dividing the Darcy velocity by the moisture content (i.e., porewater velocity = Darcy velocity/moisture content), excluding any residual moisture effects.

2.3 COMPUTER CODE

Flow and transport calculations were made using the STOMP-W (Subsurface Transport Over Multiple Phases) code, Version 3.2, which essentially has the same user's guide as Version

3.1, (*STOMP Subsurface Transport over Multiple Phases, Version 3.1 User's Guide*, PNNL-14478) for the water (W) mode. Only the water-phase mode of the code was used (STOMP-W), which is the standard mode for flow and transport calculations not involving thermal or active gas effects. STOMP-W was quality assured at Fluor Government Group by Fluor Hanford's software procedure HNF-PRO-309, *Controlled Software Management*, as described in HNF-31977, *STOMP-W Version 3.2 Requirements and Management Plan.*

Even though the required capabilities of flow and transport in unsaturated porous media exist in many codes for more than 15 years, the flow and transport simulations here are numerically difficult, requiring small time steps, but conceptually easy. The cases are more difficult than normal because of the higher water content in the initial waste location and the effect of the barrier lowering the recharge through the vadose zone over time. The extra moisture content of 4 vol% causes much faster downward flow initially than normal, and the declining recharge value due to the barrier causes the water to slow down over many years. Both of these effects add numerical difficulty to the calculations, requiring small time steps, even though the conceptual model is simple, making the cases worthy for the benchmarking of flow and transport computer codes.

2.4 NUMERICAL MODEL

A two-dimensional (2D) numerical grid was developed in the input to the STOMP-W code. Grid cell horizontal spacing was 3 m with a total of 140 cells in the horizontal direction for total horizontal domain distance of 420 m (see Figure 1). Grid cell vertical sizes of 0.5 m and 1 m were used for the vadose zone and aquifer, respectively, for a total of 214 computational cells in the vertical direction for a total vertical domain distance of 110 m. There are a total of 29,960 computational cells in the 2D numerical STOMP-W model. Key input files are shown in Appendix B. Sensitivity runs were made with a finer grid to show the sensitivity to grid size in the vertical and horizontal directions, which are discussed in Appendix B.

2.5 TEMPLATE OF EFFECTS AND PARAMETERS

Several key parameters change from one section to another (Sections 3.1 to 3.6) and in the appendices in order to provide a sensitivity analysis of these key parameters. To clarify the key parameters used for each effect, a template of the effects with key parameter values and the applicable locations in the report are shown Table 1.

Table 1. Index of Effects, Parameter Values and Location in Report

Effect	Parameter Values	Location in Report
Waste Zone Depth	30, 40, 50, 60, 70, 80, 90, 100 m	Sections 3.1 to 3.6
Historical Recharge	5 mm/yr 25 mm/yr	Sections 3.1, 3.2, 3.3, 3.4, 3.6 Sections 3.1, 3.2, 3.3, 3.4, 3.5, 3.6
Barrier Overlap Of Finite Barriers	Overlaps of waste zones: 0, 15, 30, 60 m	Sections 3.2, 3.3, Appendix C
Infinite Barrier	Infinite horizontal overlap	Sections 3.1, 3.4, 3.5, 3.6
Anisotropy	Horizontal Conductivity = 10 x Vertical Conductivity Isotropic Soil (No Anisotropy)	Sections 3.2, 3.3, Appendix C Sections 3.1, 3.4, 3.5, 3.6
Vadose Zone Thickness	74 m 104 m	Section 3.4 Sections 3.1, 3.2, 3.3, 3.5, 3.6
Adsorption	K_d of 0.1 and 1.0 mL/g No adsorption (K_d of 0.0 mL/g)	Section 3.5 Sections 3.1, 3.2, 3.3, 3.4, 3.6
Time Dependency Of Concentrations	Depths of 50, 60 m Recharges of 5 & 25 mm/yr Isotropic and Anisotropic Soil	Section 3.3
Soil Properties	One Vadose Zone Soil One Aquifer Soil	Appendix A Appendix A
Grid Resolution	Base cell size of 3 x 0.5 m Vertical. refinement of 3 x 0.1 m Horiz. refinement of 1.5 x 0.5 m	Section 2.5 Appendix B Appendix B
Time Step Size	Variable time step size of 0.0001 yr to 5 years	Appendix B
Model Application	216-B-26 Trench	Section 3.6

3.0 RESULTS

Barrier effectiveness is determined by reducing the low and high historical recharges to 0.5 mm/yr, in order to simulate barrier emplacement, and evaluating groundwater impact. The historical recharge establishes the initial background moisture content (6.9 vol% for the 5-mm/yr recharge, and 8.7 vol% for the 25-mm/yr recharge) in the vadose zone, and, thus, the initial water velocity. The pre-barrier, or antecedent, moisture content is determined from the soil properties (see Appendix A) and the recharge. When recharge is reduced to 0.5 mm/yr, caused by the barrier percolation rate of 0.5 mm/yr, the moisture content is reduced to 5.1 vol% in the vadose zone at elevations more than 2 m above the aquifer. The moisture content is larger in the very

deep vadose zone, just above the aquifer (< 2 m) due to the capillary suction of the vadose zone and the saturated water condition (no suction) in the aquifer.

3.1 BARRIER EFFECTIVENESS (INFINITE BARRIER/ISOTROPIC SOIL)

Barrier effectiveness is evaluated by calculating the peak contaminant concentration at a down-gradient monitoring well, relative to the pre-barrier waste zone contaminant concentration value of 1.0 in the vadose zone, and its arrival time, and comparing these values to the no-barrier condition.

Peak groundwater contaminant concentration at the monitoring well is shown as a function of pre-barrier waste depth in Figure 2 and tabulated in Table 2. Figure 2 shows that the peak contaminant concentrations in the groundwater (averaged over 6 m) are very close for both high and low historical recharge rates and independent of waste depth until the waste zone depth increases beyond 50 m, or more than half-way through the vadose zone. For waste zones deeper than 50 m, the peak contaminant concentration begins to steadily increase for the 25-mm/yr historical recharge. For the 5-mm/yr historical recharge, the peak concentration does not increase until the pre-barrier waste depth gets close to 70 m, which is deeper than what the 25-mm/yr historical recharge conditions show. This results from less antecedent moisture content above the waste for the 5-mm/yr historical recharge, resulting in lower downward contaminant velocity and, thus, lower contaminant transport rate into the aquifer, resulting in a lower concentration in the groundwater than the 25-mm/yr conditions. In summary, the higher historical recharge produces greater antecedent moisture content in the soil and faster initial water velocities, resulting in higher concentrations in the groundwater.

The arrival times of groundwater peak contaminant concentrations are shown in Figure 3 and tabulated in Table 2 for each pre-barrier waste depth. The delay imparted by the barrier is less for the 25-mm/yr historical recharge, than for the 5-mm/yr historical recharge. This is because there is more antecedent moisture content (8.7 vol%) for the 25-mm/yr recharge than there is for the 5-mm/yr recharge (6.9 vol%), resulting in higher downward velocities for the 25-mm/yr recharge. The antecedent moisture also causes smaller arrival times for pre-barrier waste zones deeper than 55 m and 70 m for the 25-mm/yr and 5-mm/yr historical recharges, respectively. For waste zones located above these depths, the antecedent moisture dissipates before enough contaminant mass has been flushed to the groundwater to cause the peak concentration. Thus, with the antecedent moisture gone, only the small barrier recharge of 0.5 mm/yr is available to flush the contaminants, causing arrival times to increase rapidly for shallower waste zones.

Figure 2. Effects of Waste Depth and Historical Recharge on Peak Groundwater Contaminant Concentration

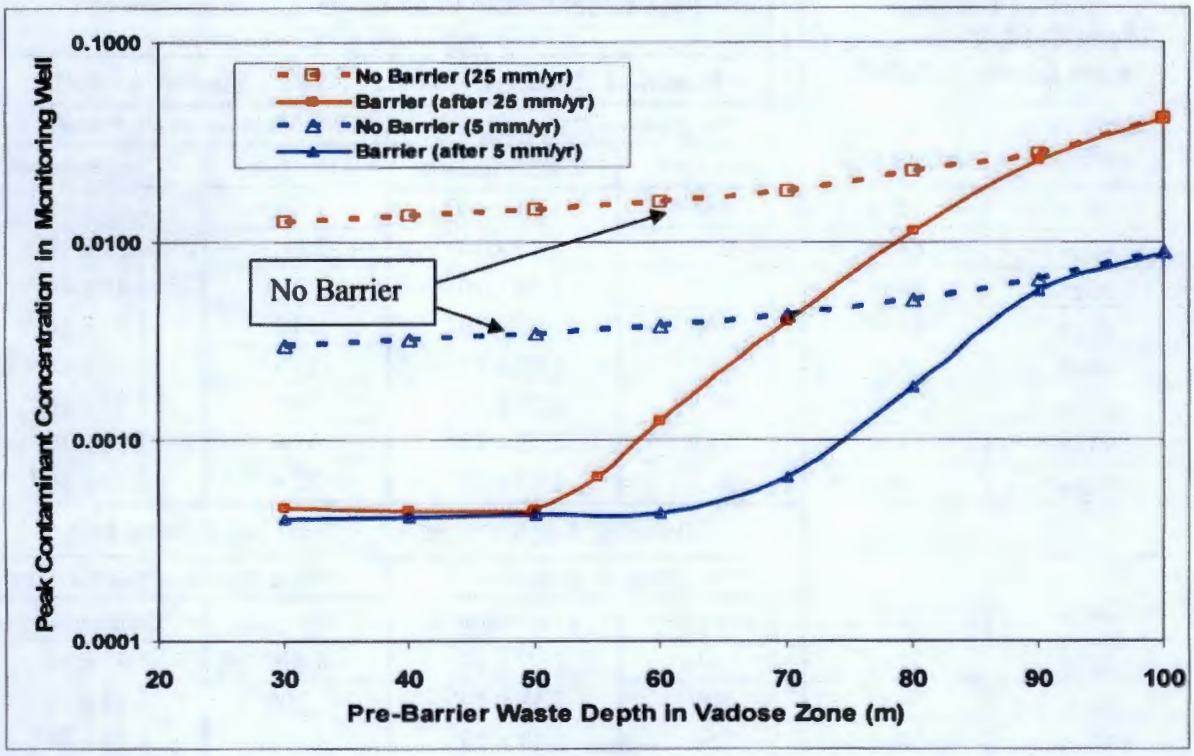


Figure 3. Effects of Waste Depth and Historical Recharge on Arrival Time of the Peak Groundwater Contaminant Concentration

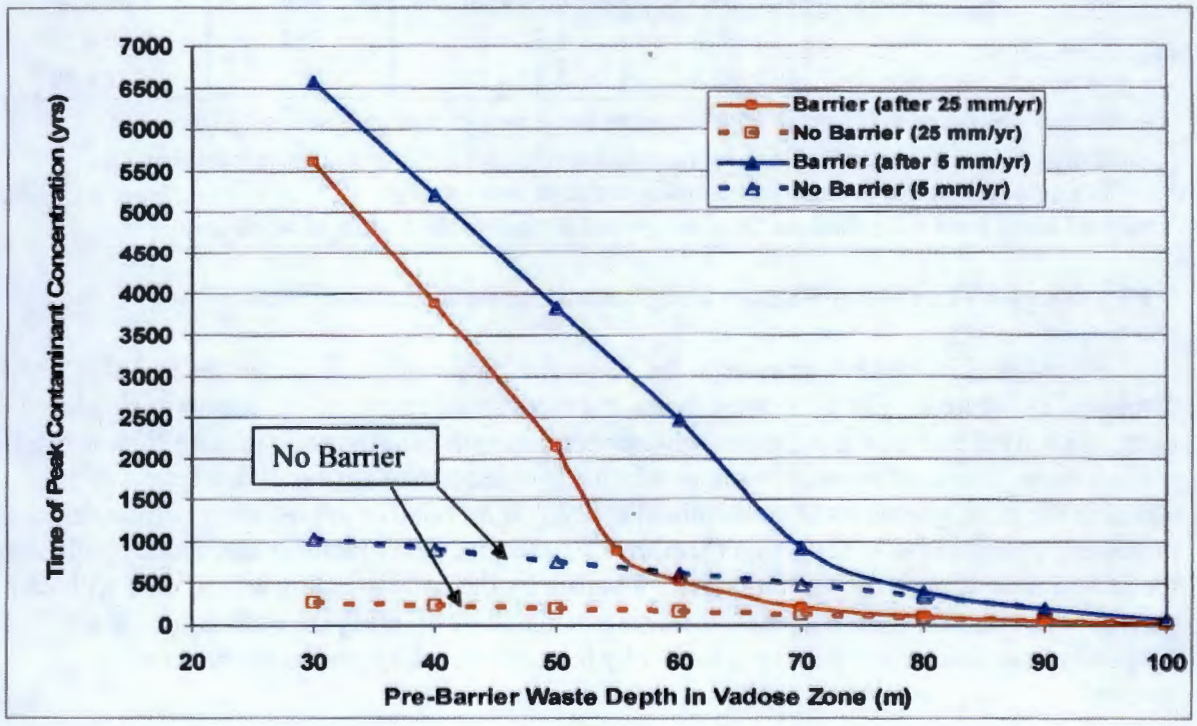


Table 2. Peak Groundwater Contaminant Concentrations and Arrival Times as a Function of Waste Depth and Historical Recharge in Vadose Zone

Waste Location in 104-m Thick Vadose Zone when Barrier Installed		Peak Groundwater Contaminant Concentration and Time of Peak Concentration Arrival			
		Historical 25-mm/yr Recharge (Wetter Pre-Barrier Soil)			
[4]Depth from surface	Elevation above GW	No Barrier (25 mm/yr)		With a Barrier ([1]0.5 mm/yr)	
		Time (yrs)	[2]Concentration	Time (yrs)	[2]Concentration
30 m	74 m	264	1.26×10^{-2}	5,600	4.52×10^{-4}
40 m	64 m	230	1.35×10^{-2}	3,880	4.39×10^{-4}
50 m	54 m	195	1.56×10^{-2}	2,150	4.45×10^{-4}
60 m	44 m	160	1.60×10^{-2}	510	1.25×10^{-3}
70 m	34 m	125	1.79×10^{-2}	210	3.94×10^{-3}
80 m	24 m	89.4	2.26×10^{-2}	101	1.13×10^{-2}
90 m	14 m	54.9	2.78×10^{-2}	53.4	2.56×10^{-2}
100 m	4 m	20.0	4.19×10^{-2}	20.0	4.19×10^{-2}
		Historical 5-mm/yr Recharge (Drier Pre-Barrier Soil)			
[4]Depth	Elevation	No Barrier (5 mm/yr)		With a Barrier ([3]0.5 mm/yr)	
		Time (yrs)	[2]Concentration	Time (yrs)	[2]Concentration
30 m	74 m	1,040	2.97×10^{-3}	6,570	3.99×10^{-4}
40 m	64 m	900	3.18×10^{-3}	5,200	4.10×10^{-4}
50 m	54 m	760	3.43×10^{-3}	3,830	4.21×10^{-4}
60 m	44 m	620	3.76×10^{-3}	2,460	4.33×10^{-4}
70 m	34 m	485	4.21×10^{-3}	930	6.52×10^{-4}
80 m	24 m	345	5.11×10^{-3}	410	1.84×10^{-3}
90 m	14 m	207	6.38×10^{-3}	201	5.65×10^{-3}
100 m	4 m	68.8	8.85×10^{-3}	68.8	8.72×10^{-3}

[1]Barrier limits recharge to 0.5 mm/yr; historical recharge was 25 mm/yr.
[2]Concentration is unit-less and relative to the initial normalized pre-barrier concentration of 1.0.
[3]Barrier limits recharge to 0.5 mm/yr; historical recharge was 5 mm/yr.
[4]Depth of waste zone is the distance from the ground surface to the bottom of waste zone.

3.1.1 Barrier Time Delay Factors and Concentration Reduction Factors

Barrier effectiveness, relative to the no-barrier performance, is quantified in Table 3 and displayed in Figure 4. The time delay factor is a measure of barrier effectiveness in slowing down the arrival time of the peak groundwater contaminant concentration relative to no-barrier performance. The concentration reduction factor is a measure of barrier effectiveness in reducing the peak groundwater contaminant concentration relative to no-barrier performance. As previously stated in the Introduction (Section 1.0), the time delay factor is calculated by dividing the arrival time of peak concentration with a barrier by the corresponding arrival time without a barrier. The concentration reduction factor is calculated by dividing the peak groundwater contaminant concentration without a barrier by the corresponding peak concentration with a barrier.

The concentration reduction factors in Table 3 (e.g., the factor 7.44) are relative to the peak concentrations from the no-barrier cases, and not relative to the larger initial concentrations in the vadose zone as noted above. For example, the peak groundwater contaminant concentration of 3.99×10^{-4} (relative to 1.0 in the pre-barrier waste zone), resulting from a pre-barrier waste depth of 30 m and the historical 5-mm/yr recharge (Table 2), means that the concentration of the contaminant is reduced by a factor of 2506 ($1/3.99 \times 10^{-4} = 2506$) in the groundwater relative to the initial vadose-zone concentration. For the no-barrier case, the peak concentration in aquifer is 2.97×10^{-3} (relative to 1.0 in the pre-barrier waste zone) which is equivalent to an overall reduction factor of 336.7 ($1/2.97 \times 10^{-3} = 336.7$) in the groundwater. Thus, with a barrier, the contaminant concentration in the aquifer is reduced an additional 7.44 times (2506/336.7 = 7.44) relative to the no-barrier case (Table 3). The aquifer's role in reducing concentrations is presented in Appendix A, Section A.2.4.

Table 3. Barrier Effectiveness as a Function of Waste Depth

Waste Location		[1]Time Delay Factor		[2]Concentration Reduction Factor	
[4]Depth	Elevation (above GW)	[3]25 mm/yr	[3]5 mm/yr	[3]25 mm/yr	[3]5 mm/yr
30 m	74 m	21.21	6.33	27.82	7.44
40 m	64 m	16.96	5.79	30.64	7.75
50 m	54 m	11.06	5.04	32.74	8.15
60 m	44 m	3.30	3.95	12.81	8.68
70 m	34 m	1.73	1.92	4.55	6.46
80 m	24 m	1.15	1.18	2.00	2.77
90 m	14 m	0.97	0.97	1.09	1.13
100 m	4 m	1.00	1.00	1.00	1.01

[1] Time Delay Factors are calculated by dividing the Time of Peak Groundwater Contaminant Concentration With a Barrier (recharge of 0.5 mm/yr) by the Time of Peak Groundwater Contaminant Concentration Without a Barrier (natural recharge).

[2] Concentration Reduction Factors are calculated by dividing the Peak Groundwater Contaminant Concentration Without a Barrier (natural recharge of 0.5 mm/yr) by the Peak Groundwater Contaminant Concentration With a Barrier (recharge of 0.5 mm/yr).

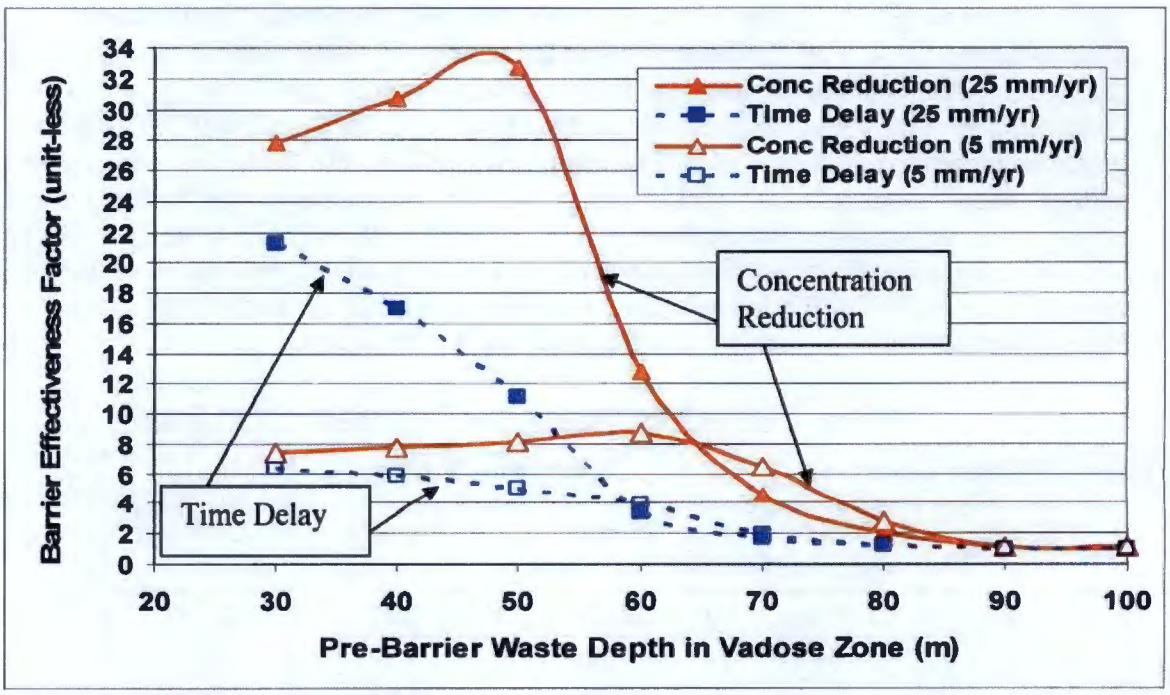
[3] Historical recharge values preceding installation of a surface barrier; i.e., pre-barrier recharge values.

