ECF-200W-15-0056
Revision 0

Estimation of the Travel Time for Migration of Aroclor 1254 from Surface Soils to Groundwater at the 216-S-10 Pond and Ditch

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

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

P.O. Box 1600
Richland, Washington 99352

Approved for Public Release;
Further Dissemination Unlimited

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Terms

CERCLA	*Comprehensive Environmental Response, Compensation, and Liability Act of 1980*
DOE	U.S. Department of Energy
EIS	environmental impact statement
PCB	polychlorinated biphenyl
RCRA	*Resource Conservation and Recovery Act of 1976*
S-10	219-S-10 Pond and Ditch

1 Purpose

This calculation documentation describes an estimation of the travel time for Aroclor 1254 (a polychlorinated biphenyl [PCB]) to migrate from the near surface soil to groundwater at the 216-S-10 Pond and Ditch (S-10). The travel time was estimated using the first derivative of the 1-dimensional advective/dispersive equation for solute transport through a porous medium (Section 3). The calculation was performed at the screening level using input parameters mostly from DOE/RL-2011-50, *Regulatory Basis and Implementation of a Graded Approach to Evaluation of Groundwater Protection*, although other sources were used when necessary. The calculation was conservative in that input parameters were chosen that minimized the travel time estimate. The conservative nature of the result was confirmed by also estimating a travel time using more realistic input values (DOE/RL-2011-50). For comparison, a third travel time estimate was made using input values identified in U.S. Department of Energy (DOE) (2005), *Technical Guidance Document for Tank Closure Environmental Impact Statement Vadose Zone and Groundwater Revised Analyses.*

2 Background

Aroclor 1254 has been a required analyte for groundwater monitoring at S-10 under the *Resource Conservation and Recovery Act of 1976* (RCRA) (DOE/RL-2008-61, *Interim Status Groundwater Monitoring Plan for the 216-S-10 Pond and Ditch*). However, PCBs have a high distribution coefficient (*Kd*), so for all practical purposes, they are essentially immobile in the subsurface. During the *Comprehensive Environmental Response, Compensation, and Liability Act of 1980* (CERCLA) remedial investigation of S-10, Aroclor 1254 was found only in the near surface soils (DOE/RL-2004-17, *Remedial Investigation Report for the 200-CS-1 Chemical Sewer Group Operable Unit*). The travel time estimate herein will support the removal of this constituent from the S-10 monitoring program because it is expected that Aroclor 1254 would not reach groundwater for thousands of years.

3 Methodology

The travel time estimate is based on the advective-dispersive equation for solute transport through a porous medium. The particular equation used considers advection in 1-dimension and dispersion in 1-dimension (i.e., longitudinal dispersion along the flow direction) (Equation 3-15 in Hemond and Fechner, 1994, *Chemical Fate and Transport in the Environment*, modified to account for retardation [i.e., flow velocity and the dispersion coefficient are divided by the retardation factor] and flow though the vadose zone [i.e., moisture content was used in place of porosity]):

$$C(x,t) = \frac{1}{\theta}\left(\frac{1}{4\pi D_x^* t}\right)^{1/2} e^{\left[-\frac{(x-u^*t)^2}{4D_x^* t}\right]} \qquad \text{Equation 1}$$

where

C = solute concentration for an instantaneous release of a unit mass from a unit area source (M/L^3)

θ = volumetric moisture content (fraction)

D_x^* = dispersion coefficient in the x-direction divided by the retardation factor (R_f) (L^2/T)

t = time (T)

x = travel distance (L)

u^* = average linear velocity divided by the retardation factor (R_f) (i.e., the contaminant migration velocity) (L/T)

For the vadose zone, the retardation factor is given by (Equation 3-22b in Hemond and Fechner [1994] modified for the vadose zone [i.e., moisture content was used in place of porosity]):

$$R_f = 1 + \frac{B_d}{\theta} K_d \qquad \text{Equation 2}$$

where

R_f = the retardation factor (i.e., ratio of the fluid migration rate to contaminant migration rate) (unitless)

β_d = bulk density (M/L^3)

θ = volumetric moisture content (fraction)

K_d = contaminant distribution coefficient (i.e., ratio of the sorbed concentration to the aqueous concentration) (L^3/M)

The dispersion coefficient is given by (Equation 3-14 in Hemond and Fechner [1994], modified by adding molecular diffusion):

$$D_x = \alpha u + D_{mol} \qquad \text{Equation 3}$$

where

α = dispersivity (L)

u = average linear velocity (L/T)

D_{mol} = molecular diffusion (L^2/T)

The time to the peak concentration can be found by taking the first derivative of Equation 1, setting it equal to zero, and solving for time (see Appendix A for derivation):

$$t_p = \frac{-D_x^* + \sqrt{(D_x^*)^2 + (u^*)^2 x^2}}{(u^*)^2} \qquad \text{Equation 4}$$

where

t_p = time to the peak concentration (T)

To use Equation 4, the average linear velocity is needed. For the vadose zone, the average linear velocity depends on the hydraulic conductivity, moisture content, and hydraulic gradient, as follows (Hemond and Fechner, 1994, Equations 3-2 and 3-4 modified for the vadose zone):

$$u = \frac{K(\theta) \cdot i}{\theta} \qquad \text{Equation 5}$$

where

$K(\theta)$ = unsaturated hydraulic conductivity (L/T)

i = hydraulic gradient (L/L)

As Equation 5 shows, hydraulic conductivity in the vadose zone is a function of moisture content. For screening level applications, vertical flow in the vadose zone can be assumed to occur under a unit hydraulic gradient (i.e., $i = 1$). In this case, the hydraulic conductivity is equal to the infiltration rate which represents the Darcy velocity (also known as seepage velocity or specific discharge) through the vadose zone. Thus, the moisture content can be calculated from the infiltration rate. The saturated and unsaturated hydraulic conductivity can be related by an empirical equation (Hillel, 1980, *Fundamentals of Soil Physics*):

$$K(\theta) = K_s \left(\frac{\theta}{n}\right)^{2b+3} \qquad \text{Equation 6}$$

where

K_s = saturated hydraulic conductivity (L/T)

n = porosity (unitless)

b = soil type coefficient (unitless)

Solving Equation 6 for moisture content yields (see Appendix A):

$$\theta = n \cdot \left(\frac{K(\theta)}{K_s}\right)^{\frac{1}{2b+3}} \qquad \text{Equation 7}$$

When applying Equation 7, if the calculated moisture content is less than field capacity, it is set equal to field capacity which represents the minimum moisture content at which flow by gravity drainage will occur.

4 Assumptions and Inputs

Equation 4 was used to calculate the travel time through the vadose zone for Aroclor 1254. Table 1 lists the input parameter values used in the calculations. Many of the hydrogeologic parameter values were taken from DOE/RL-2011-50, which lists screening level model input parameters for various environmental settings at Hanford. Hydrogeologic parameter values for the S Pond setting are given for 6 vadose zone layers in DOE/RL-2011-50, and minimum, maximum, and mean values are provided for each layer. The values chosen for the conservative travel time calculation are the ones that minimize the travel time regardless of which vadose zone layer they apply to. For the best estimate travel time, values chosen were the average of the mean values for all the layers.

Table 1. Input Parameter Values for the Travel Time Calculation

Parameter	Conservative Value	Best Value	Comment
Soil type coefficient (b)	4.05	4.05	PNL-10550, *Environmental Settings for Selected U.S. Department of Energy Installations – Support Information for the Programmatic Environmental Impact Statement and the Baseline Environmental Management Report*, Table 5.6 (200 West Environmental Setting). Value is for the Hanford formation; value for Ringold Unit E is not much different (4.38). Note: PNL-10550 was used to obtain this parameter because the soil type coefficient is not an input parameter listed in DOE/RL-2011-50.

Table 1. Input Parameter Values for the Travel Time Calculation

Parameter	Conservative Value	Best Value	Comment
Bulk density (β_d)	1.28 g/cm^3	1.74 g/cm^3	Conservative value is the lowest bulk density given in Table 4-4 of DOE/RL-2011-50 for the sedimentary layers beneath the 200 West Area S Pond setting; best value is the average of the mean values in DOE/RL-2011-50 for the same layers
Total porosity (n)	0.056	0.31	Conservative value is the lowest saturated moisture content given in Table 4-4 of DOE/RL-2011-50 for the sedimentary layers beneath the 200 West Area S Pond setting; best value is the average of the mean values in DOE/RL-2011-50 for the same layers
Field capacity*	0.072	0.041	Conservative value is the highest mean residual moisture content given in Table 4-4 of DOE/RL-2011-50 for the sedimentary layers beneath the 200 West Area S Pond setting; best value is the average of the mean values in DOE/RL-2011-50 for the same layers
Saturated hydraulic conductivity (K_s)	118 m/day	0.303 m/day	Conservative value is the highest saturated hydraulic conductivity given in Table 4-5 of DOE/RL-2011-50 for the sedimentary layers beneath the 200 West Area S Pond setting; best value is the average of the mean values in DOE/RL-2011-50 for the same layers
Infiltration rate ($K[\theta]$)	0.111 m/yr	0.047 m/yr	Conservative value is the highest infiltration rate given in Table 4-7 of DOE/RL-2011-50, which lists representative recharge rates for unvegetated or cheatgrass vegetated disturbed sites at Hanford; best value is the average of all the values in Table 4-7 of DOE/RL-2011-50 (excluding the values for pre-Hanford conditions and values identified for the tank closure EIS)
Travel distance (x)	65 m	65 m	Depth to water from the land surface at 299-W26-13 located at the 216-S-10 Pond
Dispersivity (α)	0.65 m	0.65 m	Value is 1/100th the travel distance following guidance in EPA/600/6-85/002b, *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Water – Part II (Revised 1985)*
Molecular diffusion (D_{mol})	190 cm^2/yr	190 cm^2/yr	Maximum value in Duursma (1966) as referenced by EPA/600/6-85/002b (1×10^{-6} cm^2/second * 31,557,600 seconds/yr)
Distribution coefficient (K_d)	75.6 mL/g	270 mL/g	Source is addressed in the text following this table

* The minimum moisture content at which flow in the vadose zone will occur by gravity drainage.