[4] Depth of waste zone is the distance from the ground surface to the bottom of waste zone.

Note: Each factor value includes the performance effect of a barrier relative to the performance without a barrier.

Barrier effectiveness is greater for the 25-mm/yr historical recharge because the degree of recharge reduction from 25 to 0.5 mm/yr (factor of 50) is greater than the recharge reduction for the lower historical recharge from 5 to 0.5 mm/yr (factor of 10). In other words, the higher historical recharge resulted in higher antecedent moisture content and peak groundwater contaminant concentration, so there is opportunity for more reduction. Figure 4 also shows a pronounced decline of barrier effectiveness for wastes deeper than half-way through the vadose zone, analogous to Figure 2, which shows an increase of peak concentration. More discussion of Figure 4 follows in Section 3.1.2. Also, the barrier surprisingly causes a peak concentration earlier than the no-barrier case for the waste depth of 90 m (shown in Tables 2 and 3). This is caused by the declining recharge before the no-barrier peak concentration arrives, causing a slightly lower peak concentration earlier relative to the no-barrier case (see Section 3.5.2).

Figure 4. Barrier Time Delay Factors and Concentration Reduction Factors



To gain understanding of the variability of barrier effectiveness in Figure 4, the time-dependency of the recharge was evaluated. The recharge values at a marker depth of 103 m are shown as a function of time after barrier installation for two waste-source depths (30 m and 100 m) in Figures 5 and 6 for a historical recharges of 25 mm/yr and 5 mm/yr, respectively. The 103-m marker is only 1 m above the aquifer, where the porewater velocity is all vertical or downward. This location is more suitable for recharge reporting than at the water table, where some of the water is flowing horizontally with the aquifer flow, which changes the vertical velocity slightly. For the 100-m deep waste zone, the 4 vol% extra moisture content in the waste zone causes a peak recharge value of 128 mm/yr at the 103-m mark after only 0.55 year for the 25 mm/yr recharge. Note that the recharge peaks much earlier at 0.55 year than the contaminant concentration, which peaks at 20 years at the monitoring well (see Table 2) because of the mixing of the peak concentration with the clean water below the waste zone, causing the early recharge peak to be diluted (see Appendix D for details). For the 30 m-deep waste zone, the peak recharge value is 33.7 mm/yr compared to 128 mm/yr at 103 m after 29 years, indicating that the extra 4 vol% water has spread out (both horizontally and vertically) while traveling downward. The areas under the two curves, which represent the total amount of water passing the 103-m mark, are identical after 100 years as indicated by equal recharges after 100 years.

The 25-mm/yr recharge fully decreases to the barrier recharge (percolation rate) of 0.5 mm/yr after nearly 2,000 years. In other words, it takes a long time for the antecedent moisture content to 'completely' drain from the vadose zone after the barrier is installed. However, after 1,000 years, the recharge is already down to 0.73 mm/yr. At 700 years, the initial recharge of 25 mm/yr has decreased to 1 mm/yr. At 100 years, the recharge has decreased more than half to about 11 mm/yr. The recharge starts to decrease below its historical value of 25 mm/yr at the 103-m mark at 40 years for most waste zone depths except for the 30-m depth.

Figure 5. Recharge Values over Time with Barrier after 25-mm/yr Historical Recharge

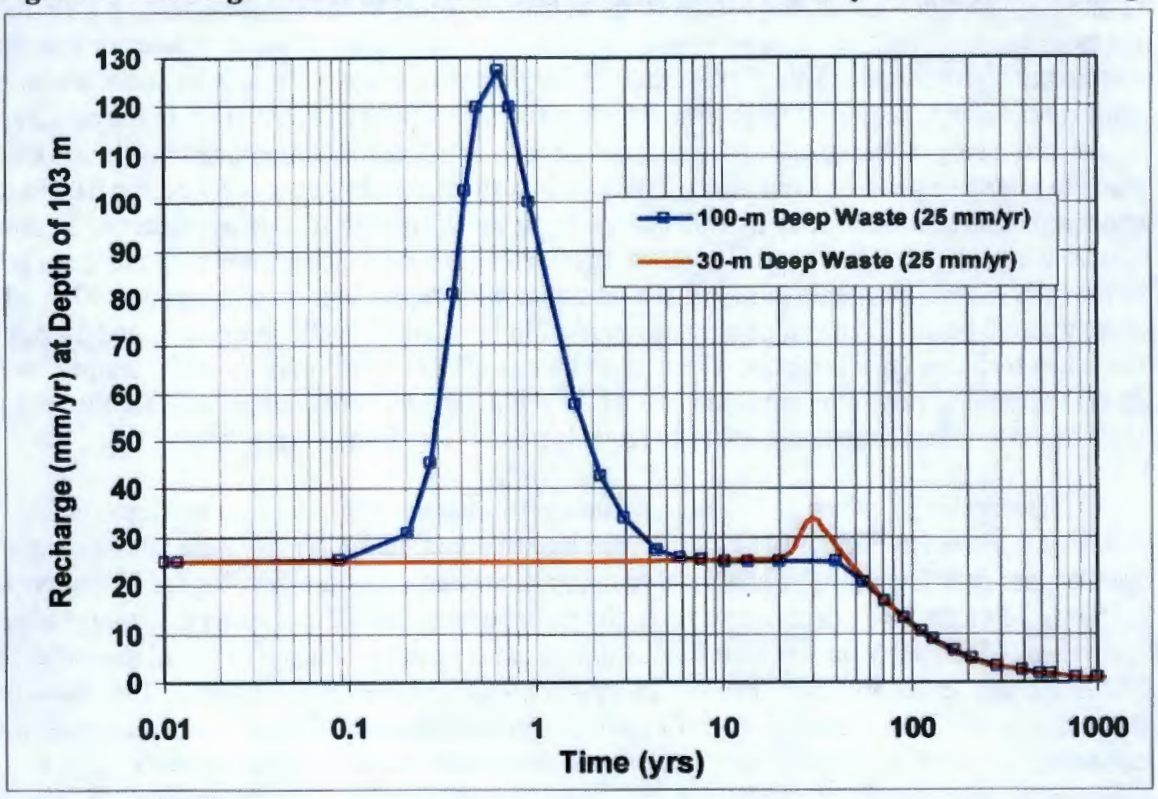
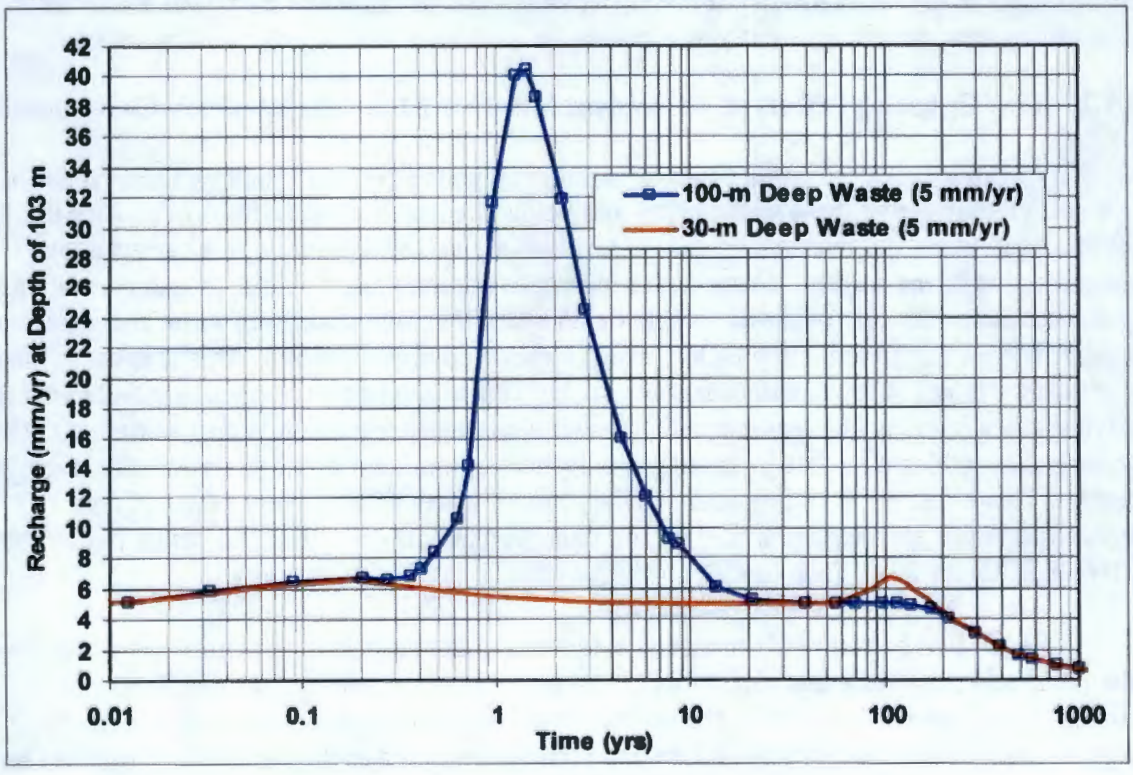


Figure 6. Recharge Values over Time with Barrier after 5-mm/yr Historical Recharge



The 25-mm/yr recharge starts to decrease after 40 to 45 years for all waste zone depths (Figure 5). In other words, the barrier takes as least 40 years to have some effect. Furthermore, the peak concentration in the groundwater arrives later than 45 years for all waste zone depths except the 100-m depth. This implies that the barrier will have some effect for those waste zones with contaminants requiring more than 45 years to reach a peak concentration in the aquifer, due to the decreasing recharge after 45 years, but no effectiveness for contaminants with less than 45 years to a reach a peak concentration. Even for a very deep waste zone at 90 m, the barrier has a concentration reduction factor of 1.09 (Table 3) for the 25-mm/yr historical recharge. In other words, the barrier still has a small concentration reduction effect for wastes zones as deep as 90 m for fully mobile contaminants. All wastes zones with depths less than or equal to 90 m take more than 50 years to reach a peak concentration in the aquifer for the no-barrier and 25-mm/yr historical recharge (see Table 2). There is no barrier effect on 100-m deep waste simply because its arrival time of peak concentration is only 20 years, which is not enough time for the recharge from the antecedent moisture content to have decreased any from 25 mm/yr.

The recharge values at 103 m over time with a barrier after the 5-mm/yr historical recharge is shown in Figure 6. The peak recharge of about 40 mm/yr from the 100-m deep waste zone occurs later for 5-mm/yr historical recharge at around 1.4 years than for the 25-mm/yr at 0.55 year. For the 30-m deep waste zone, the peak recharge at 103 m is only 6.7 mm/yr after 106 years. Thus, the 5-mm/yr historical recharge causes peak recharges (vertical velocities) at 103 m that are lower and later than the 25-mm/yr recharge for all waste zone depths. Note that the recharge at 103 m increases slightly above 5 mm/yr during the first half year, because of the enhanced moisture content pushing more water downward, thereby causing the recharge to increase slightly over the 5-mm/yr historical recharge (Figure 6). This phenomenon was not observed for the higher 25-mm/yr historical recharge because of its background moisture content being higher at 8.7 vol% instead of 6.9 vol%, which causes higher recharge values or faster water velocities, which apparently diminishes the pushing effect of enhanced moisture.

3.1.2 Two Opposing Effects of Antecedent Moisture Above the Waste on Concentrations

As described above, less antecedent moisture above the more shallow waste zones, due to less soil volume above these waste zones and below the near surface, results in a lower driving force on any waste below, causing slower infiltration into the aquifer, which causes a lower peak concentration in the aquifer. However, as shown in Figure 4 and Table 3, the concentration reduction factor actually peaks at a waste depth near 50 m, and shallower waste zones have a smaller concentration reduction factor, which appears counter-intuitive. This is because there is a secondary effect of lower antecedent moisture. This secondary and opposite effect to the lower driving-force effect is that less antecedent water also causes less dilution and mixing with the waste below, which eventually causes groundwater contaminant concentrations to be slightly higher. This effect is not as important as the primary lower driving-force effect of less antecedent water because the concentration reduction factors are still significantly higher than 1.0 (e.g., 27.8 for 30-m deep waste).

Recall that barrier performance is compared to the no-barrier performance, which always maintains a larger antecedent moisture content because of the constant 25-mm/yr recharge. Thus, for shallower waste depths, the no-barrier performance benefits more from a relatively large amount of clean water for dilution and mixing compared to the barrier performance, but not

nearly enough to counteract the larger driving force for transport from more recharge (infiltrating water) at the surface with no barrier.

In summary, less antecedent moisture above a waste zone has two effects on the eventual peak groundwater contaminant concentration:

1) lower driving force for transport of waste contaminants in vadose zone, causing lower groundwater concentrations, which is the primary effect, and
2) less dilution/mixing effects on waste contaminants in vadose zone, causing slightly higher groundwater concentrations, which is a secondary effect.

If only the lower downward driving force (velocity) of less antecedent water were considered, then the barrier concentration reduction factor would keep increasing with decreasing waste depth, which does not happen as shown in Figure 4. The time delay factors, however, do keep increasing as the waste depth decreases because the contaminants have to travel more distance for more shallow wastes, no matter how large or small the antecedent moisture is. The secondary effect is smaller for the 5-mm/yr historical recharge than the 25-mm/yr recharge (Figure 4) because there is less antecedent water to cause dilution and mixing.

3.2 EFFECTS OF FINITE BARRIER AND SOIL ANISOTROPY

The infinite barrier assumption (see Section 2.2) simplified the analysis, because no barrier edge effects needed to be defined or implemented in the model. In reality, any barrier will have some finite extension (overlap) over the waste. The overlap is the horizontal distance on each side of the underground waste zone that the barrier edge on top overhangs the waste zone. The waste zone is assumed to be centered under the barrier. In other words, the barrier overlap is the length of the barrier minus the length of the waste zone, divided by 2. The barrier does not degrade near the edge, and no water runoff is included in the model to keep it simple.

Also, anisotropic soil, where the horizontal and vertical saturated hydraulic conductivities are unequal (ratio of 10 to 1 here), is a more realistic condition that would be expected to affect contaminant transport, resulting in increased horizontal spreading of the waste. Anisotropy is expected to be important when the barrier is finite, because additional moisture may infiltrate along the barrier edges and flow underneath the barrier, causing a faster downward flow for more of the waste. The natural recharge beyond the finite barrier edges after barrier installation is assumed to be the same as the historical recharge (25 mm/yr or 5 mm/yr) before the barrier installation. More details are provided in Appendix C.

The effects of barrier overlap and anisotropic soil are itemized in Table 4, which lists the ratios of peak groundwater contaminant concentrations for the finite barrier to the infinite barrier. Figures 7 and 8 summarize the finite-to-infinite barrier concentration ratios for 25-mm/yr and 5-mm/yr historical recharges, respectively. Note that a barrier that overlaps the waste by only 15 m causes lower peak contaminant concentrations for the more shallow waste depths, which appears counter intuitive. This results from the barrier edge effects, where higher recharge "curls" underneath the barrier to intersect the waste and hasten its transport toward groundwater. This curling of water not only causes a higher mixing rate and downward velocity, but also

higher dispersion and diffusion rates. Thus, that intersected portion of the waste is removed earlier from the vadose zone than under no-curling conditions, resulting in an eventual reduced peak concentration in the aquifer. The same effect increases groundwater contaminant concentrations for waste at a depth of 40-80 m for the 15-m overlap (25 mm/yr, anisotropy), and at the 50 to 60-m waste depth for the 30 to 60-m overlap (25 mm/yr, anisotropy). In other words, for anisotropic soil and a historical recharge of 25 mm/yr, a finite barrier with a barrier overlap of 30 m is less effective (about a factor of 2) than an infinite barrier for only the 50 to 60-m deep wastes, and is essentially the same as the infinite barrier at waste depths smaller than 50 m or deeper than 60 m (Table 4). For these mid-level wastes, the edge-effect recharge intersects the majority of the waste to effectively increase contaminant flux into the groundwater.

Table 4. Ratios of Peak Groundwater Contaminant Concentrations Associated with Finite Barrier Overlap to Those for the Infinite Barrier

Waste [1]Depth in 104-m Vadose Zone	Concentration Ratios for 15 m (50 ft) Overlap Isotropic & (Anisotropic)		Concentration Ratios for 30 m (100 ft) Overlap Isotropic & (Anisotropic)		Concentration Ratios for 60 m (200 ft) Overlap Isotropic & (Anisotropic)	
	[2]25 mm/yr	[3]5 mm/yr	[2]25 mm/yr	[3]5 mm/yr	[2]25 mm/yr	[3]5 mm/yr
30 m	0.71 (0.92)	0.85 (0.75)	0.92 (0.78)	0.98 (0.76)	0.95 (0.81)	0.99 (0.92)
40 m	0.75 (1.56)	0.86 (0.89)	0.95 (1.14)	0.99 (0.86)	0.99 (0.99)	0.99 (0.96)
50 m	0.92 (2.79)	0.90 (1.16)	0.95 (2.09)	0.99 (1.06)	1.00 (1.36)	0.99 (1.04)
60 m	1.01 (2.02)	0.99 (1.64)	0.93 (1.63)	1.00 (1.39)	0.95 (1.11)	0.99 (1.15)
70 m	0.95 (1.29)	1.05 (1.66)	0.94 (1.10)	0.99 (1.39)	0.96 (0.99)	0.99 (1.09)
80 m	0.96 (0.95)	1.00 (1.12)	0.96 (0.92)	0.99 (1.05)	0.98 (0.98)	1.00 (1.01)
90 m	0.99 (1.00)	1.00 (1.00)	0.99 (1.00)	1.00 (1.00)	1.00 (1.00)	1.00 (1.00)
100 m	1.00 (1.00)	1.00 (1.00)	1.00 (1.00)	1.00 (1.00)	1.00 (1.00)	1.00 (1.00)

[1]Depth of waste zone is the distance from the ground surface to the bottom of waste zone.
Note: Concentration ratios in parentheses are for anisotropic vadose zone soil with horizontal saturated hydraulic conductivity increased by a factor of 10. Values not in parentheses are for isotropic soil.

For anisotropic soil, the ratios of finite-to-infinite barrier peak contaminant concentrations for the 25-mm/yr historical recharge are 2.09 and 1.36 for the 30-m and 60-m overlaps, respectively. As shown in Figure 7, the primary affected waste depths are only the mid-range ones, from 40 to 70 m for the high recharge. For isotropic soil, a barrier overlap of 15 m is essentially the same or better than the infinite barrier, indicating that larger barrier overlaps are needed only for anisotropic soils.

In summary, with anisotropic soil hydraulic conductivity, recharge curls beneath the barrier farther into the waste than for isotropic soil, thereby driving more of the waste into the groundwater than if isotropic soil conditions existed. However, enhancement factors of 2.09 and 1.36 for mid-range wastes in anisotropic soil (10:1 conductivity ratio) are not large factors, compared to other parameters and barrier effectiveness. Also, for waste depths of 40 m or less in anisotropic soil (10:1), a finite barrier with an overlap of 15 m (50 ft) has about the same efficiency as an infinite barrier.