EIS = environmental impact statment

There were many options for determining the distribution coefficient (K_d). A common approach is to multiply the carbon-matter partition coefficient for the compound by the fraction of organic matter in the sediments (Equation 3-24 in Hemond and Fechner [1994]):

$$K_d = K_{oc} \cdot f_{oc} \qquad \text{Equation 7}$$

where

K_{oc} = carbon-matter partition coefficient (mL/g)

f_{oc} = fraction of organic matter (unitless)

The K_d value used for the baseline risk assessment for the 216-S-10 remedial investigation was 309 mL/g[1] (Table 4-10 on page 4-112 of DOE/RL-2004-17). This was calculated from the above equation using an estimate of the carbon-matter partition coefficient and 0.001 as the fraction of organic matter. A slightly more conservative result is obtained using the average K_{oc} for three PCBs measured by Chiou et al. (1977, *Partition Coefficient and Bioaccumulation of Selected Organic Chemicals*) of $10^{6.36}$ mL/g and an organic matter fraction of 10^{-4} (page 203 of Hemond and Fechner [1994]), which yields a K_d of 230 mL/g. The value used for the updated baseline risk assessment in the CERCLA feasibility study for 216-S-10 was 75.6 mL/g (Table G-1 on page G-1 of DOE/RL-2005-63, *Feasibility Study for the 200-CS-1 Chemical Sewer Group Operable Unit*). The source was described in DOE/RL-2005-63 as the Oak Ridge National Laboratory, but a specific citation was not provided. A value 170,000 mL/g is provided in DOE (2005) for the tank closure environmental impact statement (EIS). Of these values, the lowest is 75.6 mL/g, which was used for the conservative travel time estimate. The value used for the best estimate was 270 mL/g, which is the average of 230 and 309 mL/g (i.e., average of the four values given above excluding the low and high values).

For comparison to the travel time estimates using the conservative and best values in Table 1, a travel time estimate was made consistent with guidance in DOE (2005) for the tank closure EIS. For this estimate, the input values were the same as the best values in Table 1 except the K_d was 170,000 mL/g (the value for PCBs) and the infiltration rate was 0.050 m/yr (the value for a bare sandy surface in the operational era), as recommended in DOE (2005).

The key assumption in this calculation is that moisture flow in the vadose zone occurs under a unit hydraulic gradient. Thus, the hydraulic conductivity as a function of moisture content ($K[\theta]$) is assumed to be equal to the infiltration rate. This allows the moisture content to be calculated directly from the infiltration rate using Equation 6.

5 Software Applications

Microsoft Excel[2] was used to perform the travel time calculation. Excel was used as a desktop calculator and, therefore, is exempt from controlled software management procedures.

6 Calculations

The spreadsheets used for the travel time calculations are documented in Appendix A.

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[1] It should be noted that the source documents, DOE/RL-2004-17 and DOE/RL-2005-63, lists units of L/kg for K_d, but these are numerically equivalent to mL/g.

[2] The Microsoft® products identified in this calculation are either registered trademarks or trademarks of Microsoft Corporation in the United States and/or in other countries.

7 Results

The calculated moisture content for the conservative case was less than field capacity, so it was set equal to the field capacity (0.072). For the best estimate case, the calculated moisture content was 0.15. For comparison, Figure 1 shows the neutron moisture log for well 299-W26-13 drilled in 1999 and located adjacent to the 216-S-10 and 216-S-11 Ponds. The log indicates that moisture contents range from approximately 3% for the Hanford formation, 8-9% for the Cold Creek Unit, and 5-7% for the Ringold E. These values are more similar to the conservative case than the best estimate case. This is assumed to be due to the method used to calculate the moisture content, which is a simplification and does not consider all of the processes acting in the subsurface that affect moisture content. When the moisture content was set directly equal to a value more consistent with the moisture log at 299-W26-13, i.e., 0.09, the travel time changed by less than one percent. Although decreasing the moisture content increased the average linear velocity, this was offset by an increase in the retardation factor. Thus, moisture content is not a sensitive parameter in the travel time calculation.

The retardation factor for the conservative case was 1,345 indicating that Aroclor 1254 would migrate 1,345 times slower than the natural movement of moisture in the vadose zone. For the best estimate case, the retardation factor was 3,051. The average linear velocities were 1.54 m/yr for the conservative case and 0.31 m/yr for the best estimate case, however the contaminant migration velocities were much lower at 1.1×10^{-3} m/yr and 1.0×10^{-4} m/yr, respectively. The travel time for Aroclor 1254 to groundwater was 56,000 years for the conservative case (a migration rate of 1.2 meters per thousand years) and 643,000 years for the best estimate case (a migration rate of 0.1 meters per thousand years). This demonstrates the conservative nature of the 56,000 year travel time estimate. The travel time using the tank closure EIS values for distribution coefficient and infiltration rate was substantially longer at 380 million years (a migration rate of 0.2 millimeters per thousand years). This was due to the very high distribution coefficient for this case (170,000 mL/g which yielded a retardation factor of 1.9 million).

The 56,000 year travel time calculated for the conservative case is a lower bound. The actual travel time is expected to be longer as shown by the much higher result for the best estimate case (643,000 years). These calculations demonstrate that for all practical purposes Aroclor 1254 is not mobile in the subsurface so this constituent can be removed from the 216-S-10 Pond and Ditch RCRA groundwater monitoring program because it will not migrate from the surface soils to groundwater within any reasonable timeframe.

Neutron-Neutron Moisture Survey

Waste Management Technical Services

Project: S-Pond
Borehole: 299-W26-13

Log Date : December 10, 1999
Depth Datum: Ground Level

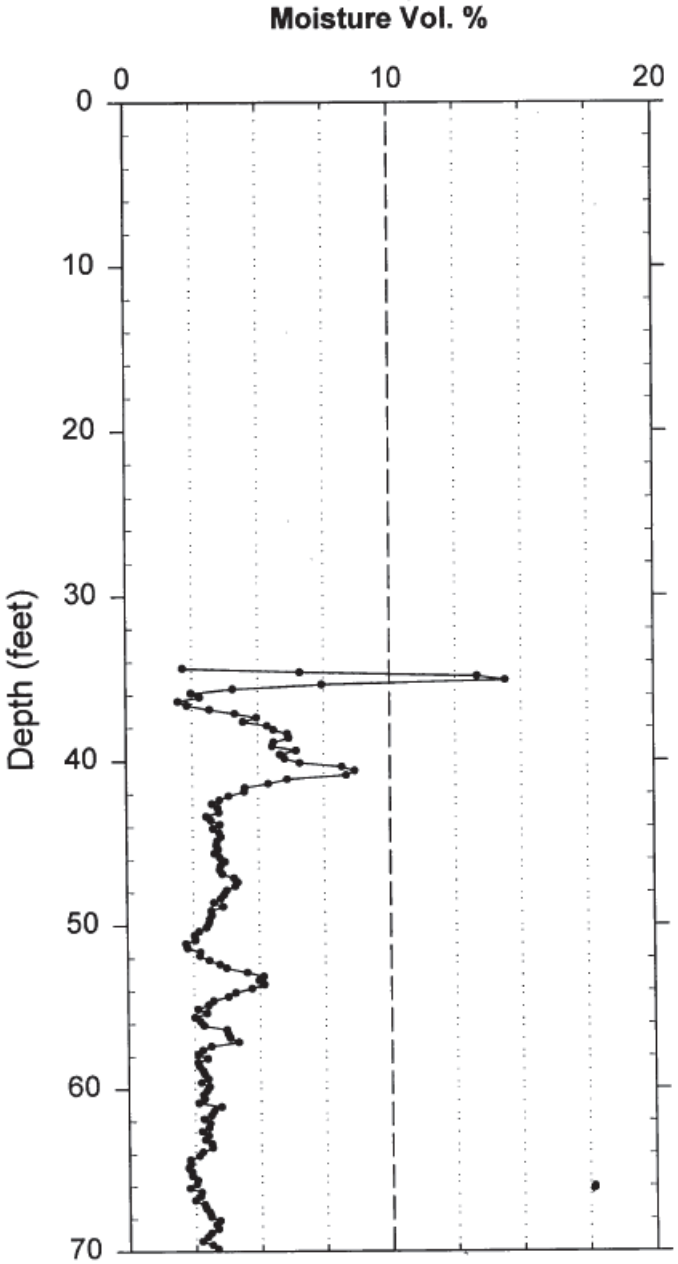

Figure 1. Neutron Moisture Log for 299-W26-13 (3 sheets)