Figure 7. Ratio of Groundwater Contaminant Concentrations for 25-mm/yr Recharge

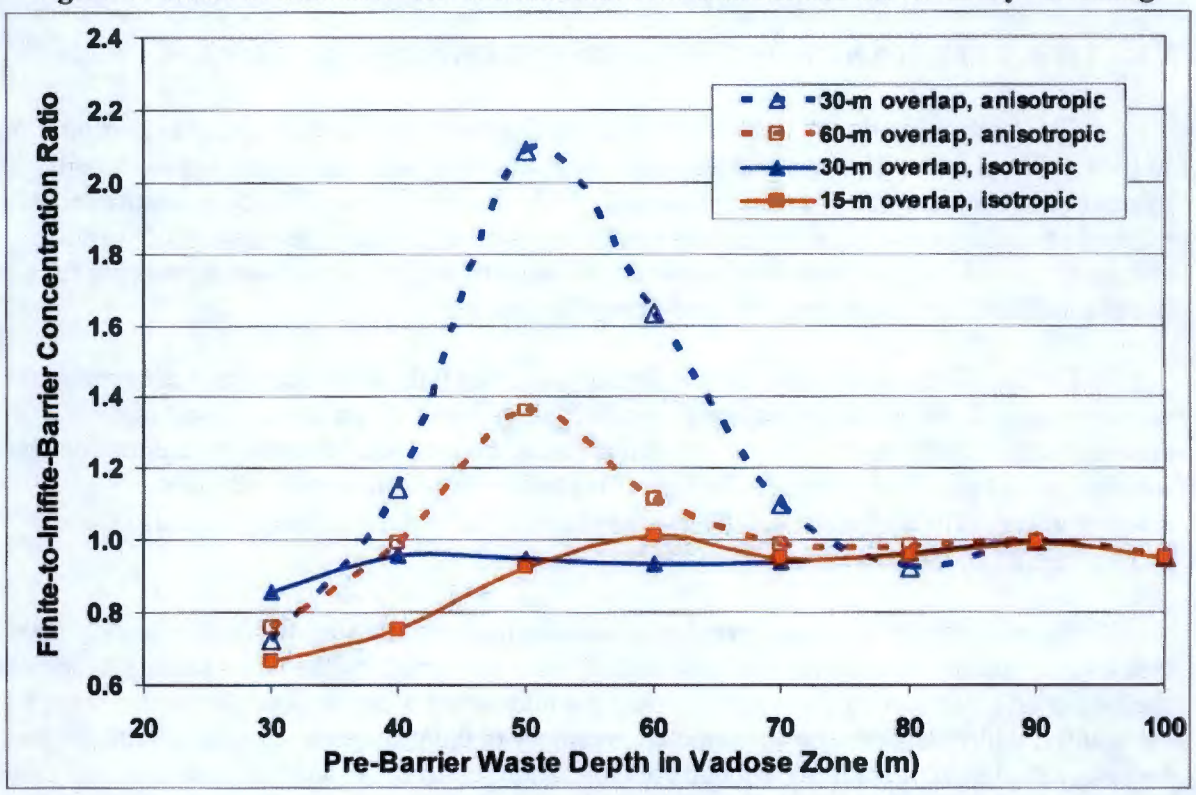
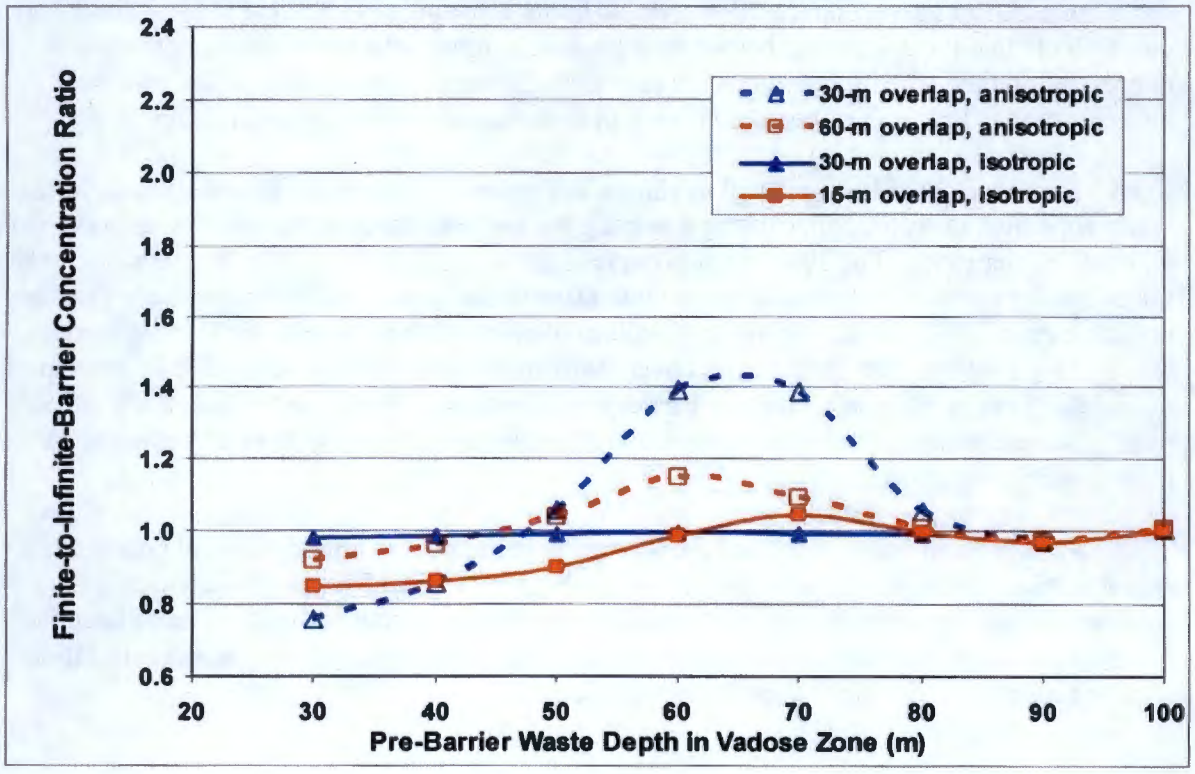


Figure 8. Ratio of Groundwater Contaminant Concentrations for 5-mm/yr Recharge



3.3 TIME DEPENDENCY OF CONTAMINANT CONCENTRATIONS

This section shows the time dependency of the instantaneous contaminant concentration in the aquifer to better illustrate barrier effectiveness for both anisotropic and isotropic soils. The extent of the barrier overlap is also considered. Only the cases for a 60-m deep waste zone with a 5-mm/yr recharge and for a 50-m deep waste zone with a 25-mm/yr recharge (both historical and future) are shown because these waste depths showed high peak concentrations and, thus, are better candidates for illustrating the time-dependent behavior.

For the 60-m waste depth and the 5-mm/yr recharge, the time-dependent contaminant concentrations in the groundwater are shown in Figures 9 and 10 for isotropic soil and anisotropic soil, respectively. Some simulations were stopped after the peak concentration was reached, so not all of the curves in the figures continue onward to zero or very low concentrations. The no-barrier cases have the highest peak concentration, which also occurs sooner than all of the other peaks from the barrier cases.

Figure 9 shows the time-dependent contaminant concentrations for isotropic soils. The 0-m overlap causes some of the contaminants to wash out earlier by the water curling underneath the barrier and intersecting the waste, causing the intersected waste to flow downward faster to the aquifer, which depletes the contaminant inventory in the vadose zone sooner. With the fast inventory depletion, there is not enough contamination left to cause another peak at a later time. Thus, the peak concentration with the 0-m overlap occurs sooner and is smaller than for larger overlaps and the infinite barrier as shown in Figure 9. The 15-m overlap curve is very close to the infinite barrier curve, and the 30-m overlap curve is essentially identical to the infinite barrier curve. Note that the no-overlap barrier case predicts a lower peak groundwater contaminant concentration than when some overlap is provided. However, the duration of the near-peak concentration is longer (i.e., broader curve top) than those cases with some overlap.

However, for anisotropic soil as shown in Figure 10, more water intersects more of the waste zone than isotropic soil, causing a larger peak concentration for the no-overlap curve than all other barrier cases. The 30-m overlap curve is not as close to the infinite barrier curve as the 60-m overlap curve is. All overlap sizes up to 60 m cause higher peak concentrations than the infinite barrier in Figure 10. However, the 60-m overlap curve is close to the infinite barrier curve. This suggests that finite barriers over 'anisotropic' soils may need to have an overlap of 60 m (200 ft) to be close to an infinite barrier's performance. On the other hand, finite barriers over 'isotropic' soils may need to have an overlap of at most 15 m (50 ft) to approximate an infinite barrier's performance.

For the 50-m waste depth and the 25-mm/yr recharge, the time-dependent contaminant concentrations in the groundwater are shown in Figures 11 and 12 for isotropic soil and anisotropic soil, respectively. All of the peak concentrations occur earlier than those from the 5-mm/yr recharge, but otherwise are very similar. The anisotropic soil causes more deviation from the infinite barrier cases than the isotropic soil.

Figure 9. Effect of Barrier Overlap on Groundwater Contaminant Concentrations versus Time (Isotropic Soil, 5-mm/yr Recharge, Waste Depth of 60 m)

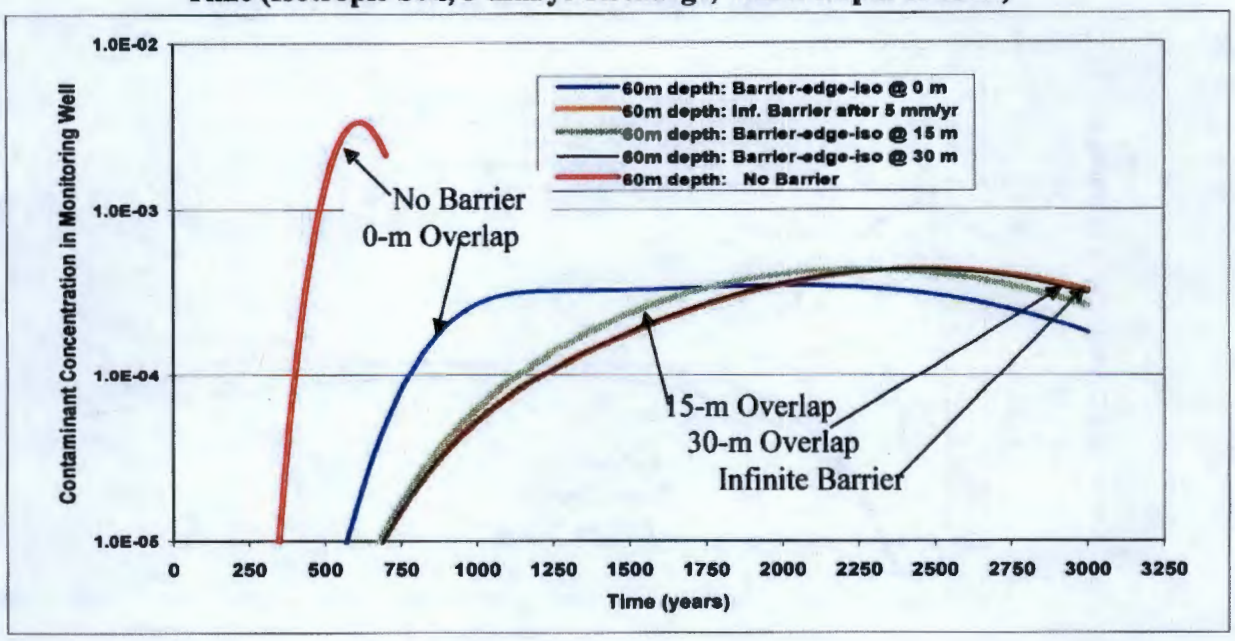


Figure 10. Effect of Barrier Overlap on Groundwater Contaminant Concentrations versus Time (Anisotropic Soil, 5-mm/yr Recharge, Waste Depth of 60 m)

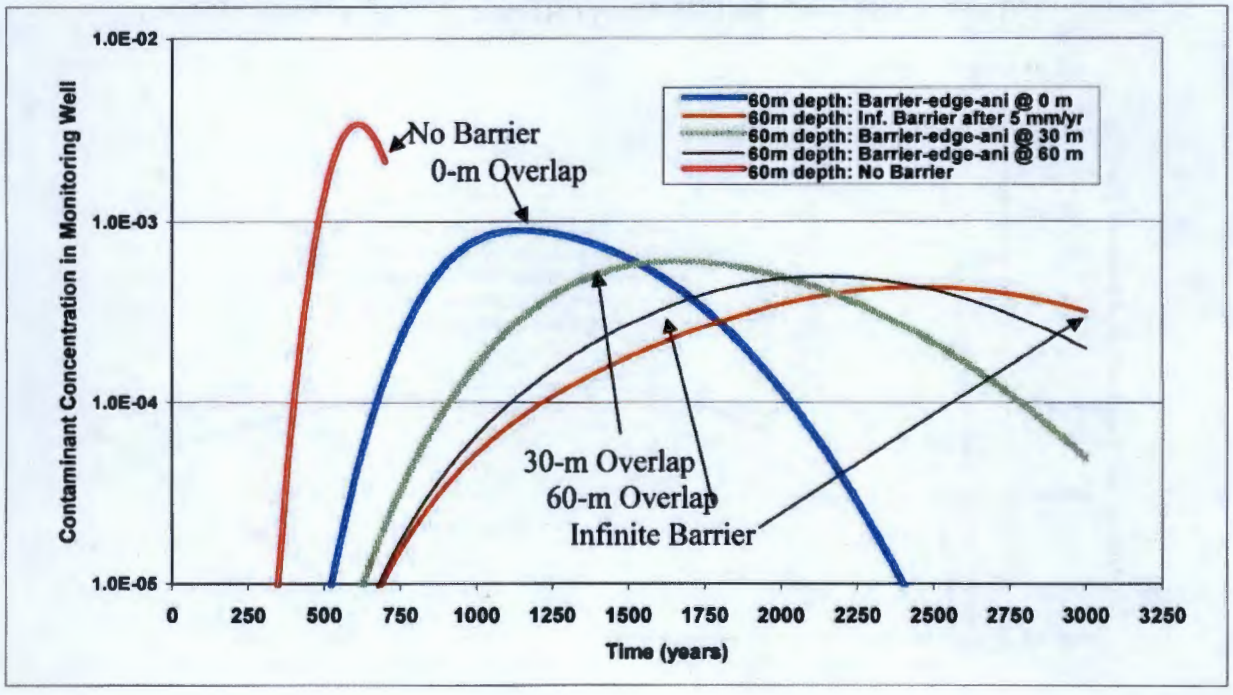


Figure 11. Effect of Barrier Overlap on Groundwater Contaminant Concentrations versus Time (Isotropic Soil, 25-mm/yr Recharge, Waste Depth of 50 m)

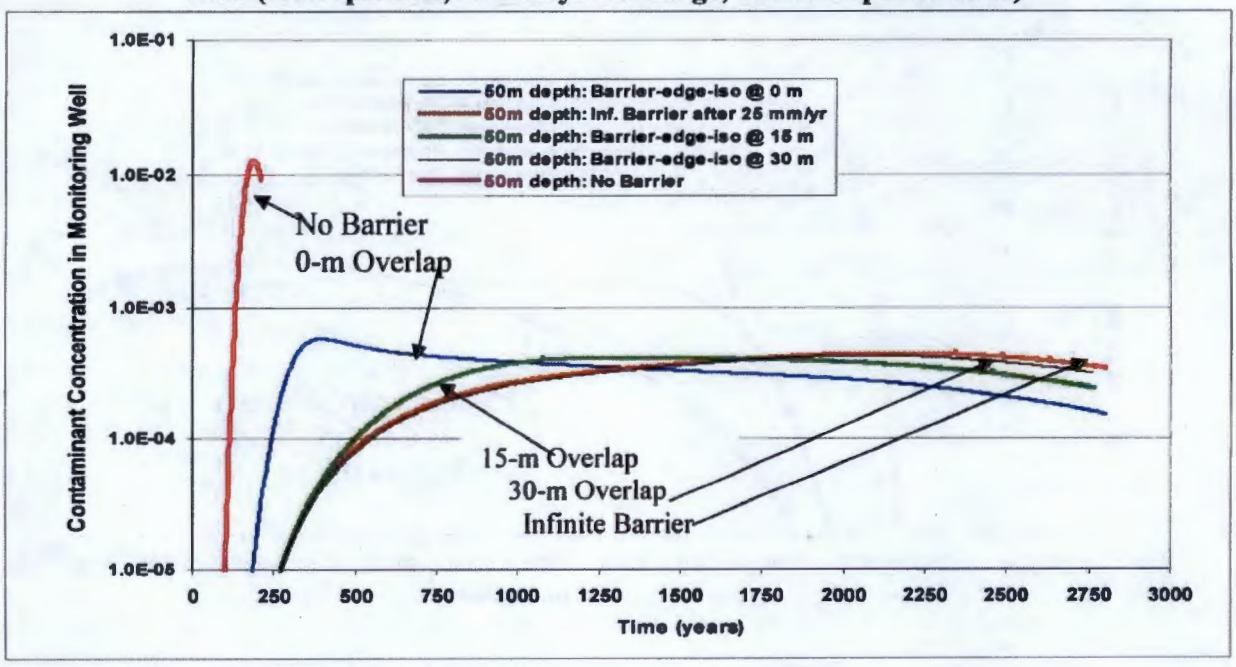
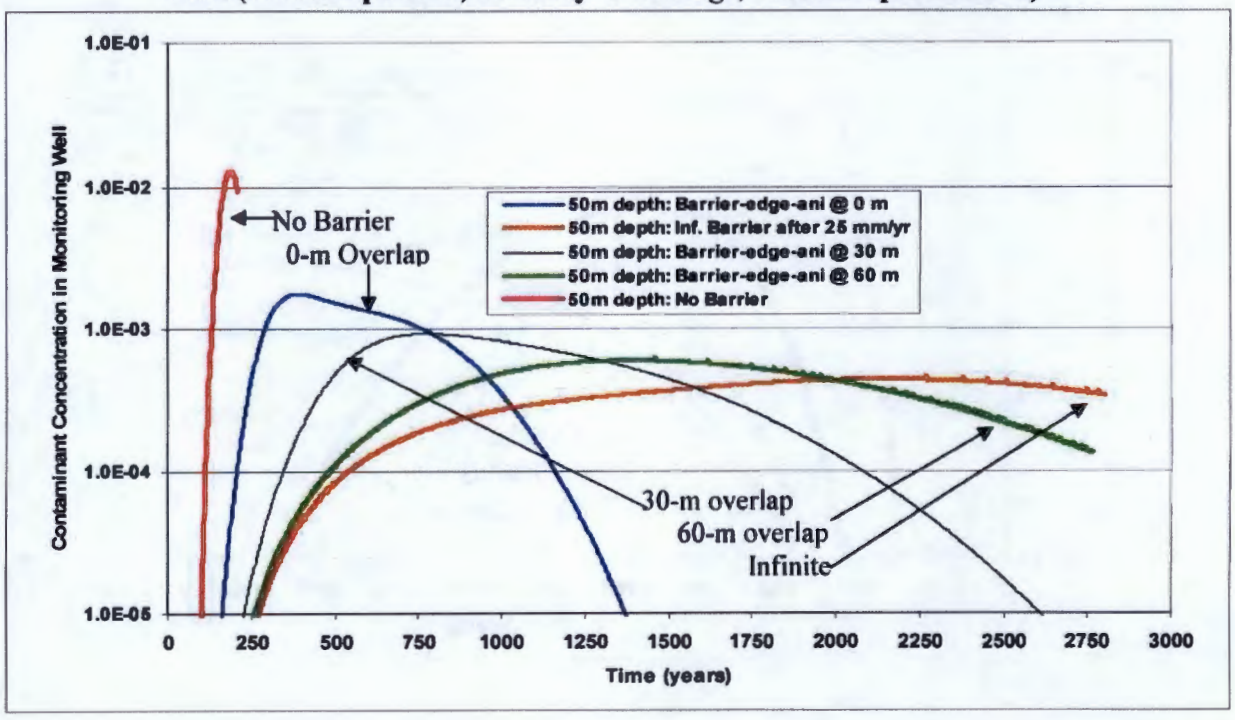


Figure 12. Effect of Barrier Overlap on Groundwater Contaminant Concentrations versus Time (Anisotropic Soil, 25-mm/yr Recharge, Waste Depth of 50 m)



3.4 EFFECT OF VADOSE ZONE THICKNESS

Because much of the Hanford Central Plateau vadose zone is thinner than 104 m, the effect of vadose zone thickness was evaluated. For example, the vadose zone is approximately 75 to 90 m thick in portions of the 200 West Area in the vicinity of the U Plant. The barrier is assumed to be infinite in length and the soil is assumed to be isotropic.

A thinner vadose zone implies that the barrier is closer to the waste for a given waste elevation above the aquifer, causing less antecedent water to be above the waste zone. The effect of a thinner vadose zone was evaluated by performing barrier simulations with a 74-m thick vadose zone with high historical recharge (25 mm/yr). This evaluation is compared to the analogous (high recharge) barrier simulations for the 104-m thick vadose zone in Table 5.

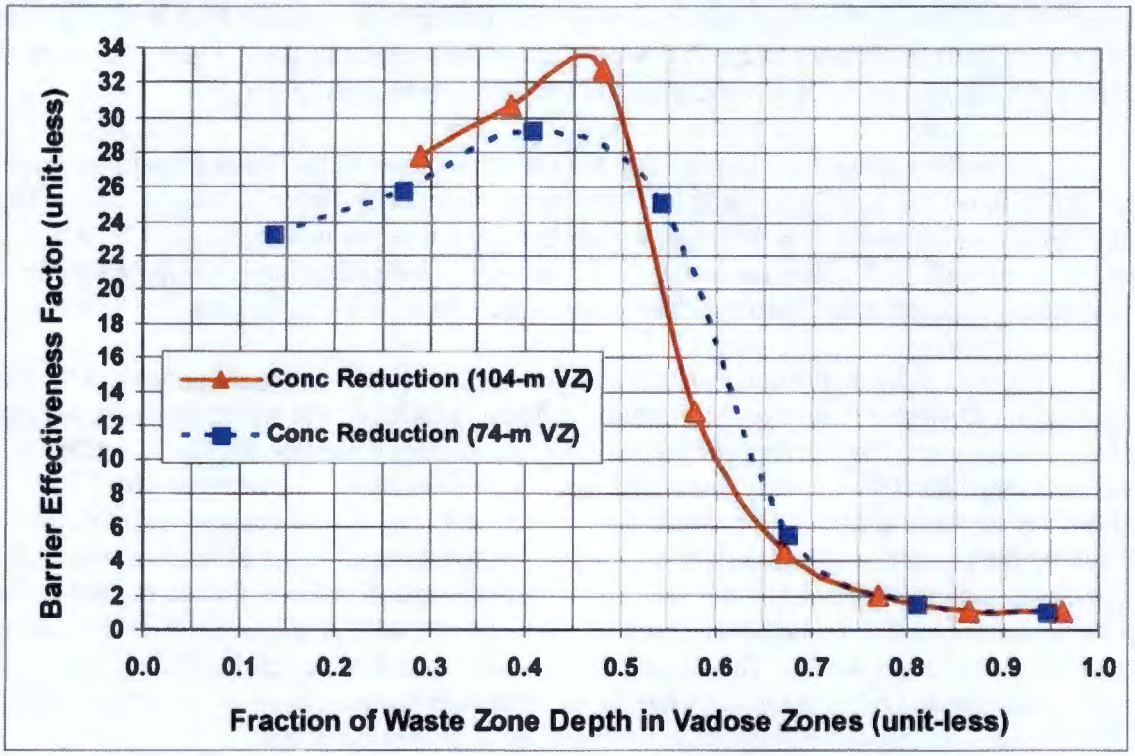
Figure 13 shows the concentration reduction factors in both vadose zones as a function of the fraction of vadose zone that the waste zone depth is located. For waste depths in the top half of the vadose zone, the barrier over the 74-m vadose zone is generally slightly less effective than a barrier over the 104-m vadose, because there is less distance for the waste to travel downward in the thinner vadose zone. As a result, the contaminant mass doesn't spread out as much before reaching the aquifer, causing slightly higher peak concentrations in the groundwater and lower barrier effectiveness. Note that the peak concentration reduction factor for the thinner vadose zone is also located about half-way down the vadose zone, dropping quickly after the half-way mark as shown in Figure 13. This trend is very similar to that observed for the thicker vadose zone. This trend is expected to continue for even thinner vadose zones, with the barrier effectiveness factors decreasing as the vadose zone thickness decreases.

Table 5. Effect of Vadose Zone Thickness on Barrier Effectiveness

Waste [4]Elevation (for both 74-m & 104-m thick vadose zones)	[1]Time Delay Factor ([3]25 mm/yr)		[2]Concentration Reduction Factor ([3]25 mm/yr)	
	104-m Vadose	74-m Vadose	104-m Vadose	74-m Vadose
74 m	21.2	-	27.8	-
64 m	17.0	26.9	30.6	23.3
54 m	11.1	22.9	32.7	25.8
44 m	3.3	17.2	12.8	29.3
34 m	1.7	4.8	4.6	25.1
24 m	1.2	1.7	2.0	5.5
14 m	1.0	1.0	1.1	1.5
4 m	1.0	1.0	1.0	1.0

[1] Time Delay Factors are calculated by dividing the Time of Peak Groundwater Contaminant Concentration With a Barrier (0.5 mm/yr recharge) by the Time of Peak Groundwater Contaminant Concentration Without a Barrier (recharge of 25 mm/yr).
[2] Concentration Reduction Factors are calculated by dividing the Peak Groundwater Contaminant Concentration Without a Barrier (recharge of 25 mm/yr) by the Peak Groundwater Contaminant Concentration With a Barrier (0.5 mm/yr recharge).
[3] Historical recharge value preceding installation of a surface barrier.
[4] Waste elevation is the vertical distance from the water table (top of aquifer) to the bottom of waste zone.

Figure 13. Concentration Reduction Factors for Waste Depths in Different Vadose Zones



The 25-m/yr recharge decreases sooner in the thinner vadose than in the thicker vadose because there is less antecedent water in the thinner vadose zone due to less soil. As a result, the barrier effectiveness is larger for the thinner vadose for waste depths in the bottom half of vadose zone, except for very deep wastes where barriers aren't very effective for both vadose zones.

3.5 EFFECT OF SMALL CONTAMINANT ADSORPTION

The analysis in this section assumes the base parameters of an infinite barrier and isotropic soil, but the contaminants are assumed to have some adsorption to soil, which reduces their transport velocity relative to water. In reality, many contaminants in the vadose zone are partially adsorbed onto the solid particles and are not all in aqueous solution. A parameter, called the distribution coefficient and denoted by K_d, is often used to describe how much of a species is adsorbed on the solid versus how much is in aqueous solution. The definition of the distribution coefficient is as follows:

K_d = [adsorbed contaminant mass per unit mass (g) of solid]
/ [contaminant mass in aqueous solution per unit volume (mL) of solution], (1)

which has units of mL/g. A K_d value of 1.0 mL/g indicates that there is as much contaminant mass in a gram of soil as there is in a mL of pore water (solution). A K_d value of zero indicates that no contaminant mass is adsorbed on the soil, which is a fully mobile contaminant. For example, ^{99}Tc is usually modeled as fully mobile in the soil with a K_d value of zero, which is the lower bound value. In PNNL-14702, *Vadose Zone Hydrogeology Data Package for the 2004*

Composite Analysis, the upper bound value of the K_d of ^{99}Tc (as pertechnetate) in Hanford soil is 0.1 mL/g, except where reducing agents are present, which results in higher values. In contrast to ^{99}Tc, uranium has a higher K_d range of 0.2 mL/g to 4.0 mL/g for most Hanford soil impact zones and source categories (PNNL-14702).

The K_d values of 0.1 mL/g and 1.0 mL/g are assumed in the simulations with and without an infinite barrier for the high historical recharge of 25 mm/yr. Also, for the 1 mL/g K_d value, only deep waste depths of 70 m or more were simulated due to the increasing long arrival times of peak concentration for more shallow waste zones. Arrival times of peak contaminant concentration in the groundwater and the peak concentrations are shown in Table 6. Time delay factors and concentration reduction factors are shown in parentheses, and are also plotted in Figures 14 and 15, respectively. The barrier is very effective down to very deep waste depths of 90 to 100 m in the 104-m thick vadose zone for the K_d value of 1.0 mL/g. Even for the smaller distribution coefficient of 0.1 mL/g, the barrier is more effective down to 90 m, which has a concentration reduction factor of 10, compared to 2 for the fully-mobile contaminants. The barrier is clearly more effective for contaminants with some adsorption than with no adsorption, especially for very deep wastes, as indicated by larger barrier effectiveness factors for all waste zone depths, especially for the very deep (> 70 m) waste zones.

3.5.1 Reason for Higher Barrier Effectiveness for Contaminants with Absorption

To gain understanding of the increased barrier effectiveness for adsorbed contaminants, the partitioning of contaminant mass on soil particles and in solution is evaluated. In a unit volume of unsaturated soil, the ratio of adsorbed contaminant mass to solution contaminant mass can be deceptively large, even with small K_d values. This is because there is so little moisture content in a unit soil volume relative to the larger soil mass. For example, with a K_d value of 1.0 mL/g, for moisture contents of 12.7 and 8.7 vol%, and a soil bulk density of 1.773 g/mL (see Appendix B), the ratio of adsorbed contamination to contamination in solution is 14 and 20.4 for moisture contents of 12.7 to 8.7 vol%, respectively, which are calculated as follows:

Ratio = Adsorbed contaminant mass/Contaminant mass in solution in unit soil volume,

$$= K_d \times (\text{soil mass in 1 mL of soil})/(\text{water volume in 1 mL of soil}), \quad (2)$$

$$= 1.0 \text{ mL/g} \times 1.773 \text{ g}/0.127 \text{ mL} = 14 \text{ for 12.7 vol\% moisture content}, \quad (2a)$$

$$= 1.0 \text{ mL/g} \times 1.773 \text{ g}/0.087 \text{ mL} = 20.4 \text{ for 8.7 vol\% moisture content}. \quad (2b)$$

These results show that the amount of required clean water to flush out the eventual peak concentration value of the contamination having a K_d of 1.0 could be up to 21.4 times more (20.4 from Equation (2a) plus 1.0 for contaminant in solution) than if the contaminant were fully mobile. As a result, the time of peak concentration arrival is much greater for adsorbing contaminants than for mobile contaminants. Note that the arrival time of peak concentration for the no-barrier case (70-m depth, K_d of 1 mL/g) is 2665 years, which is about 21.32 times longer than for the corresponding fully mobile contaminant case (125 years). This indicates that 21.32 times (2665 years/125 years) more clean water is required for the adsorbed contaminant (K_d of 1 mL/g) to be flushed enough out of the vadose zone to cause the peak contaminant concentration in the groundwater than for the fully mobile contaminant for this no-barrier case.

Table 6. Effect of Small Adsorption of Contaminant on Concentration with High Historical Recharge (25 mm/yr), Infinite Barrier and Isotropic Soil

Waste Depth in 104-m Vadose Zone	No Barrier (K_d = 0.1 mL/g)		With a Barrier (0.5 mm/yr) (K_d = 0.1 mL/g)	
	Time of Peak Concentration (years)	Peak Concentration (relative to 1)	Time of Peak Concentration ([1]Delay Factor)	Peak Concentration ([2]Reduct. Factor)
30 m	806	1.10×10^{-2}	31,800 (39.5)	3.21×10^{-4} (34.3)
40 m	700	1.18×10^{-2}	26,550 (37.9)	3.40×10^{-4} (34.8)
50 m	592	1.28×10^{-2}	21,280 (35.9)	3.68×10^{-4} (34.8)
60 m	487	1.41×10^{-2}	16,000 (32.9)	4.00×10^{-4} (35.2)
70 m	379	1.59×10^{-2}	10,760 (28.4)	4.34×10^{-4} (36.6)
80 m	275	1.85×10^{-2}	5,455 (19.8)	5.10×10^{-4} (36.4)
90 m	169	2.33×10^{-2}	316 (1.9)	2.36×10^{-3} (9.9)
100 m	61	3.81×10^{-2}	57 (0.93)	3.52×10^{-2} (1.1)
	No Barrier (K_d = 1.0 mL/g)		With a Barrier (0.5 mm/yr) (K_d = 1.0 mL/g)	
70 m	2,665	1.52×10^{-2}	119,600 (44.8)	3.88×10^{-4} (39.1)
80 m	1.924	1.88×10^{-2}	82,350 (42.8)	4.56×10^{-4} (39.0)
90 m	1,180	2.25×10^{-2}	45,080 (38.2)	5.81×10^{-4} (38.7)
100 m	429	3.68×10^{-2}	7,280 (17.0)	9.75×10^{-4} (37.8)
101 m	353	3.98×10^{-2}	350 (0.99)	2.36×10^{-3} (16.9)

[1] Time Delay Factors are calculated by dividing the Time of Peak Groundwater Contaminant Concentration With a Barrier (0.5-mm/yr recharge) by the Time of Peak Groundwater Contaminant Concentration Without a Barrier (natural recharge of 25 mm/yr).

[2] Concentration Reduction Factors are calculated by dividing the Peak Groundwater Contaminant Concentration Without a Barrier (natural recharge of 25 mm/yr) by the Peak Groundwater Contaminant Concentration With a Barrier (0.5 mm/yr recharge) for each distribution coefficient, K_d, value and waste depth.

For the barrier case, the recharge into the aquifer decreases over time to 0.5 mm/yr, which is 50 times smaller than 25 mm/yr, meaning much more time is needed for the same amount of flushing clean water. For example, the barrier case for 70-m deep waste has a peak concentration arrival time of 119,600 years, which is 44.8 times higher than the corresponding no-barrier case arrival time of 2,665 years. The time delay factor of 44.8 is less than 50 because the antecedent moisture prevents the recharge from immediately reducing to 0.5 mm/yr.

Figure 14. Barrier Concentration Reduction Factors for Small-Adsorption Contaminants

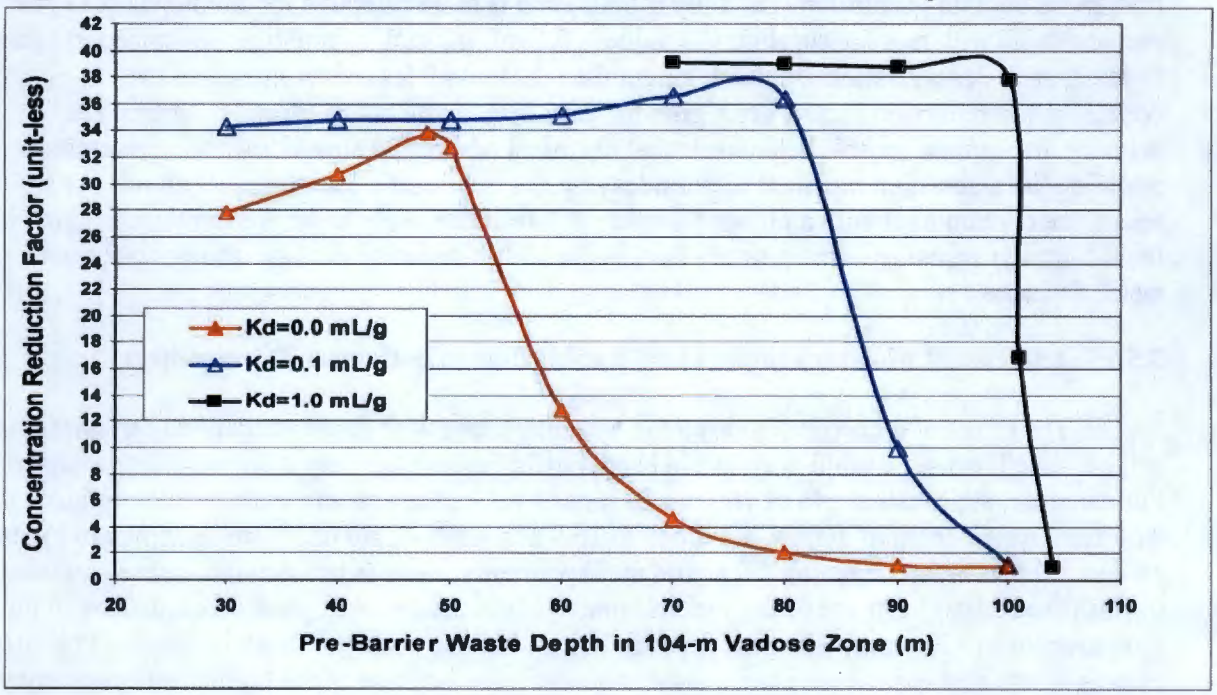
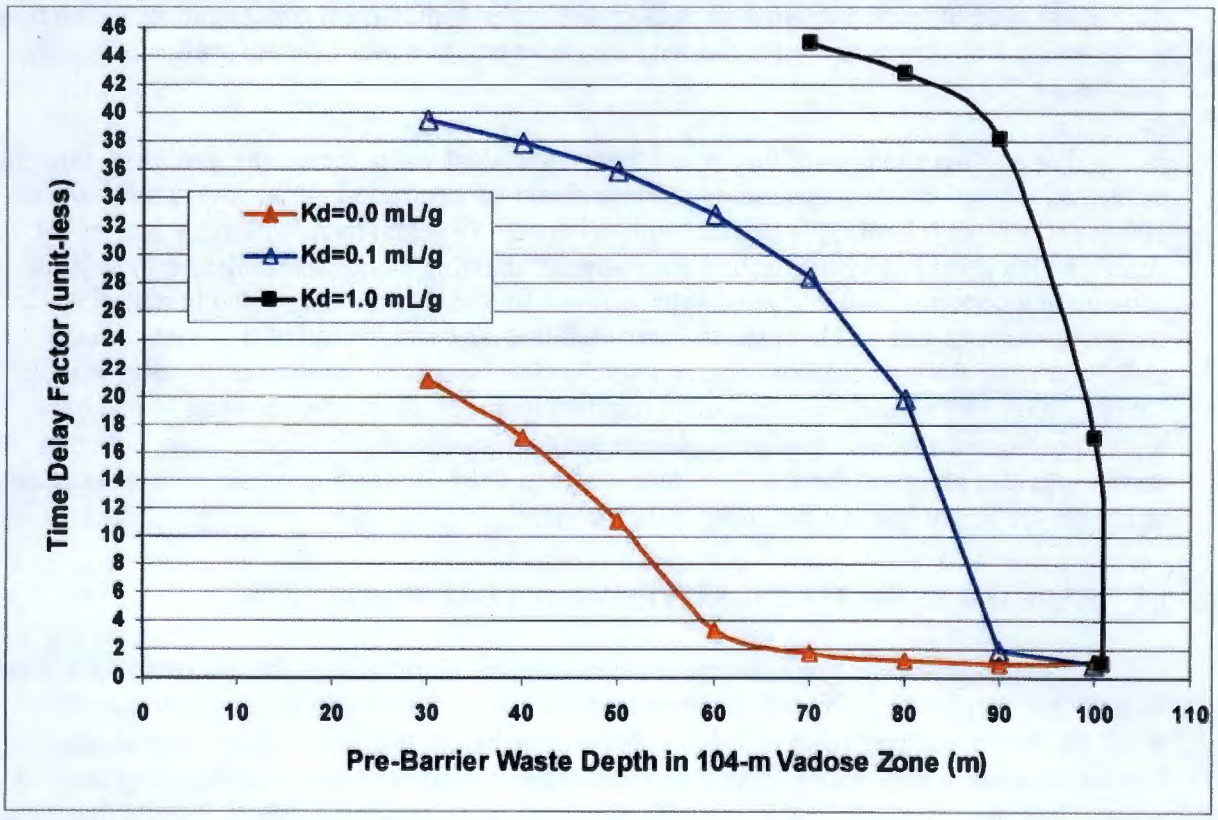


Figure 15. Barrier Time Delay Factors for Small-Adsorption Contaminants



In summary, a barrier is more effective for contaminants with some adsorption on the soil than those with no adsorption (i.e., fully mobile) and is more effective for deeper wastes. For contaminants with more adsorption (K_d value > 0.1 mL/g), such as uranium, the transport times to reach peak concentration are much longer than those with less adsorption, and the concentration reduction factors are higher for very deep waste zones (depth > 70 m). The primary mechanism for this behavior is that chemical adsorption slows down the contaminant allowing the antecedent moisture to drain leaving the bulk of the contaminant behind. As a result, the contaminant with a higher K_d value will be more likely to be primarily transported in the 0.5-mm/yr recharge domain rather than in the higher-recharge domain during antecedent water drainage.