Neutron-Neutron Moisture Survey

Waste Management Technical Services

Project: S-Pond
Borehole: 299-W26-13

Log Date : December 10, 1999
Depth Datum: Ground Level

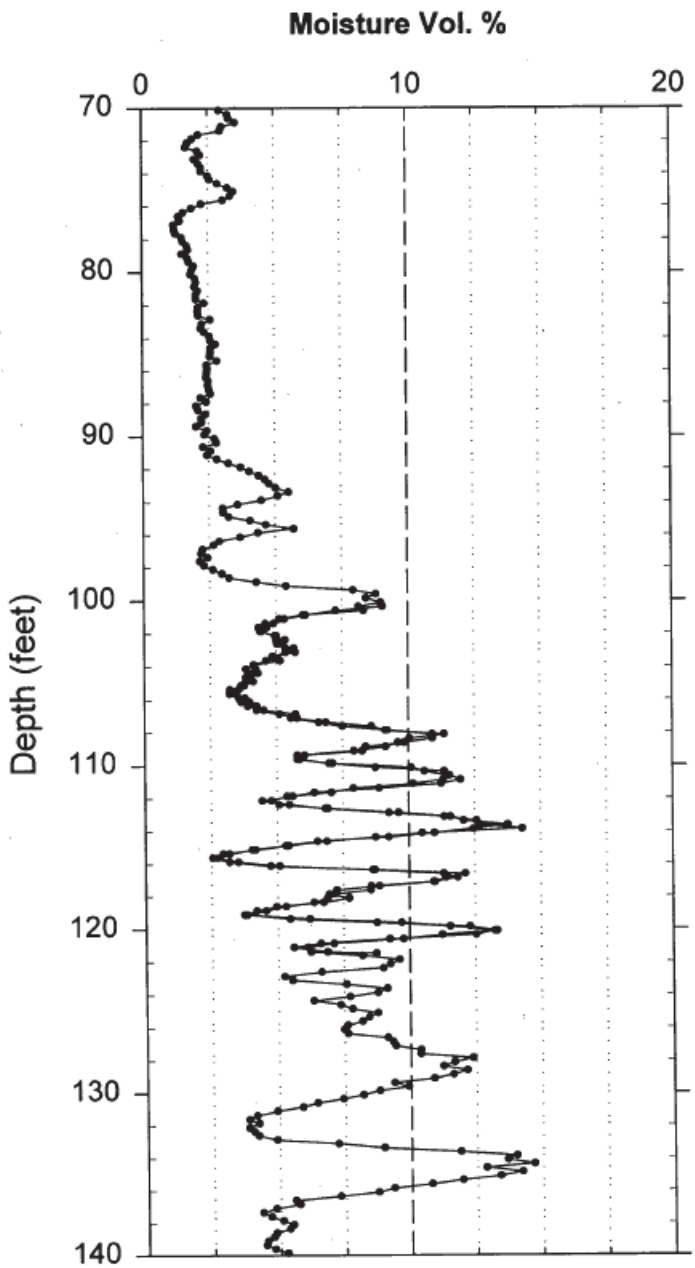

Figure 1. Neutron Moisture Log for 299-W26-13 (3 sheets)

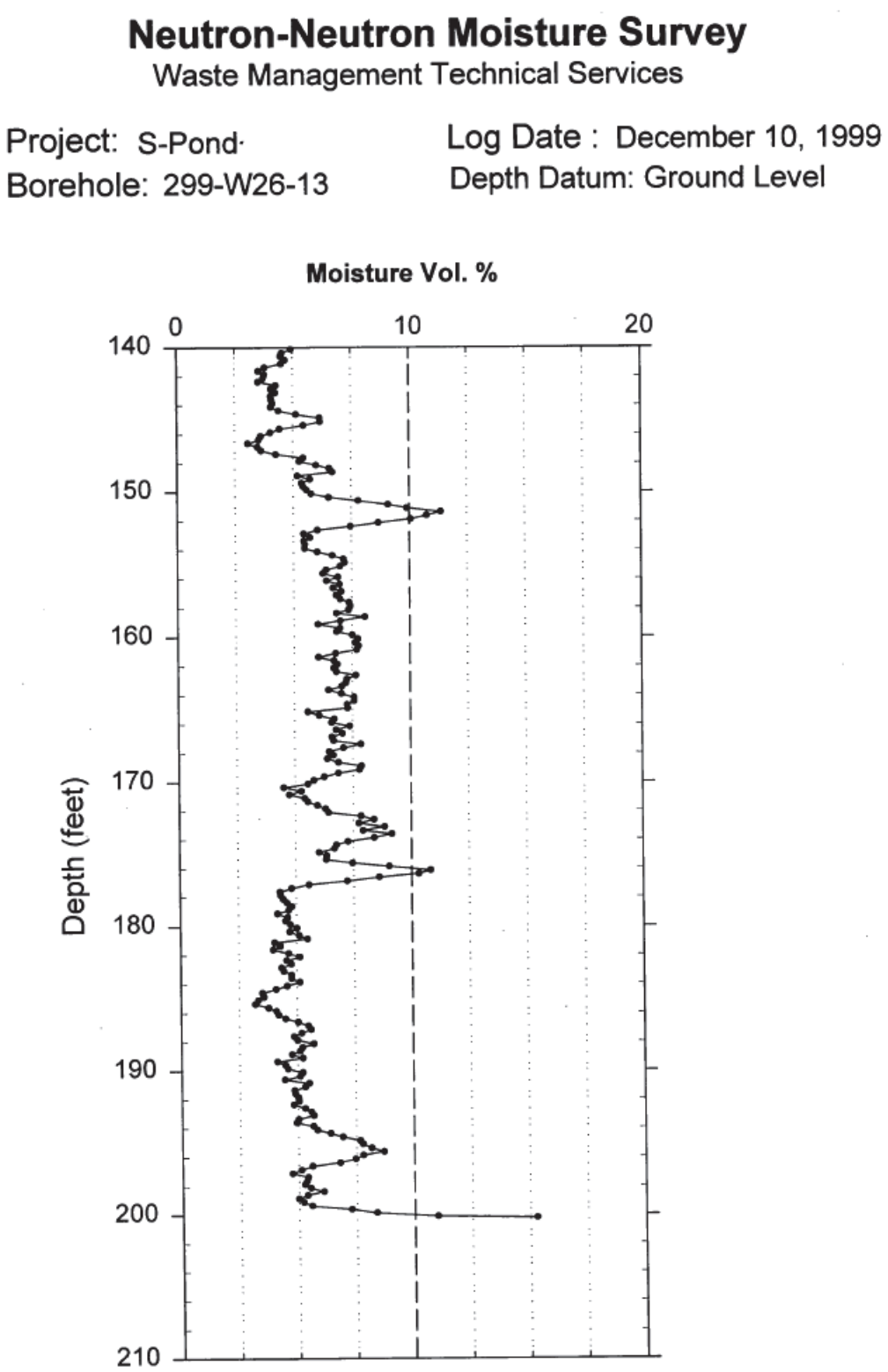

Figure 1. Neutron Moisture Log for 299-W26-13 (3 sheets)

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Appendix A

Travel Time Calculation Spreadsheets and Equation Derivations

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This appendix presents the spreadsheets used to calculate the travel time for Aroclor 1254 from surface soils to groundwater at the 216-S-10 Pond and Ditch. The spreadsheets use named cells instead of cell addresses to refer to specific cells. The cell names used are the variable names in the equations of the main text. The names and the corresponding cell references are shown in Table A-1.

Each spreadsheet consists of 3 sections: input data, computed data, and the calculation result. The input data section is where the input data listed in Table 1 of the main text are entered into the spreadsheet. The computed data section contains intermediate calculation results for moisture content, retardation factor, longitudinal dispersion, longitudinal dispersion divided by the retardation factor, average linear velocity, and average linear velocity divided by the retardation factor. The result section is where the travel time is calculated. Figure A-1 shows the spreadsheet displaying the formulas entered into each cell. Figures A-2 through A-4 show the spreadsheets with the data and calculation results for the conservative travel time estimate, the best estimate, and the travel time calculated with the tank closure EIS infiltration rate and distribution coefficient for PCB, respectively.

This appendix also provides the derivation of the time to peak equation (Equation 4 of the main text) from the advective-dispersive equation (Equation 1 of the main text) (Figure A-5), and it shows how Equation 6 of the main text is solved for moisture content (Equation 7 of the main text) (Figure A-6). At the peak concentration on the breakthrough curve, the first derivative of the advective-dispersive equation is equal to zero. Thus, the time to peak equation is derived by taking the first derivative of the advective-dispersive equation, then setting it equal to zero and solving for time.

Table A-1. List of Named Cells in the Travel Time Spreadsheets

Name	Cell Reference
alpha	C13
b	C8
Bd	C7
Dmol	C15
Dx	C21
Dx_star	C22
fc	C10
K_theta	C12
Kd	C6
Ksat	C11
n	C9
Rf	C20
theta	C19
u	C23
u_star	C24
x	C14

	A	B	C	D	E
1	**Travel Time Equation (1-Dimensional Advection, 1-Dimensional Dispersion)**				
2	Conservative Travel Time Estimate				
3					
4		**Input Data**			
5					
6		Contaminant Distribution Coefficient [Kd]:	75.6	mL/g	
7		Bulk Density [Bd]:	1.28	g/cm^3	
8		Soil Type Coefficient [b]:	4.05	unitless	
9		Porosity [n]:	0.056	fraction	
10		Field Capacity [fc]:	0.072	fraction	
11		Saturated Hydraulic Conductivity [Ksat]:	118	m/day	
12		Infiltration Rate [K_theta]:	0.111	m/yr	
13		Longitudinal Dispersivity [alpha]:	0.65	m	
14		Travel Distance [x]:	65	m	
15		Molecular Diffusion [Dmol]:	190	cm^2/yr	
16					
17		**Computed Data**			
18					
19		Volumetric Moisture Content [theta]:	=IF(n*((K_theta/(Ksat*365.25))^(1/(2*b+3)))<fc,fc,n*((K_theta/(Ksat*365.25))^(1/(2*b+3))))	fraction	Equation 6
20		Retardation Factor [Rf]:	=1+Bd/theta*Kd	unitless	Equation 2
21		Longitudinal Dispersion Coefficient [Dx]:	=alpha*u+Dmol/(100^2)	m^2/yr	Equation 3
22		Longitudinal Dispersion Coefficient Divided by Rf [Dx_star]:	=Dx/Rf	m^2/yr	
23		Average Linear Velocity [u]:	=K_theta/theta	m/yr	Equation 5
24		Average Linear Velocity Divided by Rf [u_star]:	=u/Rf	m/yr	
25					
26		**Result**			
27					
28		Time to the Peak Concentration:	=((-1)*Dx_star+SQRT(Dx_star^2+(u_star^2)*(x^2)))/(u_star^2)	yrs	Equation 4