3.5.2 Antecedent Moisture Impact and Rapid Change in Barrier Effectiveness

The effect of antecedent moisture is very important with small contaminant adsorption to soil because it causes a rapid decrease in barrier effectiveness for very deep waste zone depths. For example, at a waste depth of 100 m and K_d of 1 mL/g, the concentration reduction factor is 37.8 for a waste depth of 100 m, but drops to 16.9 at a waste depth of 101 m as shown in Figure 14 and Table 6 before reaching 1.0 at 104 m. Apparently, there is just enough antecedent water to flush the contaminant out of the vadose zone to cause the eventual peak concentration in the groundwater in 350 years, when the depth is 101 m, but not when the depth is 100 m. The 101-m deep waste also experiences more dispersion/diffusion because of the higher moisture content above the aquifer. As a result, for the 100-m deep waste, a very low water rate (recharge of 0.5 mm/yr due to the barrier), is all the recharge that is left to flush enough contaminant mass out of the vadose zone to cause the eventual peak groundwater contaminant concentration, which takes 7,300 years. The downward water velocity has decreased to about 2.6 mm/yr after 340 years (see Figure 5).

For another example of the impact from antecedent water decreasing over time, note that the arrival time of the peak groundwater contaminant concentration, for a waste zone depth of 100 m and a K_d of 0.1 mL/g, is shorter 'with' a barrier (57 years) than 'without' a barrier (61 years), which is caused by the declining recharge of draining antecedent moisture. The peak contaminant concentration in groundwater is lower for the barrier case, which is caused by the declining recharge and just happens to occur earlier at 57 years instead of 61 years. For the no-barrier case, the contaminant concentration has the same concentration at 57 years, but the concentration keeps on increasing, due to constant recharge, for four more years to reach the higher peak concentration. A slightly shorter peak arrival time with a barrier than without a barrier was also observed for the 90-m deep waste in Table 2, which occurs for the same reason as above; the beginning of a declining recharge value.

3.6 BARRIER EFFECTIVENESS FOR AN ACTUAL WASTE SITE

Conservative peak groundwater contaminant concentrations can be estimated for a given waste depth (or elevation) by substituting the measured peak contaminant concentration in the waste for the normalized value of 1.0, in other words, by multiplying the peak groundwater contaminant concentrations in Table 2 by the measured concentration in the vadose-zone pore water. However, the model assumes a 120 m by 3 m waste zone size with 12.7 vol% moisture. To apply the concentrations from this report to different size waste sites/zone with different moisture contents, a modified concentration would have to be developed, based on the waste

zone's contaminant mass, moisture content and size. All of the contaminant mass above a depth can be placed into the waste zone at that depth to be conservative. The waste zone size in this report is characteristic of the 216-B-26 Trench in the BC Cribs and Trenches Area (D&D-31659, *Geophysical Investigations by High-Resolution Resistivity for the BC Cribs and Trenches Area, 2004-2006*). Thus, in applying the model to the 216-B-26 Trench or a similar site, one only has to multiply the peak concentrations in Table 2 by the measured peak concentration in the pore water.

For example, soil sampling at the 216-B-26 Trench revealed a peak ^{99}Tc concentration in vadose-zone pore water of 1.4 million pCi/L at a depth of 31 m (RPP-20303). Multiplying the calculated concentrations (relative to 1.0) in Table 2 by 1.4 million pCi/L of ^{99}Tc in aqueous solution, predicts ^{99}Tc concentrations in the groundwater as shown in Table 7. Since the half-life of ^{99}Tc is much larger than the vadose transport time, decay effects are excluded.

Note that the ^{99}Tc drinking water standard (900 pCi/L) cannot be met without a barrier. Also the drinking-water standard can be met by emplacing a barrier, if the ^{99}Tc is no deeper than approximately 55 m for the conservatively high historical recharge of 25 mm/yr. If the historical recharge were 5 mm/yr or less, which is likely, then the drinking-water standard could potentially be met when ^{99}Tc is almost 70 m deep prior to barrier installation.

Table 7. Peak Contaminant Concentration of ^{99}Tc as a Function of Pre-barrier Waste Depth/Elevation in Vadose Zone (Infinite Barrier and Isotropic Soil)

Waste Location		[1]Peak Concentration of ^{99}Tc in Monitoring Well (pCi/L)			
[3]Depth Below Surface 104-m vadose	Elevation Above GW	No Barrier		With a Barrier (0.5 mm/yr)	
		25 mm/yr recharge	5 mm/yr recharge	[2]25 mm/yr recharge	[2]5 mm/yr recharge
30 m	74 m	**17,600**	**4,300**	**680**	**559**
40 m	64 m	**18,800**	**4,600**	**675**	**574**
50 m	54 m	**20,400**	**5,000**	**623**	**589**
60 m	44 m	**22,400**	**5,400**	**1,750**	**606**
70 m	34 m	**25,100**	**6,100**	**5,520**	**912**
80 m	24 m	**31,700**	**7,400**	**15,800**	**2,580**
90 m	14 m	**39,000**	**9,000**	**35,800**	**7,910**
100 m	4 m	**58,700**	**12,800**	**58,700**	**12,400**

[1]Using a vadose zone peak ^{99}Tc Concentration in Aqueous Solution of 1.4×10^6 pCi/L (RPP-20303).
[2]Historical recharge values before barrier installation.
[3]Depth of waste zone is the distance from the ground surface to the bottom of waste zone.

Since the ^{99}Tc at the BC Cribs and Trenches Area waste sites is located approximately 30 to 40 m deep, it is predicted that a surface barrier that limits recharge to 0.5 mm/yr over the long-term, could be sufficient in keeping the groundwater ^{99}Tc concentration below the drinking-water standard.

Following barrier installation, the estimated peak ^{99}Tc concentration in groundwater ranges from 560 to 680 pCi/L (Table 7), resulting from contamination in the vadose depth range

of 30 to 50 m. The minimum calculated peak concentration of 560 pCi/L is higher than the ^{99}Tc concentration previously calculated, 480 pCi/L, using a more detailed model reported in PNNL-14907, *Vadose Zone Contaminant Fate-and-Transport Analysis for the 216-B-26 Trench*. It was expected that the concentrations calculated here are conservative, which is confirmed by the comparison to the peak concentration calculated in PNNL-14907. Both calculations may be conservative, but the calculation in this report is more conservative. In regards to arrival time of the peak ^{99}Tc concentration, the arrival time is estimated here to range from 2,150 to 6,570 years for waste depths of 50 to 30 m (Table 2), respectively, whereas the arrival time calculated by the more detailed model (PNNL-14907) was approximately 4,000 years for a ^{99}Tc depth of about 40 m. The arrival time of the peak concentration varies considerably with the depth of the waste, so comparison between the calculations for this variable is not conclusive.

Site-specific analysis is recommended when more precise information is necessary for decision-making or for remedial design. To estimate how the results calculated here may change with more detailed analysis, the assumptions described earlier must be examined.

Using an actual layered stratigraphy that includes multiple soil types, such as silt loam that has greater water retention capability, would tend to slow contaminant transport to groundwater and decrease the peak contaminant concentration. Also, adding water transport anisotropy to the soils (i.e., allowing for increased lateral moisture transport relative to downward transport), decreasing the length of the waste zone, and increasing the dispersion coefficients are expected to slow contaminant transport to the groundwater and decrease the contaminant concentration in the groundwater. Conversely, a finite barrier and a thicker or longer waste zone would likely increase the contaminant concentrations shown in Table 7. However, all of the site-specific changes for BC Cribs and Trenches Area waste sites would likely decrease the concentrations shown in Table 7.

4.0 CONCLUSIONS AND SUMMARY

The effectiveness of a barrier to mitigate groundwater impact from vadose-zone contamination can be estimated from the depth of the waste and the historical recharge. A barrier that limits the water recharge into the vadose zone to 0.5 mm/yr or less is shown to be very effective in reducing the groundwater contaminant concentration for fully-mobile contaminants located in the top half of the vadose zone. A barrier can reduce the groundwater peak contaminant concentration by more than a factor of 30, compared to no-barrier performance. Barrier effectiveness is lower for depths located more than half way toward the groundwater. However, some barrier effectiveness (more than a factor of 2 over no-barrier performance) is still predicted at a waste depth of 80 m in a 104-m thick vadose zone for fully-mobile contaminants.

Waste depth begins to adversely affect barrier effectiveness when the waste zone is more than half-way toward the groundwater at the time the barrier is installed. Historical long-term recharge determines the pre-barrier moisture content (antecedent moisture) and the early contaminant transport rate following barrier installation. The closer the waste zone is to the barrier, the less antecedent water above the waste. Less antecedent water provides a lower driving force (recharge) on the contaminants, thereby, slowing down the contaminant transport rate to the groundwater and decreasing the eventual peak concentration in the groundwater.

Barrier effectiveness is enhanced for contaminants with some adsorption on the soil particles, especially for very deep wastes (depths > 70 m). The main reason for this behavior is that chemical adsorption slows down the contaminant, allowing the antecedent moisture to drain past the contaminants, leaving the bulk of the contaminant behind. As a result, the contaminants with higher K_d values will be more likely to be primarily transported in the small 0.5-mm/yr recharge domain rather than in the higher-recharge domain during antecedent water drainage.

For soil exhibiting isotropic hydraulic conductivity, a barrier overlap of 15 m (50 ft) approximates an infinite barrier for all waste depths. Greater barrier overlap is required when soil possesses 10:1 hydraulic anisotropy, particularly when combined with high historic recharge. However, a finite barrier with an overlap of 30 m on anisotropic soil with 25-mm/yr historical recharge amplifies the infinite barrier's peak contaminant concentration in the groundwater by at most a factor of 2.09 for only the mid-depth waste zones.

For the 216-B-26 Trench, a barrier could reduce the eventual peak concentrations of ^{99}Tc in the groundwater to be less than 900 pCi/L (the drinking water standard) for both historical recharges at waste depths of 50 m or less.

4.1 TECHNICAL SUMMARY OF PARAMETER IMPORTANCE

The most important parameters for calculating peak contaminant concentrations in the groundwater and a surface barrier's effectiveness in reducing contaminant concentrations in the groundwater, based on this analysis, are the following:

1) Waste depth at the time of barrier installation. Barrier effectiveness varies considerably as a function of waste depth. Relative to the no-barrier condition, the concentration reduction factor ranges from 1 to 32.7 for a relative high historical recharge of 25-mm/yr as a function of waste depth, making the waste depth a very important parameter.

2) Pre-barrier antecedent moisture content or, equivalently, historical recharge. The antecedent moisture content is important for the deeper waste zones because it is a large driving force on deep waste with the barrier unable to stop it or slow it down much. However, antecedent moisture is less important for waste zones in the top half of the vadose zone. The higher historical recharge allows a barrier to be more effective than the lower historical recharge. For historical recharges greater than 25 mm/yr, a barrier has more potential for concentration reduction and time delay.

3) Vadose zone thickness. For the 25-mm/yr historical recharge, the concentration reduction factors for a barrier over a 74-m thick vadose are large (> 20) for all waste zone depths located in the top half of the thinner vadose zone, but not as large as the thicker vadose zone's barrier effectiveness factors (> 30) at the half way depth or above. Furthermore, the peak barrier efficiency is lower for the thinner vadose zone, but the thinner vadose zone has larger barrier efficiencies for waste depths more than half way deep inherently due to less antecedent water in less (vertical) soil.

4) Contaminant adsorption on the soil. The distribution coefficient, K_d, was shown to be very important in enhancing barrier effectiveness, especially for deeper wastes. Even a small K_d value of 0.1 mL/g showed significant enhancement of longer travel times and larger concentration reduction factors, especially for deeper wastes. For a larger K_d value of 1.0 mL/g, the concentration reduction factor is larger for all waste depths, and exceptionally larger for very deep waste zones at depths of 90 to 100 m. Likewise, the time delay factors are larger for larger distribution coefficients. These results suggest that more time can be allowed for barrier installation over waste zones with adsorbed contaminants than for waste zones with fully mobile contaminants in order to achieve the same barrier effectiveness. The reasons for higher barrier efficiency for partially adsorbed contaminants is that more mass has to be flushed out of the vadose zone, due to adsorption on soil, with a small recharge of only 0.5 mm/yr, as summarized in Section 4.0.

5) Barrier overlap and soil anisotropy. The barrier overlap size is more important for the anisotropic soil than for the isotropic soil, and more important for the high 25-mm/yr historical recharge than for the 5-mm/yr recharge. Hydraulic anisotropy is more important for wetter soils. The effects of 10:1 anisotropic soil are not large (about 2.09 for the worst waste-zone depth) compared to the effects of other parameters, when the barrier overlap is 30 m or more. In other words, anisotropy is not as important as some other parameters. The effects of larger ratios (>10) of horizontal to vertical conductivity were not analyzed. A finite barrier reduces the peak concentration relative to the infinite barrier performance for many waste zone depths because of the curling of water under the barrier washing out some of the waste early, thereby reducing the waste mass that causes the peak concentration.

6) Extra moisture content in waste zone. Extra waste-zone moisture content, associated with liquid forms of waste, shortens the arrival time of peak concentration by less than 150 years for waste depths in the top half of the vadose zone, which is not a large impact. However, larger volumes (larger than 120 m by 3 m) of high moisture content regions are potentially more important. The extra moisture content also results in an initial larger contaminant mass in the waste zone, and eventually larger contaminant concentrations in the groundwater, because the concentration, not the mass, is set in the waste-zone pore water in the model. However, even though the concentration is affected by contaminant mass size, the barrier effectiveness is not affected by the extra moisture content or contaminant mass size because any increased amount of moisture or contaminant mass is the same for the barrier and no-barrier cases.

7) Other parameters. Other parameters expected to influence barrier effectiveness or groundwater contaminant concentration, but were not analyzed here, include the following:

   a) spatial size of the waste zone (length, width and thickness), along with the contaminant concentration over this space, which are both very waste site specific. Larger waste zones cause larger peak contaminant concentrations in the aquifer, and vice versa. However, the barrier effectiveness is not expected to change much because the waste mass is the same for barrier and no-barrier conditions. An increase in the horizontal dimension of waste zone is expected to have more impact than increases in the vertical dimension because the depth changes with the vertical dimension.

   b) soil layers and heterogeneities. Soil layering and heterogeneities can cause enhanced

lateral flow, which can be important for the finite barrier cases. These effects are expected to reduce the contaminant groundwater concentrations, but funneling effects could increase the concentrations.

c) dispersivity and diffusion have more importance for wetter soils. Thus, the 100-m deep waste zone is penalized more than shallower waste zones because the soil is wetter near the aquifer. Also, dispersivity/diffusion processes may be important for finite barriers with anisotropic soil in affecting the curling of water under the barrier's shadow. The model included dispersivity/diffusion effects, but no attempt was made to determine their relative impact from advection of water.

d) percolation rate (recharge) through the barrier, which was fixed at 0.5 mm/yr in this analysis. Smaller percolation rates would increase the barrier effectiveness and higher rates would decrease the effectiveness. Also, short-term and long-term temporal variation in the barrier percolation rate was not considered.

e) residual moisture content could play a role in very dry soils, which result from the deployment of a barrier.

f) flow rate and thickness of the aquifer directly influences the groundwater contaminant concentration. Faster water flow causes lower contaminant concentrations in the aquifer. Thicker aquifers allow more mixing of the vadose-zone contaminant flux. However, the barrier effectiveness should be independent of the aquifer flow rate and thickness because both the no-barrier and barrier cases will result in lower groundwater contaminant concentrations with a faster aquifer flow and larger thickness.

5.0 REFERENCES

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APPENDIX A - ADDITIONAL ASSUMPTIONS AND PARAMETER VALUES

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A.1 INTRODUCTION

The main assumptions for the modeling are presented in Sections 2.1 and 2.2. This appendix discusses more assumptions and/or specific parameter values.

A.2 SOIL PARAMETERS FOR FLOW AND TRANSPORT CALCULATIONS

1) Soil Hydraulic Parameters

Assumed soil properties are shown in Table A-1. Values for the single soil type, that is representative of sand and gravel, were obtained from PNNL-14702. The Hanford H1 soil samples in PNNL-14702 show a mean-value conductivity of 1.09 x 10^{-3} cm/sec (344 m/yr). The van-Genuchten parameters, alpha and N, which are described in the STOMP users' manual (PNNL-14478), are given the mean values from PNNL-14702, as well as the residual saturation and porosity for the vadose zone. The 'extended' van-Genuchten model was chosen, which is better suited for very dry soils (PNNL-14702, Fayer and Simmons 1995). Hysteresis effects of the unsaturated soil characteristic properties were not included in the model.

For completeness, unsaturated properties are also listed for the aquifer, even though the aquifer is always saturated in this analysis. The effective porosity of the aquifer layer is assumed to consist of only large pores. With the small pores excluded from the model, the effective porosity is small (assumed to be 12 vol%) in the model, which causes faster contaminant flow (i.e., higher porewater velocity). A large conductivity value of 0.13 cm/sec (112 m/day) for the aquifer was chosen because it is consistent with the small porosity value, and was also obtained from PNNL-14702. These aquifer parameter values promote a fast flow through the large pores in order to minimize the arrival time of the contaminants to the monitoring well. These aquifer parameters only affect the travel time, not the concentration in the well. The aquifer Darcy velocity, in a uniform aquifer, determines the amount of concentration reduction in the well.

Table A-1. Physical Properties of Soils

Soil Type	Porosity (m^3/m^3)	Hydraulic Conductivity	Alpha (1/cm)	N	Residual Saturation	Longitudinal Dispersivity
Hanford (sandy gravel)	0.318	0.00109 cm/sec (343.7 m/yr)	0.0415	1.759	0.077	0.02 m
Aquifer Soil (Ringold)	0.12	0.13 cm/sec (112 m/day)	0.0132	1.753	0.077	0.1 m

Other parameters used in the model are described here, but for a complete list of parameter values, see the actual code input file in Appendix B. The soil density is only used when there is adsorption to the soil, which affects only the non-zero K_d cases in Section 3.5; the particle density is the input (see Appendix B) and the code calculates the bulk density from the porosity and particle density. A typical particle density for sand of 2,600 kg/m^3 was used, giving a bulk density of 1,773 kg/m^3 (=2,600 x (1-0.318)) for the Hanford soil.

2) Low Longitudinal Dispersion Length of 0.02 m And Transverse Length of 0.002 m

These values are used in the Quirk-Millington contaminant dispersion model (PNNL-14478) and are considered small and conservative. Larger dispersion lengths would cause the contaminants to spread out faster, which usually lowers the peak concentration in the soil water. The Peclet number for the model grid is around 5, which means that the advection transport rate is about 5 times larger than the dispersion transport rate. The contaminants in the aquifer are given a larger longitudinal dispersion length of 0.1 m and a transverse length of 0.01 m, which is still considered small and conservative. These assumed dispersivity values are smaller and more conservative than the mean value, 0.203 m, listed in PNNL-14702 for the vadose zone soil chosen here. The contaminant molecular diffusion coefficient in water is the commonly used value of 2.5×10^{-5} cm^2/sec.

3) No Contaminant Flux or Moisture through Side Boundaries

The vertical side boundaries of the model domain (see Figure 1) do not allow contaminant flux or moisture to pass out of or into the model domain, except for the 6-m thick aquifer, where water and contaminants flow out on the right (down-gradient) side of model domain, and clean water flows in on the left (up-gradient) side.

4) Groundwater Flow Rate (Darcy Velocity) is 0.024 m/day

This parameter value was justified in Section 2.2, and is discussed in more detail. The Darcy velocity affects the waste concentration directly as follows: contaminant concentration in the groundwater = contaminant influx into region divided by the product of Darcy velocity and cross-sectional area (e.g., $C = Q / V * A$, where Q is contaminant influx with units like Ci/day, V is the Darcy velocity, m/day, and A is the cross-sectional flow area, m^2). Due to additional pre-barrier water from the vadose zone reaching the groundwater (25 mm/yr and 5 mm/yr), the Darcy flow velocity was lowered on the left side boundary (incoming groundwater) of model domain to 0.0203 m/day and 0.0235 m/day for the 25 mm/yr and 5 mm/yr recharge values, respectively. The recharge water entering the aquifer enhances the groundwater flow rate to about 0.024 m/day at the 100-m down-gradient well and the right-most (outgoing) boundary. In summary, the contaminant concentration in the aquifer is calculated by dividing the contaminant flux into an aquifer region by the groundwater volumetric flow rate (V * A) into the region, where the flux and flow rate are both calculated by the model over time. Even though the Darcy velocity is fixed on the left-side boundary, the interior domain has varying Darcy velocity because of the varying incoming vadose water flux when the barrier is installed.