Figure A-1. Travel Time Spreadsheet with Formulas Displayed

	A	B	C	D	E
1	**Travel Time Equation (1-Dimensional Advection, 1-Dimensional Dispersion)**				
2	Conservative Travel Time Estimate				
3					
4		**Input Data**			
5					
6		Contaminant Distribution Coefficient [Kd]:	75.6	mL/g	
7		Bulk Density [Bd]:	1.28	g/cm^3	
8		Soil Type Coefficient [b]:	4.05	unitless	
9		Porosity [n]:	0.056	fraction	
10		Field Capacity [fc]:	0.072	fraction	
11		Saturated Hydraulic Conductivity [Ksat]:	118	m/day	
12		Infiltration Rate [K_theta]:	0.111	m/yr	
13		Longitudinal Dispersivity [alpha]:	0.65	m	
14		Travel Distance [x]:	65	m	
15		Molecular Diffusion [Dmol]:	190	cm^2/yr	
16					
17		**Computed Data**			
18					
19		Volumetric Moisture Content [theta]:	0.072	fraction	Equation 7
20		Retardation Factor [Rf]:	1345	unitless	Equation 2
21		Longitudinal Dispersion Coefficient [Dx]:	1.021083333	m^2/yr	Equation 3
22		Longitudinal Dispersion Coefficient Divided by Rf [Dx_star]:	0.00075917	m^2/yr	
23		Average Linear Velocity [u]:	1.541666667	m/yr	Equation 5
24		Average Linear Velocity Divided by Rf [u_star]:	0.001146221	m/yr	
25					
26		**Result**			
27					
28		Time to the Peak Concentration:	56133.21876	yrs	Equation 4

Figure A-2. Travel Time Spreadsheet for the Conservative Estimate

	A	B	C	D	E
1	**Travel Time Equation (1-Dimensional Advection, 1-Dimensional Dispersion)**				
2	Best Travel Time Estimate				
3					
4		**Input Data**			
5					
6		Contaminant Distribution Coefficient [Kd]:	270	mL/g	
7		Bulk Density [Bd]:	1.74	g/cm^3	
8		Soil Type Coefficient [b]:	4.05	unitless	
9		Porosity [n]:	0.31	fraction	
10		Field Capacity [fc]:	0.041	fraction	
11		Saturated Hydraulic Conductivity [Ksat]:	0.303	m/day	
12		Infiltration Rate [K_theta]:	0.047	m/yr	
13		Longitudinal Dispersivity [alpha]:	0.65	m	
14		Travel Distance [x]:	65	m	
15		Molecular Diffusion [Dmol]:	190	cm^2/yr	
16					
17		**Computed Data**			
18					
19		Volumetric Moisture Content [theta]:	0.154022357	fraction	Equation 7
20		Retardation Factor [Rf]:	3051.206527	unitless	Equation 2
21		Longitudinal Dispersion Coefficient [Dx]:	0.217347828	m^2/yr	Equation 3
22		Longitudinal Dispersion Coefficient Divided by Rf [Dx_star]:	7.12334E-05	m^2/yr	
23		Average Linear Velocity [u]:	0.305150504	m/yr	Equation 5
24		Average Linear Velocity Divided by Rf [u_star]:	0.00010001	m/yr	
25					
26		**Result**			
27					
28		Time to the Peak Concentration:	642853.4868	yrs	Equation 4

Figure A-3. Travel Time Spreadsheet for the Best Estimate

	A	B	C	D	E
1	**Travel Time Equation (1-Dimensional Advection, 1-Dimensional Dispersion)**				
2	Travel Time Estimate with Tank Closure EIS Values for Distribution Coefficieint and Infiltration Rate				
3					
4		**Input Data**			
5					
6		Contaminant Distribution Coefficient [Kd]:	170000	mL/g	
7		Bulk Density [Bd]:	1.74	g/cm^3	
8		Soil Type Coefficient [b]:	4.05	unitless	
9		Porosity [n]:	0.31	fraction	
10		Field Capacity [fc]:	0.041	fraction	
11		Saturated Hydraulic Conductivity [Ksat]:	0.303	m/day	
12		Infiltration Rate [K_theta]:	0.05	m/yr	
13		Longitudinal Dispersivity [alpha]:	0.65	m	
14		Travel Distance [x]:	65	m	
15		Molecular Diffusion [Dmol]:	190	cm^2/yr	
16					
17		**Computed Data**			
18					
19		Volumetric Moisture Content [theta]:	0.154883331	fraction	Equation 7
20		Retardation Factor [Rf]:	1909825.627	unitless	Equation 2
21		Longitudinal Dispersion Coefficient [Dx]:	0.228835363	m^2/yr	Equation 3
22		Longitudinal Dispersion Coefficient Divided by Rf [Dx_star]:	1.1982E-07	m^2/yr	
23		Average Linear Velocity [u]:	0.322823635	m/yr	Equation 5
24		Average Linear Velocity Divided by Rf [u_star]:	1.69033E-07	m/yr	
25					
26		**Result**			
27					
28		Time to the Peak Concentration:	380369474.9	yrs	Equation 4

Figure A-4. Travel Time Spreadsheet with the Distribution Coefficient and Infiltration Rate for the Tank Closure EIS

CH2MHILL SUBJECT Derivation of the time to peak equation (with dispersion) BY J P McDonald SHEET NO. 1 of 3 DATE 2/25/2016 PROJECT NO.