Note that the aquifer can potentially provide a large contaminant concentration reduction in the groundwater. For example, a narrow contaminant stream entering the aquifer from the vadose zone with a recharge of 5 mm/yr, has its concentration potentially reduced to a small calculated fraction, 5.7×10^{-4}, of its initial vadose zone concentration of 1.0. The small concentration fraction is simply calculated by dividing the recharge (5 mm/yr) by the groundwater flow velocity (0.024 m/day) and converting units [i.e., 5.7×10^{-4} = (5 mm/yr * 0.001 m/mm) / (0.024 m/day * 365 days/yr)]. The concentration fraction of 5.7×10^{-4} is equivalent to an aquifer dilution factor of 1750 ($1.0/5.7 \times 10^{-4}$), assuming only clean groundwater

picks up the narrow contaminant stream. However, the aquifer dilution factor is much lower than 1750 when the contaminant flux entering the aquifer is wide, because the groundwater is no longer clean when flowing under a wide stream of incoming contaminants. For example, in Section 3.1.1, an overall (vadose zone and groundwater effects) reduction factor of 336.7 is calculated for the no-barrier case with a 5-mm/yr recharge for 30-m deep waste zone that is 120 meters wide. For deeper wastes, the overall reduction factor decreases (< 336.7), demonstrating that a wide contaminant stream cannot achieve the high aquifer dilution factor of 1750 for a narrow waste stream. With a barrier, the recharge into the aquifer eventually decreases to 0.5 mm/yr, resulting in larger potential concentration reduction than natural conditions. In effect, this is the reason why barriers are effective; they slow down the water infiltration rate with contaminants into the groundwater, thereby causing more reduction from the flowing groundwater.

A3.0 REFERENCES

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APPENDIX B - STOMP-W INPUT FILES AND GRID SENSITIVITIES

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B.1 Key Input Files

The base STOMP-W barrier input file is listed below in its entirety to show all the detailed parameter values. The input file simulates a barrier with a 0.5 mm/yr recharge and a waste depth of 30 m, with the contaminant zone being 120 m by 3 m. The restart file called out in the input file below sets up the initial or pre-barrier moisture content and water velocity for the 25-mm/yr historical recharge.

The input file that created this restart file is also listed. The restart-file flow conditions were determined by simulating the 25-mm/yr recharge for 240 years, when steady-state conditions were reached. The Darcy velocity was set lower on the inlet side of aquifer at 0.02031 m/day than on the outlet side at 0.024 m/day in order to account for the recharge adding to the aquifer flow rate and achieving the desired 0.024 m/day velocity. The aquifer pressure calculated at the bottom right side of model domain (151,669 Pascal) by restart-file-creation run was used as a pressure input for all of the other input files with 25-mm/yr recharge. This method is equivalent to using a hydraulic gradient across the length of the aquifer, but was thought to be easier for the reader to see a fixed velocity of 0.24 m/day than a fixed hydraulic gradient.

The input files with an adsorption K_d coefficient of 1.0 mL/g and a finite barrier case with an overlap of 15 m and anisotropic soil are also listed. The waste depth in these files is 100 m, and the historical recharge is 25 mm/yr.

Several simulations were made using a finer grid in order to quantify these effects. The input file for the 100-m deep waste is listed; the finer grid has a 0.1-m vertical cell size through and below the waste zone (3 m and 4 m distances, respectively) and a 0.2-m vertical cell size for 2 m of distance above the waste zone, instead of the normal size of 0.5 m.

Horizontal grid size was also addressed for the anisotropic soil cases with the 25-mm/yr recharge and waste depths of 30 and 50 m. The horizontal grid cell size was changed to 1.5 m, instead of the base 3 m. The groundwater contaminant concentrations did not change for the finer horizontal grid sensitivity cases, indicating that the lateral grid size was not sensitive. However, the vertical grid size is important as shown in next section (B.2).

B.2 Results of Cases with Finer Vertical Grid

Only two waste depths, 100 m and 30 m, were simulated in order to obtain sensitivity results for shallow and very-deep wastes, assuming that other waste depths would be bounded by these two extremes. Only the high 25-mm/yr historical recharge was used. The groundwater contaminant concentration increased for the finer-grid cases as shown in Table B-1. In separate cases, the aquifer grid was also refined, but this refinement showed little change.

For a waste zone depth of 30 m, the finer grid causes the concentration to increase by 13% for the no-barrier case and by 15% for the barrier case. As a result, the concentration reduction factor for the finer-grid cases decreases slightly to 27.5 for the finer grid from 27.8 for

the base grid. The arrival time of peak concentration was slightly smaller for the 30-m deep waste with the finer grid.

For the 100-m deep waste, the concentrations for the finer grid increase 30% over those calculated with the base grid with or without a barrier. As a result, the concentration reduction factor stays the same at 1.0. The arrival time of the peak concentration is about 9% longer with the finer grid than with the base grid, but the time delay factors (1.0) are the same.

In summary, the finer grid causes higher concentrations than the base grid with largest increase occurring at large waste depths and a smaller increase for the small waste depths. However, the concentrations reduction factors stay about the same because the increases are similar for no-barrier and barrier cases. The finer grid causes the peak concentration arrival time to increase for the large waste depths, but to decrease slightly for the small waste depths.

Table B-1. Results of Finer-Grid and Base-Grid Cases

Waste Location in 104-m Thick Vadose Zone when Barrier Installed		Peak Groundwater Contaminant Concentration and Time of Peak Concentration Arrival			
		Historical 25-mm/yr recharge (Wetter Pre-Barrier Soil)			
Depth from surface		No Barrier (25 mm/yr)		With a Barrier ([1]0.5 mm/yr)	
		Time (yrs)	[2]Concentration	Time (yrs)	[2]Concentration
30 m	Finer Grid	263	1.43×10^{-2}	5,530	5.18×10^{-4}
30 m	Base Grid	264	1.26×10^{-2}	5,600	4.52×10^{-4}
100 m	Finer Grid	21.8	5.45×10^{-2}	21.8	5.45×10^{-2}
100 m	Base Grid	20.0	4.19×10^{-2}	20.0	4.19×10^{-2}
		[3]Time Ratio	[4]Concentration Ratio	[3]Time Ratio	[4]Concentration Ratio
30 m	Finer-to-Base Ratio	1.0	1.13	0.99	1.15
100 m	Finer-to-Base Ratio	1.09	1.30	1.09	1.30
				Time Delay Factor	Concentration Reduction Factor
30 m	Finer Grid			21.0	27.5
30 m	Base Grid			21.2	27.8
100 m	Finer Grid			1.0	1.0
100 m	Base Grid			1.0	1.0

[1]Barrier limits recharge to 0.5 mm/yr; historical recharge was 25 mm/yr.

[2]Concentration is unit-less and relative to the initial normalized pre-barrier concentration of 1.0.

[3]Time Ratio is the arrival time of peak concentration calculated with the finer-grid divided by the base grid arrival time of peak concentration.

[4]Concentration Ratio is the concentration from the finer-grid calculation divided by base-grid concentration.

B.3 Time Step Size Variation

Time step sizes were also changed, but the time step size variation did not change the results very much. Relatively small time step sizes were used in all cases. The time step size started at 0.0001 year and increased by 15% every converged time step until 0.1 to 5 years were reached for the 100-m and 30-m deep waste zone, respectively. For the slow moving adsorbed contaminant transport case, the time step size was gradually increased to 10 years.

B.4 Base Input File for 30-m Deep Waste

```
~Simulation Title Card
1,
Flow and Transport  2D model,
Dr. Mel Piepho,
Fluor Gov. Group,
April 12 2006,
10:00 AM PST,
2,
This problem represents a 2D model for flow & transport calcs
It covers a distance of about 420 m or 1385 feet.
#-----------------------------------------------
~Solution Control Card
#-----------------------------------------------
Restart file,flow-final2-2p5cm.rst240yr,
# Normal,
Water w/transport,
1,
0,yr,6000.0,yr,0.0001,yr,5.0,yr,1.15,16,1.e-6,
3000000,
# variable aqueous diffusion,
# variable gas diffusion,
1,
effective permeability,geometric,

~Grid Card
tilted cartesian,0,deg,0,deg,
140,1,214,
#
# X Grid
0.0,m,140@3.0,m,
#
# y Grid
0.0,m,1@1.0,m,
#
# Z Grid
-600,cm,6@100.0,cm,
208@50,cm,
#
~Rock/Soil Zonation Card
2,
Ringold-sat,1,140,1,1,1,6,
Hanford,1,140,1,1,7,214,
#
```

```
~Mechanical Properties Card
Ringold-sat,2740,kg/m^3,0.12,0.12,0,,Millington and Quirk,
Hanford,2600,kg/m^3,0.318,0.318,0,,Millington and Quirk,
#
~Hydraulic Properties Card
Ringold-sat,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,
Hanford,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,
#
~Saturation Function Card
Ringold-sat,Extended van Genuchten,0.0132,1/cm,1.753,0.077,,
Hanford,Extended van Genuchten,0.0415,1/cm,1.759,0.077,,
#
~Aqueous Relative Permeability Card
Ringold-sat,Mualem,,,,
Hanford,Mualem,,,,
#
#-----------------------------------------
~Solute/Fluid Interaction Card
1,
Tc-99,Conventional,2.5E-5,cm^2/s,Continuous,1E20,yr,
0,
#
~Solute/Porous Media Interaction Card
Ringold-sat,0.1,m,0.01,m,
Tc-99,0.0,ml/g,1.0,
Hanford,0.02,m,0.002,m,
Tc-99,0.0,ml/g,1.0,
#
~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
3,
Aqueous Pressure Overwrite,92360,Pa,,,,,,41,80,1,1,155,160, # pressure for an extra 4% moisture
solute aqueous volumetric concentration Overwrite,Tc-99,0.0,1/L,,,,,,1,140,1,1,1,214,
solute aqueous volumetric concentration OVerwrite,Tc-99,1.0,1/L,,,,,,41,80,1,1,155,160,  #~3 m thick,27 m to 30 m
deep
#
~Boundary Conditions Card
#-----------------------------------------
6,
top,Neumann Aqueous,Zero Flux,
1,80,1,1,214,214,2,
0,yr,-0.5,mm/yr,,,,,
12005,yr,-0.5,mm/yr,,,,,
top,Neumann Aqueous,Zero Flux,
81,140,1,1,214,214,2,
0,yr,-0.5,mm/yr,,,,,
12005,yr,-0.5,mm/yr,,,,,
west,neumann aqueous,Zero Flux,
1,1,1,1,1,6,1,
0,yr,0.02031,m/day,,,,,
west,Zero Flux,Zero Flux,
1,1,1,1,7,214,1,
0,yr,78000,Pa,,,,,
east,Hydraulic Gradient,Outflow,
140,140,1,1,1,6,1,
0,yr,151669,Pa,,,,,
```

```
east,Zero Flux,Zero Flux,
140,140,1,1,7,214,1,
0,yr,78000,Pa,,,,
#-----------------------------------------
#-----------------------------------------
~Output Options Card
#-----------------------------------------
1,
113,1,1,
2,2,yr,cm,4,4,4,
6,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous pressure,,
solute aqueous conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
1,
7550,yr,
8,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous relative permeability,,
Aqueous pressure,,
solute aqueous conc,Tc-99,1/L,
solute volumetric conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
#-----------------------------------------
~Surface Flux Card
#-----------------------------------------
6,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,214,214,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,7,7,
Aqueous Volumetric,L/day,L,West,113,113,1,1,1,6,
Solute Flux,Tc-99,1/day,,Top,1,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,Top,81,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,West,113,113,1,1,1,6,
```

B.5 Restart-File-Creation Input File

```
~Simulation Title Card
1,
Flow 2D model,
Dr. Mel Piepho,
Fluor Gov. Group,
April 12 2006,
10:00 AM PST,
2,
This problem represents a 2D model for initial flow conditions
It covers a horizontal distance of 420 m
#-----------------------------------------
~Solution Control Card
#-----------------------------------------
# Restart file,big6-edit.rst500yr,
```

```
Normal,
Water,  w/transport,
1,
0,yr,240.0,yr,0.01,yr,4.0,yr,1.25,16,1.e-6,
3000000,
#variable aqueous diffusion,
#variable gas diffusion,
1,
effective permeability,geometric,

~Grid Card
cartesian,0,deg,0,deg,
140,1,214,
#
# X Grid
0.0,m,140@3.0,m,
#
# y Grid
0.0,m,1@1.0,m,
#
# Z Grid
-600,cm,6@100.0,cm,
208@50,cm,
#
~Rock/Soil Zonation Card
2,
Ringold-sat,1,140,1,1,1,6,
Hanford,1,140,1,1,7,214,
#
~Mechanical Properties Card
Ringold-sat,2740,kg/m^3,0.12,0.12,0,,Millington and Quirk,
Hanford,2600,kg/m^3,0.318,0.318,0,,Millington and Quirk,
#
~Hydraulic Properties Card
Ringold-sat,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,
Hanford,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,
#
~Saturation Function Card
Ringold-sat,Extended van Genuchten,0.0132,1/cm,1.753,0.077,,
Hanford,Extended van Genuchten,0.0415,1/cm,1.759,0.077,,
#
~Aqueous Relative Permeability Card
Ringold-sat,Mualem,,,,
Hanford,Mualem,,,,
#
#-----------------------------------------
# ~Solute/Fluid Interaction Card
# 1,
# Tc-99,Conventional,2.5E-5,cm^2/s,Continuous,1E20,yr,
# 0,
#
# ~Solute/Porous Media Interaction Card
# R# ingold-sat,1,m,0.1,m,
# Tc-99,0.0,ml/g,1.0,
# Hanford,0.2,m,0.02,m,
# Tc-99,0.0,ml/g,1.0,
```

```
#
~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
2,
#Gas Pressure,100000,Pa,,,,,,1,140,1,1,1,214,
Aqueous Pressure,88000,Pa,,,,,,1,140,1,1,1,214,
Aqueous Pressure,140000,Pa,,,,,,1,140,1,1,1,6,
# solute aqueous volumetric concentration,Tc-99,1.0,1/l,,,,,,1,80,1,1,106,154,  #~17 m thick, 25 m to 42 m deep
#
~Boundary Conditions Card
#-----------------------------------------------
5,
top,Neumann Aqueous,Zero Flux,
1,140,1,1,214,214,2,
0,yr,-2.5,cm/yr,,,,,
12005,yr,-2.5,cm/yr,,,,,
west,neumann aqueous,Zero Flux,
1,1,1,1,1,6,1,
0,yr,0.02031,m/day,,,,,
west,Dirichlet aqueous,Zero Flux,
1,1,1,1,7,214,1,
0,yr,78000,Pa,,,,,
east,neumann aqueous,Outflow,
140,140,1,1,1,6,1,
0,yr,0.024,m/day,,,,,
east,Dirichlet aqueous,Zero Flux,
140,140,1,1,7,214,1,
0,yr,78000,Pa,,,,,
#-----------------------------------------------
~Output Options Card
#-----------------------------------------------
29,
70,1,214,
70,1,212,
70,1,210,
70,1,200,
70,1,196,
70,1,192,
70,1,186,
70,1,179,
70,1,175,
70,1,168,
70,1,158,
70,1,146,
70,1,138,
70,1,130,
70,1,122,
70,1,115,
70,1,100,
70,1,90,
70,1,80,
70,1,40,
70,1,25,
70,1,8,
70,1,7,
140,1,7,
```

```
70,1,6,
140,1,6,
1,1,1,
70,1,1,
140,1,1,
2,2,yr,cm,6,6,6,
4,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous relative permeability,,
Aqueous pressure,,
1;
1500,yr,
4,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous relative permeability,,
Aqueous pressure,,

#-----------------------------------------
~Surface Flux Card
#-----------------------------------------
4,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,214,214,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,7,7,
Aqueous Volumetric,L/day,L,East,139,139,1,1,1,6,
Aqueous Volumetric,L/day,L,East,139,139,1,1,7,214,
```

B.6 Input File for Adsorption Kd of 1 mL/g for 100-m Deep Waste

```
~Simulation Title Card
1,
Flow and Transport 2D model,
Dr. Mel Piepho,
Fluor Gov. Group,
April 12 2006,
10:00 AM PST,
2,
This problem represents a 2D model for flow & transport calcs
It covers a distance of 420 m or 1385 feet.
#-----------------------------------------
~Solution Control Card
#-----------------------------------------
Restart file,flow-final2-2p5cm.rst240yr,
# Normal,
Water w/transport,
1,
0,yr,7500.0,yr,0.0001,yr,10.0,yr,1.15,16,1.e-6,
3000000,
# variable aqueous diffusion,
# variable gas diffusion,
1,
effective permeability,geometric,

~Grid Card
```

```
tilted cartesian,0,deg,0,deg,
140,1,214,
#
# X Grid
0.0,m,140@3.0,m,
#
# y Grid
0.0,m,1@1.0,m,
#
# Z Grid
-600,cm,6@100.0,cm,
208@50,cm,
#
~Rock/Soil Zonation Card
2,
Ringold-sat,1,140,1,1,1,6,
Hanford,1,140,1,1,7,214,
#
~Mechanical Properties Card
Ringold-sat,2740,kg/m^3,0.12,0.12,0,,Millington and Quirk,
Hanford,2600,kg/m^3,0.318,0.318,0,,Millington and Quirk,
#
~Hydraulic Properties Card
Ringold-sat,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,
Hanford,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,
#
~Saturation Function Card
Ringold-sat,Extended van Genuchten,0.0132,1/cm,1.753,0.077,,
Hanford,Extended van Genuchten,0.0415,1/cm,1.759,0.077,,
#
~Aqueous Relative Permeability Card
Ringold-sat,Mualem,,,,
Hanford,Mualem,,,,
#
#-----------------------------------------------
~Solute/Fluid Interaction Card
1,
Tc-99,Conventional,2.5E-5,cm^2/s,Continuous,1E20,yr,
0,
#
~Solute/Porous Media Interaction Card
Ringold-sat,0.1,m,0.01,m,
Tc-99,1E-3,m^3/kg,1.0,
Hanford,0.02,m,0.002,m,
Tc-99,1E-3,m^3/kg,1.0,
#
~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
3,
Aqueous Pressure overwrite,92360,Pa,,,,,,,41,80,1,1,15,20,
solute aqueous volumetric concentration overwrite,Tc-99,0.0,1/L,,,,,,,1,140,1,1,1,214,
solute aqueous volumetric concentration overwrite,Tc-99,1.0,1/L,,,,,,,41,80,1,1,15,20,  #~3 m thick,97 m to 100 m
deep
#
~Boundary Conditions Card
#-----------------------------------------------
```

```
6,
top,Neumann Aqueous,Zero Flux,
1,80,1,1,214,214,2,
0,yr,-0.5,mm/yr,,,,,
42005,yr,-0.5,mm/yr,,,,,
top,Neumann Aqueous,Zero Flux,
81,140,1,1,214,214,2,
0,yr,-0.5,mm/yr,,,,,
42005,yr,-0.5,mm/yr,,,,,
west,neumann aqueous,Zero Flux,
1,1,1,1,1,6,1,
0,yr,0.02031,m/day,,,,,
west,Zero Flux,Zero Flux,
1,1,1,1,7,214,1,
0,yr,78000,Pa,,,,,
east,Hydraulic Gradient,Outflow,
140,140,1,1,1,6,1,
0,yr,151669,Pa,,,,,
east,Zero Flux,Zero Flux,
140,140,1,1,7,214,1,
0,yr,78000,Pa,,,,,
#-----------------------------------------
#-----------------------------------------
~Output Options Card
#-----------------------------------------
41,
60,1,214,
60,1,180,
60,1,170,
60,1,160,
60,1,150,
60,1,140,
60,1,130,
60,1,120,
60,1,100,
60,1,90,
60,1,80,
60,1,70,
60,1,60,
60,1,50,
60,1,40,
60,1,30,
60,1,25,
60,1,20,
60,1,15,
60,1,10,
60,1,9,
60,1,8,
60,1,7,
60,1,6,
60,1,5,
60,1,4,
60,1,3,
60,1,2,
60,1,1,
41,1,6,
```

```
51,1,6,
61,1,6,
71,1,6,
81,1,6,
113,1,7,
113,1,6,
113,1,5,
113,1,4,
113,1,3,
113,1,2,
113,1,1,
1,1,yr,cm,4,4,4,
6,
Aqueous moisture content,,
solute inventory,Tc-99,,
solute volumetric conc,Tc-99,1/L,
solute aqueous conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
1,
1000,yr,
8,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous pressure,,
solute inventory,Tc-99,,
solute aqueous conc,Tc-99,1/L,
solute volumetric conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
#-----------------------------------------------
~Surface Flux Card
#-----------------------------------------------
6,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,214,214,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,7,7,
Aqueous Volumetric,L/day,L,West,113,113,1,1,1,6,
Solute Flux,Tc-99,1/day,,Top,1,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,Top,81,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,West,113,113,1,1,1,6,
```

B.7 Input File for Barrier Overlap of 15 m and Anisotropic Soil for 100-m Deep Waste

```
~Simulation Title Card
1,
Flow and Transport 2D model,
Dr. Mel Piepho,
Fluor Gov. Group,
April 12 2006,
10:00 AM PST,
2,
This problem represents a 2D model for flow & transport calcs
It covers a distance of about 420 m or 1385 feet.
#-----------------------------------------------
```

```
~Solution Control Card
#-----------------------------------------------
Restart file,flow-final2-2p5cm.rst240yr,
# Normal,
Water w/transport,
1,
0,yr,30.0,yr,0.0001,yr,0.1,yr,1.15,16,1.e-6,
3000000,
# variable aqueous diffusion,
# variable gas diffusion,
1,
effective permeability,geometric,

~Grid Card
tilted cartesian,0,deg,0,deg,
140,1,214,
#
# X Grid
0.0,m,140@3.0,m,
#
# y Grid
0.0,m,1@1.0,m,
#
# Z Grid
-600,cm,6@100.0,cm,
208@50,cm,
#
~Rock/Soil Zonation Card
2,
Ringold-sat,1,140,1,1,1,6,
Hanford,1,140,1,1,7,214,
#
~Mechanical Properties Card
Ringold-sat,2740,kg/m^3,0.12,0.12,0,,Millington and Quirk,
Hanford,2600,kg/m^3,0.318,0.318,0,,Millington and Quirk,
#
~Hydraulic Properties Card
Ringold-sat,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,
Hanford,1.090E-02,hc:cm/s,1.090E-02,hc:cm/s,1.090E-03,hc:cm/s,
#
~Saturation Function Card
Ringold-sat,Extended van Genuchten,0.0132,1/cm,1.753,0.077,,
Hanford,Extended van Genuchten,0.0415,1/cm,1.759,0.077,,
#
~Aqueous Relative Permeability Card
Ringold-sat,Mualem,,,,
Hanford,Mualem,,,,
#
#-----------------------------------------------
~Solute/Fluid Interaction Card
1,
Tc-99,Conventional,2.5E-5,cm^2/s,Continuous,1E20,yr,
0,
#
~Solute/Porous Media Interaction Caord
Ringold-sat,0.1,m,0.01,m,
```

```
Tc-99,0.0,ml/g,1.0,
Hanford,0.02,m,0.002,m,
Tc-99,0.0,ml/g,1.0,
#
~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
3,
Aqueous Pressure overwrite,92360,Pa,,,,,,,41,80,1,1,15,20,
solute aqueous volumetric concentration overwrite,Tc-99,0.0,1/L,,,,,,,1,140,1,1,1,214,
solute aqueous volumetric concentration overwrite,Tc-99,1.0,1/L,,,,,,,41,80,1,1,15,20,  #~3 m thick,97 m to 100 m
deep
#
~Boundary Conditions Card
#-----------------------------------------------------
7,
top,Neumann Aqueous,Zero Flux,
1,35,1,1,214,214,1,
0,yr,-25.0,mm/yr,,,,,
top,Neumann Aqueous,Zero Flux,
36,85,1,1,214,214,1,
0,yr,-0.5,mm/yr,,,,,
top,Neumann Aqueous,Zero Flux,
86,140,1,1,214,214,1,
0,yr,-25.0,mm/yr,,,,,
west,neumann aqueous,Zero Flux,
1,1,1,1,1,6,1,
0,yr,0.02031,m/day,,,,,
west,Zero Flux,Zero Flux,
1,1,1,1,7,214,1,
0,yr,78000,Pa,,,,,
east,Hydraulic Gradient,Outflow,
140,140,1,1,1,6,1,
0,yr,151669,Pa,,,,,
east,Zero Flux,Zero Flux,
140,140,1,1,7,214,1,
0,yr,78000,Pa,,,,,
#-----------------------------------------------------
#-----------------------------------------------------
~Output Options Card
#-----------------------------------------------------
41,
60,1,214,
60,1,180,
60,1,170,
60,1,160,
60,1,150,
60,1,140,
60,1,130,
60,1,120,
60,1,100,
60,1,90,
60,1,80,
60,1,70,
60,1,60,
60,1,50,
60,1,40,
```

```
60,1,30,
60,1,25,
60,1,20,
60,1,15,
60,1,10,
60,1,9,
60,1,8,
60,1,7,
60,1,6,
60,1,5,
60,1,4,
60,1,3,
60,1,2,
60,1,1,
41,1,6,
51,1,6,
61,1,6,
71,1,6,
81,1,6,
113,1,7,
113,1,6,
113,1,5,
113,1,4,
113,1,3,
113,1,2,
113,1,1,
1,1,yr,cm,4,4,4,
6,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous pressure,,
solute aqueous conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
4,
250,yr,
500,yr,
750,yr,
1000,yr,
8,
Aqueous moisture content,,
Aqueous saturation,,
Aqueous relative permeability,,
Aqueous pressure,,
solute aqueous conc,Tc-99,1/L,
solute volumetric conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
#-----------------------------------------------
~Surface Flux Card
#-----------------------------------------------
6,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,214,214,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,7,7,
Aqueous Volumetric,L/day,L,West,113,113,1,1,1,6,
Solute Flux,Tc-99,1/day,,Top,1,140,1,1,7,7,
```

```
Solute Flux,Tc-99,1/day,,Top,81,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,West,113,113,1,1,1,6,
```

B.8 Base Input File with Finer Grid for 100-m Deep Waste

```
~Simulation Title Card
1,
Flow and Transport  2D model,
Dr. Mel Piepho,
Fluor Gov. Group,
April 12 2006,
10:00 AM PST,
2,
This problem represents a 2D model for flow & transport calcs
It covers a distance of 420 m or 1385 feet.
#-----------------------------------------------
~Solution Control Card
#-----------------------------------------------
Restart file,flow-2007-2p5cm.rst240yr,
# Normal,
Water w/transport,
1,
0,yr,40.0,yr,0.0001,yr,0.1,yr,1.15,16,1.e-6,
3000000,
# variable aqueous diffusion,
# variable gas diffusion,
1,
effective permeability,geometric,

~Grid Card
tilted cartesian,0,deg,0,deg,
140,1,276,
#
# X Grid
0.0,m,140@3.0,m,
#
# y Grid
0.0,m,1@1.0,m,
#
# Z Grid
-600,cm,6@100.0,cm,
70@10,cm,10@20,cm,190@50,cm,
#
~Rock/Soil Zonation Card
2,
Ringold-sat,1,140,1,1,1,6,
Hanford,1,140,1,1,7,276,
#
~Mechanical Properties Card
Ringold-sat,2740,kg/m^3,0.12,0.12,0,,Millington and Quirk,
Hanford,2600,kg/m^3,0.318,0.318,0,,Millington and Quirk,
#
~Hydraulic Properties Card
Ringold-sat,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,1.3E-01,hc:cm/s,
```

```
Hanford,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,1.090E-03,hc:cm/s,
#
~Saturation Function Card
Ringold-sat,Extended van Genuchten,0.0132,1/cm,1.753,0.077,,
Hanford,Extended van Genuchten,0.0415,1/cm,1.759,0.077,,
#
~Aqueous Relative Permeability Card
Ringold-sat,Mualem,,,,
Hanford,Mualem,,,,
#
#-----------------------------------------------
~Solute/Fluid Interaction Card
1,
Tc-99,Conventional,2.5E-5,cm^2/s,Continuous,1E20,yr,
0,
#
~Solute/Porous Media Interaction Card
Ringold-sat,0.1,m,0.01,m,
Tc-99,0,m^3/kg,1.0,
Hanford,0.02,m,0.002,m,
Tc-99,0,m^3/kg,1.0,
#
~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
3,
Aqueous Pressure overwrite,92360,Pa,,,,,,,41,80,1,1,47,77,
solute aqueous volumetric concentration overwrite,Tc-99,0.0,1/L,,,,,,,1,140,1,1,1,276,
solute aqueous volumetric concentration overwrite,Tc-99,1.0,1/L,,,,,,,41,80,1,1,47,77,  #~3 m thick,97.0 m to 100.0
m deep
#
~Boundary Conditions Card
#-----------------------------------------------
6,
top,Neumann Aqueous,Zero Flux,
1,80,1,1,276,276,2,
0,yr,-0.5,mm/yr,,,,,
42005,yr,-0.5,mm/yr,,,,,
top,Neumann Aqueous,Zero Flux,
81,140,1,1,276,276,2,
0,yr,-0.5,mm/yr,,,,,
42005,yr,-0.5,mm/yr,,,,,
west,neumann aqueous,Zero Flux,
1,1,1,1,1,6,1,
0,yr,0.02031,m/day,,,,,
west,Zero Flux,Zero Flux,
1,1,1,1,7,276,1,
0,yr,78000,Pa,,,,,
east,Hydraulic Gradient,Outflow,
140,140,1,1,1,6,1,
0,yr,151669,Pa,,,,,
east,Zero Flux,Zero Flux,
140,140,1,1,7,276,1,
0,yr,78000,Pa,,,,,
#-----------------------------------------------
#-----------------------------------------------
~Output Options Card
```

```
#-----------------------------------------
41,
60,1,276,
60,1,180,
60,1,170,
60,1,160,
60,1,150,
60,1,140,
60,1,130,
60,1,120,
60,1,100,
60,1,90,
60,1,80,
60,1,70,
60,1,60,
60,1,50,
60,1,40,
60,1,30,
60,1,25,
60,1,20,
60,1,15,
60,1,10,
60,1,9,
60,1,8,
60,1,7,
60,1,6,
60,1,5,
60,1,4,
60,1,3,
60,1,2,
60,1,1,
41,1,6,
51,1,6,
61,1,6,
71,1,6,
81,1,6,
113,1,7,
113,1,6,
113,1,5,
113,1,4,
113,1,3,
113,1,2,
113,1,1,
1,1,yr,cm,4,4,4,
6,
Aqueous moisture content,,
solute inventory,Tc-99,,
solute volumetric conc,Tc-99,1/L,
solute aqueous conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
1,
1000,yr,
8,
Aqueous moisture content,,
Aqueous saturation,,
```

```
Aqueous pressure,,
solute inventory,Tc-99,,
solute aqueous conc,Tc-99,1/L,
solute volumetric conc,Tc-99,1/L,
xnc aqueous vol,m/day,
znc aqueous vol,mm/yr,
#-----------------------------------------------
~Surface Flux Card
#-----------------------------------------------
6,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,276,276,
Aqueous Volumetric,m^3/yr,m^3,Top,1,140,1,1,7,7,
Aqueous Volumetric,L/day,L,West,113,113,1,1,1,6,
Solute Flux,Tc-99,1/day,,Top,1,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,Top,81,140,1,1,7,7,
Solute Flux,Tc-99,1/day,,West,113,113,1,1,1,6,
```

APPENDIX C - FINITE BARRIERS AND SOIL ANISTROPY

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C.1 INTRODUCTION

The effects of a finite barrier and soil anisotropy are analyzed. Anisotropic soil is characterized by unequal vertical and horizontal (the larger one) hydraulic conductivities, which potentially causes more horizontal spreading of underground waste, or, on the other hand, potentially causes more waste to converge towards its center if higher water fluxes are present in outer waste-free regions. Anisotropic soil properties are more important when the barrier is finite, with moisture infiltrating around the barrier edges and flowing underneath the barrier, causing a faster downward flow for more of the waste, transporting it faster to the aquifer, and increasing the contaminant concentration in the groundwater. The barrier overlap is the horizontal distance on each side of the underground waste zone that the barrier edge on top overhangs the waste zone. The waste zone is assumed to be centered under the barrier with equal barrier overlaps. In other words, the barrier overlap is the length of the barrier minus the length of the waste zone, divided by 2.

All assumptions and parameters in Section 2.0 were employed except the infinite barrier and isotropic soil assumptions. Groundwater contaminant concentration was calculated for both the low and high historical recharge values of 5 mm/yr and 25 mm/yr, respectively. It is assumed that there is no tilt to the barrier and no water runoff from the barrier beyond its edge. The natural recharge or water flux beyond the barrier edge is simply kept at the historical recharge value. Even though there is more potential water flux near the edge past the barrier, the natural recharge value beyond the edge was kept uniform at 5 or 25 mm/yr.

The anisotropic soil conductivities are simply modeled by increasing the horizontal conductivity by a factor of 10 and keeping the vertical conductivity the same (see Appendix A for vadose-zone soil properties). Use of a more elaborate anisotropic model, such as described in PNNL-15443 (*Vadose Zone Transport Field Study Summary Report*), is not considered here because this analysis is for a generic site. The simple 10-to-1 horizontal-to-vertical conductivity ratio is implemented and has been used many times in the past (e.g., *Vadose Zone Hydrogeology Data Package for the 2004 Composite Analysis*, PNNL-14702, Appendix C).

C.2 ISOTROPIC SOIL AND BARRIER OVERLAP RESULTS

The peak groundwater contaminant concentrations are shown in Figure C-1 for the historical recharge value of 5 mm/yr, and in Figure C-2 for the higher historical recharge value of 25 mm/yr. Table C-1 tabulates these effects. Calculations show that the extent of barrier overlap does not strongly affect groundwater contaminant concentrations for isotropic soils. Also, at waste depths less than 60 m (top half) and the 5-mm/yr recharge, the peak groundwater contaminant concentration is actually lower when the barrier edge coincides with the edge of the waste than for the infinite barrier. This results from the higher recharge at the barrier edge intersecting the edges of the waste, which moves that portion of the waste down faster than the middle part of the waste. Hence, this edge waste is removed earlier from the vadose zone than the middle (central) portion of the waste, causing a reduced peak concentration from the reduced waste source.

Figure C-1. Peak Groundwater Contaminant Concentration for Isotropic Soil and 5-mm/yr Recharge as a Function of Waste Depth and Barrier Overlap

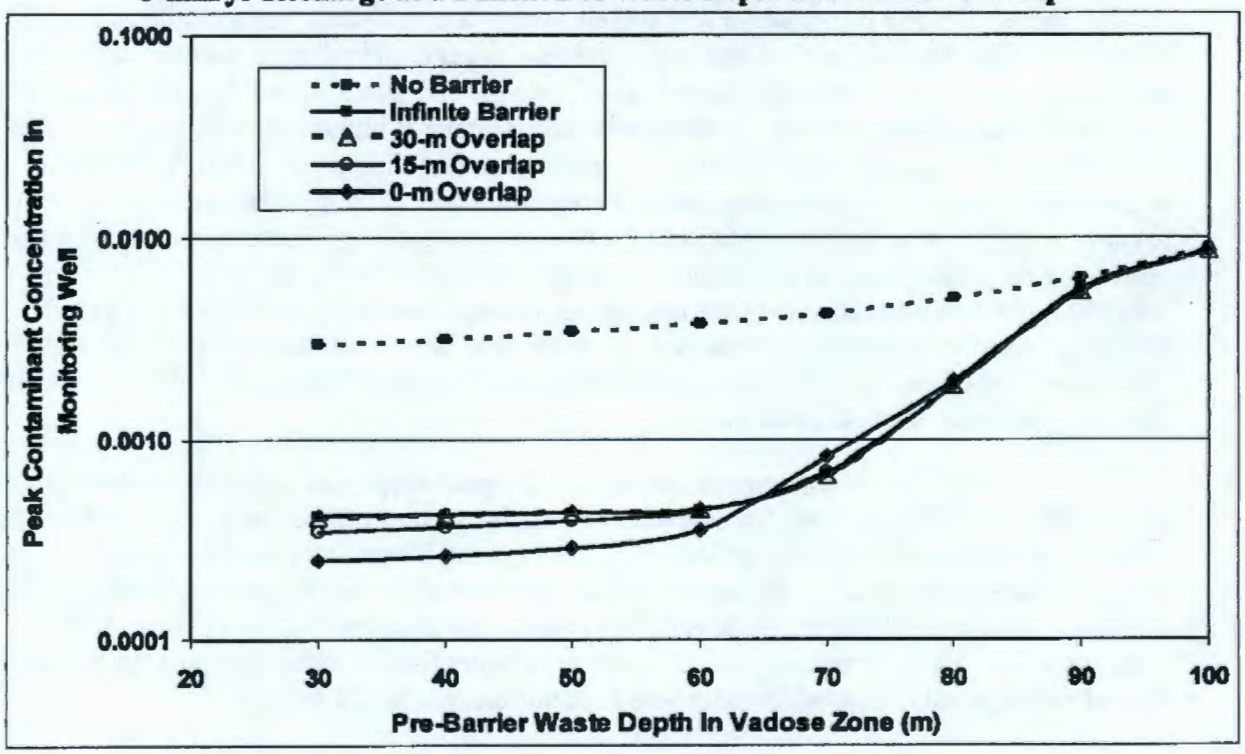


Figure C-2. Peak Groundwater Contaminant Concentration for Isotropic Soil and 25-mm/yr Recharge as a Function of Waste Depth and Barrier Overlap

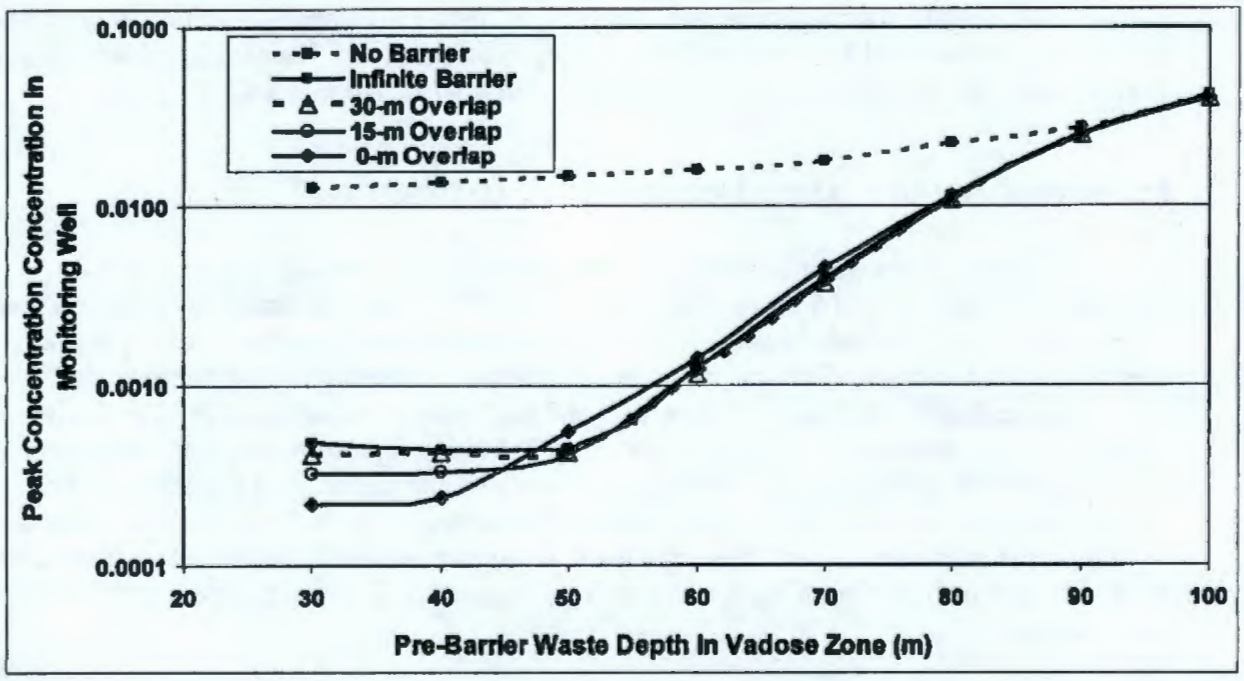


Figure C-1 and Table C-1 (for isotropic soil), show that for any barrier overlap, the peak contaminant concentration in the groundwater is close to the peak concentration with the infinite barrier with lower concentrations if the recharge is no more than 5 mm/yr.

Figure C-2 and Table C-1 indicate that groundwater peak contaminant concentration is only slightly raised for waste depths of 50 and 60 m (~26%, see Table C-1), high historical recharge and no barrier overlap, but is lowered for waste depths of 30 and 40 m. For the high recharge of 25 mm/yr and any barrier overlap, the peak concentrations are close to those with the infinite barrier and are lower for waste depths of 40 m or less (Figure C-2, for isotropic soil). Also, for very deep waste at depths of 80 m or more, there is no effect resulting from barrier overlap because of the large spatial region of antecedent water content located above the waste.

Figures C-1 and C-2 show that the effect of the barrier overlap is minor compared to the overall effect of the barrier.

Table C-1. Ratios of Peak Groundwater Contaminant Concentrations Associated with Finite Barrier Overlap to Those for the Infinite Barrier over Isotropic Soil

Waste Depth in 104-m Vadose Zone	[1]Concentration Ratios for 0-m Overlap		[1]Concentration Ratios for 15-m (50 ft) Overlap		[1]Concentration Ratios for 30-m (100 ft) Overlap	
[2]Isotropic	25 mm/yr	5 mm/yr	25 mm/yr	5 mm/yr	25 mm/yr	5 mm/yr
30 m	0.49	0.61	0.71	0.85	0.92	0.98
40 m	0.54	0.63	0.75	0.86	0.95	0.99
50 m	1.26	0.67	0.92	0.90	0.95	0.99
60 m	1.14	0.80	1.01	0.99	0.93	1.00
70 m	1.14	1.26	0.95	1.05	0.94	0.99
80 m	0.99	1.06	0.96	1.00	0.96	0.99
90 m	1.00	0.97	0.99	1.00	0.99	1.00
100 m	0.95	1.00	1.00	1.00	1.00	1.00

[1]Concentration Ratios are the peak groundwater concentration with finite barrier overlap divided by the peak concentration with infinite barrier.
[2]Vadose zone is isotropic;
Recharges are long-term historical recharges and future recharges beyond the edges of finite barriers; the finite and infinite barriers have an assumed recharge value of 0.5 mm/yr.

C.3 ANISOTROPIC SOIL AND BARRIER OVERLAP RESULTS

Peak groundwater contaminant concentrations are shown in Figures C-3 and C-4 for the 5-mm/yr and 25-mm/yr recharge values, and are summarized in Table C-2. Compared to isotropic soil, more barrier overlap is required for keeping the concentrations close to those realized with the infinite barrier. At low waste depths of 30 m or 40 m, and lower recharge, the peak groundwater contaminant concentration is lower for the 15-m overlap cases than those for

Figure C-3. Peak Groundwater Contaminant Concentration for Anisotropic Soil & 5-mm/yr Recharge as a Function of Waste Depth & Barrier Overlap

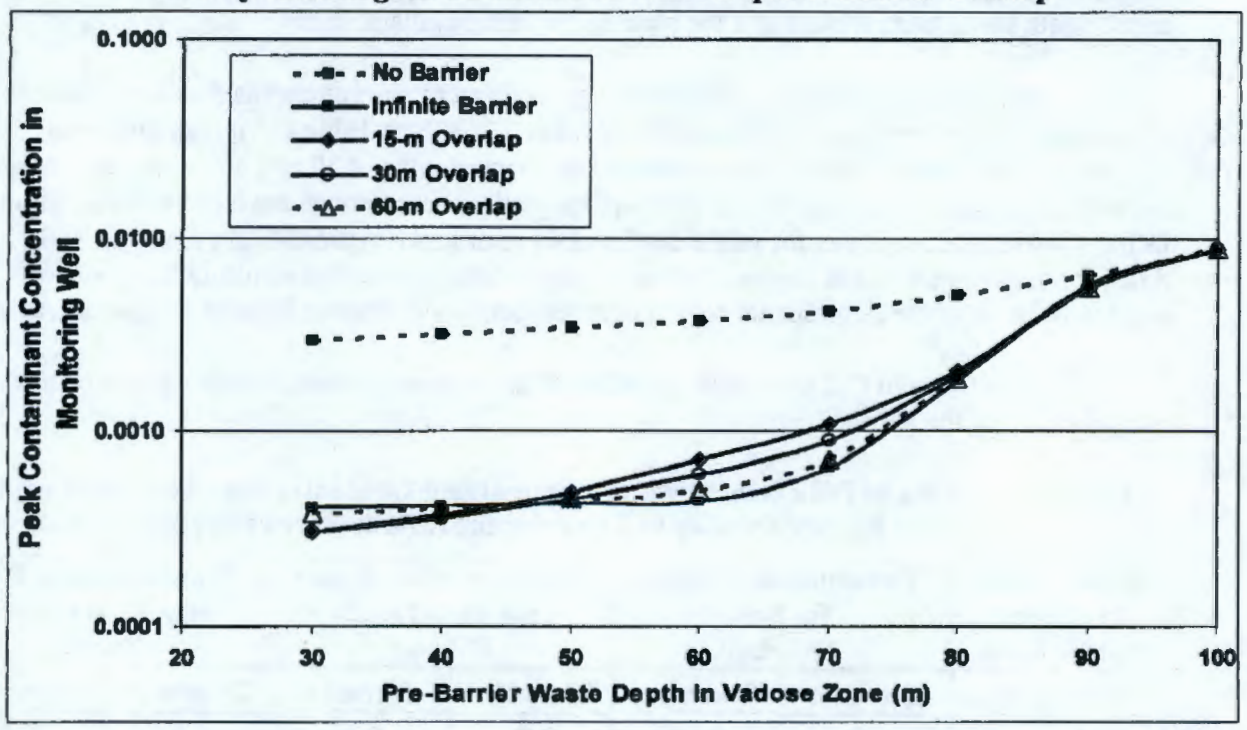
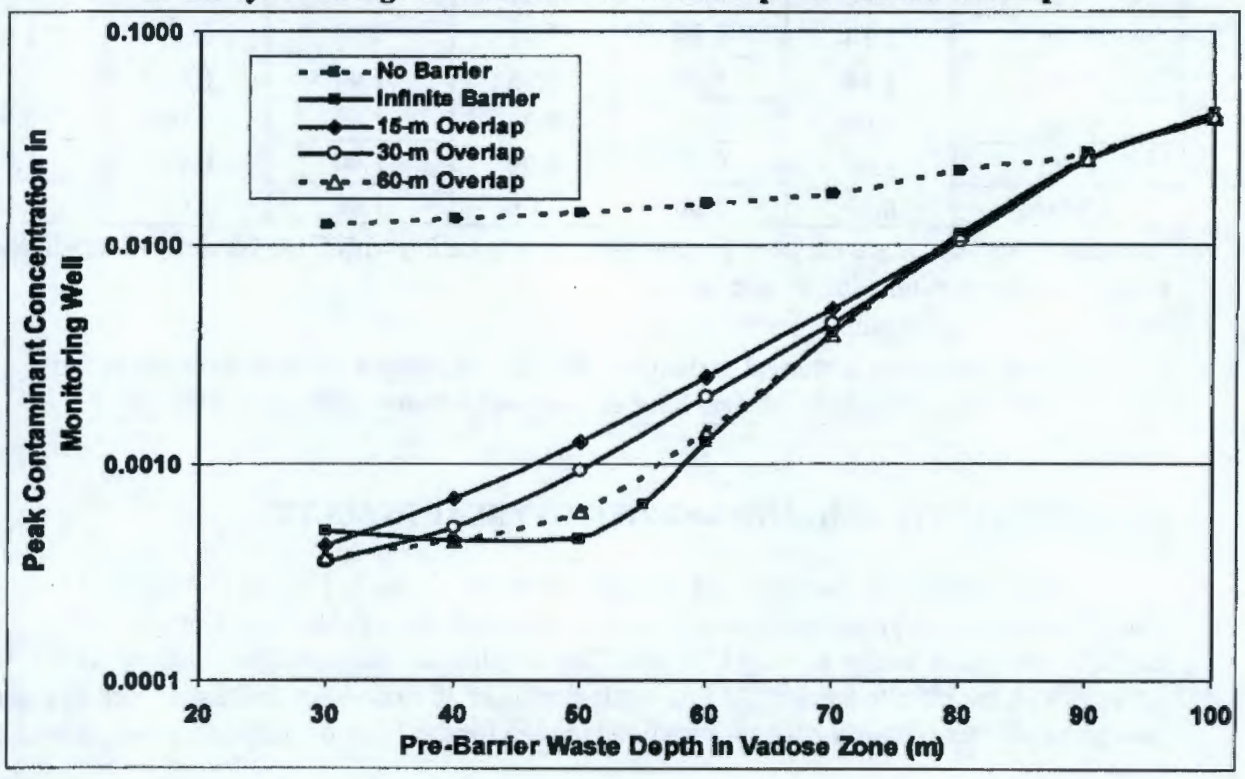


Figure C-4. Peak Groundwater Contaminant Concentration for Anisotropic Soil & 25-mm/yr Recharge as a Function of Waste Depth & Barrier Overlap



the infinite overlap cases. This is primarily because the natural recharge beyond the barrier edges causes a faster water flow near the edges of the waste, which moves that portion of the waste down faster than the middle or central portion of waste. This end waste is removed earlier from the vadose zone than the middle portion of the waste, causing a reduced peak concentration from the reduced waste source.

Table C-2 shows the peak groundwater contaminant concentration ratios of the finite barrier overlap cases to the infinite barrier cases. If the barrier overlap is 30 m (100 ft) or more, and the recharge is 5 mm/yr or less, then the peak groundwater contaminant concentration in the groundwater is close (within 39%) to the infinite barrier's peak concentration for all waste depths. For the high recharge of 25 mm/yr and a barrier overlap of 30 m (100 ft) or more, the peak concentration is close to that for the infinite barrier for waste depths other than 50 and 60 m, which have about a factor of 2 higher peak concentrations. Also, for very deep waste with a depth of 80 m or more, there is little difference caused by the barrier overlap, because there is 80 m or more of the vadose zone with antecedent moisture above the waste. For waste depths from 40 to 70 m in anisotropic soil, a 15-m barrier overlap causes higher peak concentrations than the infinite barrier and the 30-m barrier overlap.

Table C-2. Ratios of Peak Groundwater Contaminant Concentrations Associated with Finite Barrier Overlap to those for the Infinite Barrier Over Anisotropic Soil

Waste Depth in 104-m Vadose Zone	*Concentration Ratios for 15-m (50 ft) Overlap		*Concentration Ratios for 30-m (100 ft) Overlap		*Concentration Ratios for 60-m (200 ft) Overlap	
**Anisotropic	25 mm/yr	5 mm/yr	25 mm/yr	5 mm/yr	25 mm/yr	5 mm/yr
30 m	0.92	0.75	0.78	0.76	0.81	0.92
40 m	1.56	0.89	1.14	0.86	0.99	0.96
50 m	2.79	1.16	2.09	1.06	1.36	1.04
60 m	2.02	1.64	1.63	1.39	1.11	1.15
70 m	1.29	1.66	1.10	1.39	0.99	1.09
80 m	0.95	1.12	0.92	1.05	0.98	1.01
90 m	1.00	1.00	1.00	1.00	1.00	1.00
100 m	1.00	1.00	1.00	1.00	1.00	1.00

*Concentration Ratios are the peak groundwater concentration with finite barrier overlap divided by the peak concentration with infinite barrier.

**Vadose zone is isotropic;

Recharges are long-term historical recharges and future recharges past the edges of finite barriers; the finite and infinite barriers have an assumed recharge value of 0.5 mm/yr.

C.4 SUMMARY

The extent of barrier overlap is more important for anisotropic soil than for isotropic soil, and more important for high historical and future natural recharge than for lower historical and

future natural recharge. The natural recharge is the water infiltration rate past the edges of the barrier. It is suggested that a barrier overlap of 30 m (100 ft) may be sufficient for all waste depths, especially for those less than 50 m deep. On the other hand, an overlap of 15 m (50 ft) may not be sufficient for waste depths in the center part of vadose zone (50 to 60 m deep) unless the soil is more isotropic than anisotropic or the recharges are low.

C.5 REFERENCES

PNNL-14702, 2004, *Vadose Zone Hydrogeology Data Package for the 2004 Composite Analysis*, Rev. 0, Pacific Northwest National Laboratory, Richland, Washington.

PNNL-15443, 2006, *Vadose Zone Transport Field Study Summary Report*, Pacific Northwest National Laboratory, Richland, Washington.

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APPENDIX D - TIME RELATIONSHIP OF PEAK RECHARGE AND PEAK CONCENTRATION AT DIFFERENT LOCATIONS

D.1 INTRODUCTION

The recharge value peaks much earlier than the contaminant concentration in the groundwater. For the 100-m deep waste zone, the peak recharge at the 103-m depth peaks in only 0.55 year after barrier emplacement for the 25-mm/yr historical recharge, and in only 1.4 years for the 5-mm/yr historical recharge (see Figures 5 and 6). For the 100-m deep waste zone, the contaminant concentration at the monitoring well peaks in 20 years for the 25-mm/yr recharge and in 68.8 yeas for the 5-mm/yr recharge. For shallower waste zones, the differences between the time of peak recharge and peak concentration gets larger. This appendix gives some reasons for this phenomenon, focusing on the 100-m deep waste zone and the 25-mm/yr recharge.

D.2 COMPARISON OF PEAK CONCENTRATIONS AT DIFFERENT LOCATIONS

The peak recharge into the aquifer is caused by the enhanced moisture content in the waste zone. The peak concentration location for reporting purposes in this report has been at the down-gradient monitoring well with a 6-m averaging screen because the average concentration in the monitoring well is representative of drinking water from a well. Recall that all of the contaminant mass conservatively goes through the 6-m well screen. Peak concentrations at other locations in the vadose zone and aquifer are compared.

For comparative purposes, peak concentration locations, other than at the monitoring well, include the following:

1) the pore water of the vadose zone just above the aquifer (e.g., 103 m deep),

2) the top aquifer water below the middle of the waste zone, and

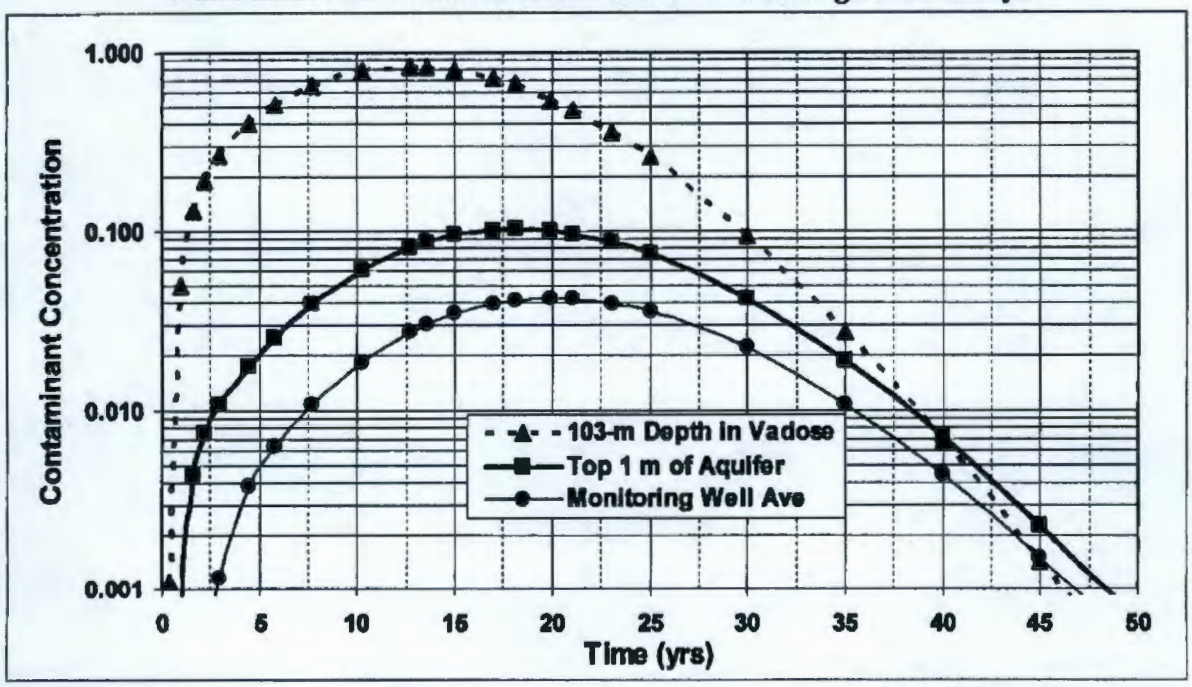
3) the top aquifer water below the outer edge of waste zone.

The contaminant concentration in the top part of the aquifer is larger than the average concentration over the 6-m aquifer thickness because the top-most contaminant concentration is the contaminant flux from the vadose zone as it enters the aquifer divided by the aquifer flow rate, and the well is averaged over the 6-m screen. The top part of the aquifer is 1 meter thick in the numerical model. The concentration is averaged over the 6-m aquifer depth at a down-gradient location by dividing the contaminant flux by the water flux at the location. Both contaminant flux and water flux are calculated by the computer code over time.

The time and magnitude of peak concentrations are compared at different locations for the 100-m deep waste zone and 25-mm/yr historical recharge. The recharge at 103 m (essentially the same at 104 m at top of aquifer) peaks very early at 0.55 year as shown in Figure 5 in Section 3.1.2. The extra moisture content (4 vol%) in the waste zone causes the large peak recharge at this early time. However, the peak concentration at the 103-m mark occurs later (12.5 years) than the peak recharge. The peak concentrations in the top of aquifer, below the middle and right outer edge of the waste zone, occur later, and the peak concentration at the monitoring well occurs the latest at 20 years. The time-dependent concentrations at the well

(averaged over 6-m well screen), vadose zone, and top part of the aquifer below the middle of the waste zone are shown in Figure D-1. Note that the peak concentrations occur much later than the peak recharge (Figure 5), which occurs at 0.55 yr. The peak recharge occurs much earlier than the peak concentration because much of the contaminant mass in the waste zone must move downward to cause a peak concentration. For example, about 45% of the contaminant mass has gone by the monitoring well before the peak concentration is reached there at 20 years. The contaminant mass at the 103-m mark at the time of peak recharge (0.55 year) is much smaller than when the peak concentration later occurs. This is because the contaminated water in the waste zone mixes with the clean water (recharge) entering the zone above and with the clean water located below the waste zone. As a result, the concentration is low at early times at 103-m, and only after much (e.g., ~45%) of the contaminant mass has mixed with the clean water below the waste zone, is a peak concentration finally reached.

Figure D-1. Contaminant Concentrations Over Time at Three Locations for 100-m Deep Waste Zone with a Barrier After Historical Recharge of 25 mm/yr



The peak concentration value at 103 m in the vadose zone is about 8 times higher than in the top aquifer below the middle of waste zone due to dilution from flowing aquifer water. The concentration in the top of the aquifer below the right (down-gradient) edge of waste zone (Figure 1) is the highest concentration in the aquifer, due to the horizontal continuation of infiltrating contaminants into the aquifer from the long waste zone. The infiltrating contaminants continue to join the contaminant mass in the top aquifer water as the water flows under the waste zone and its infiltrating contaminants. The peak concentration at the monitoring well is about 40% of the peak concentration in the top aquifer below the middle of the waste zone, due to averaging over the 6-m well screen. The peak concentration at the monitoring well is about the same at all aquifer locations down-gradient from the right edge of the waste zone because the contaminant mass moves downward in the aquifer 6-m thickness, but cannot escape below the aquifer. There is very little contamination spreading laterally in the vadose zone in the model,

such that very little contaminant flux enters the aquifer from beyond the waste zone side edges, causing the average concentration in the aquifer to not change after the groundwater flows by the bottom of the waste zone.

D.3 CONCLUSION

At the 103-m depth in the vadose zone, the recharge peaks much earlier than the peak concentration. This is mainly because the peak recharge value is caused by the enhanced moisture content in the waste zone, which quickly flows downward, despite the presence of the barrier. The peak concentrations at different locations occur much later because 45 to 50% of the contaminant mass in the waste zone has to pass by the location before a peak is observed. The peak recharge water is carrying less concentrated waste than in the waste zone because of the dilution of clean water above and below the waste zone.

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