1-D Advective / Dispersive Equation (Equation 3-15 in Hemond and Fechner (1994) for a unit mass):

$$c = \frac{1}{\theta\sqrt{4\pi D t}} \cdot e^{\frac{-(x-ut)^2}{4Dt}}$$

$$\frac{dc}{dt} = \frac{d}{dt}\left[\frac{1}{\theta\sqrt{4\pi D t}}\right] e^{\frac{-(x-ut)^2}{4Dt}} + \frac{1}{\theta\sqrt{4\pi D t}} \frac{d}{dt}\left[e^{\frac{-(x-ut)^2}{4Dt}}\right]$$

$$\frac{d}{dt}\frac{1}{\theta\sqrt{4\pi D t}} = \frac{1}{\theta} \cdot \frac{d}{dt}(4\pi D t)^{-1/2}$$

$$= \frac{1}{\theta}\left(-\frac{1}{2}\right)(4\pi D t)^{-3/2} \cdot 4\pi D$$

$$= \left(-\frac{1}{2\theta}\right)(4\pi D)\left[\frac{1}{(4\pi D t)^3}\right]^{1/2}$$

$$= \left(-\frac{1}{2\theta}\right)\left[\frac{(4\pi D)^2}{(4\pi D)^3 t^3}\right]^{1/2}$$

$$= -\frac{1}{2\theta} \cdot \left[\frac{1}{4\pi D t^3}\right]^{1/2}$$

$$= -\frac{1}{2\theta t\sqrt{4\pi D t}}$$

$$\frac{d}{dt} e^{\frac{-(x-ut)^2}{4Dt}} = e^{\frac{-(x-ut)^2}{4Dt}} \cdot \frac{d}{dt}\frac{-(x-ut)^2}{4Dt}$$

$$\frac{d}{dt}\frac{-(x-ut)^2}{4Dt} = \frac{\frac{d}{dt}\left[-(x-ut)^2\right] \cdot 4Dt - \frac{d}{dt}[4Dt] \cdot \left[-(x-ut)^2\right]}{(4Dt)^2}$$

$$= \frac{-2(x-ut)(-u) \cdot 4Dt - 4D\left[-(x-ut)^2\right]}{(4Dt)^2}$$

$$= \frac{(2u)(\cancel{4D}t)(x-ut) + \cancel{4D}(x-ut)^2}{(4D)^2 t^2}$$

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Figure A-5. Derivation of the Travel Time Equation (3 sheets)

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$$= \frac{2Dt(x-ut)+(x-ut)^2}{4Dt^2}$$

$$= \frac{(x-ut)[2ut+(x-ut)]}{4Dt^2}$$

$$= \frac{(x-ut)(x+ut)}{4Dt^2}$$

$$\frac{dC}{dt} = -\frac{1}{2\theta t\sqrt{4\pi Dt}}\cdot e^{\frac{-(x-ut)^2}{4Dt}} + \frac{1}{\theta\sqrt{4\pi Dt}}\cdot e^{\frac{-(x-ut)^2}{4Dt}}\cdot\frac{(x-ut)(x+ut)}{4Dt^2}$$

$$= e^{\frac{-(x-ut)^2}{4Dt}}\cdot\left[-\frac{1}{2\theta t\sqrt{4\pi Dt}} + \frac{(x-ut)(x+ut)}{4Dt^2\theta\sqrt{4\pi Dt}}\right]$$

$$= e^{\frac{-(x-ut)^2}{4Dt}}\cdot\left[-\frac{2Dt}{4Dt^2\theta\sqrt{4\pi Dt}} + \frac{(x-ut)(x+ut)}{4Dt^2\theta\sqrt{4\pi Dt}}\right]$$

$$= e^{\frac{-(x-ut)^2}{4Dt}}\cdot\frac{(x-ut)(x+ut)-2Dt}{4Dt^2\theta\sqrt{4\pi Dt}}$$

At the time of the peak concentration, the first derivative (dC/dt) will be equal to zero. So, set the above equation equal to zero and solve for t:

$$e^{\frac{-(x-ut)^2}{4Dt}}\cdot\frac{(x-ut)(x+ut)-2Dt}{4Dt^2\theta\sqrt{4\pi Dt}} = 0$$

Because $e^{\frac{-(x-ut)^2}{4Dt}}$ can never be zero, the above equation reduces to:

$$\frac{(x-ut)(x+ut)-2Dt}{4Dt^2\theta\sqrt{4\pi Dt}} = 0$$

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Figure A-5. Derivation of the Travel Time Equation (3 sheets)

CH2MHILL SUBJECT Derivation of the time to peak equation (with dispersion) BY I.P. McDonald SHEET NO. 3 of 3 DATE 2/25/2016 PROJECT NO.

For the fraction to be equal to zero, the numerator must be zero, so:

$$(x-ut)(x+ut) - 2Dt = 0$$
$$x^2 - u^2t^2 - 2Dt = 0$$
$$-u^2t^2 - 2Dt + x^2 = 0$$
$$u^2t^2 + 2Dt - x^2 = 0$$

By the quadratic formula:

$$t = \frac{-2D \pm \sqrt{4D^2 - 4u^2(-x^2)}}{2u^2}$$

$$= \frac{-2D \pm \sqrt{4(D^2 + u^2x^2)}}{2u^2}$$

$$= \frac{-\cancel{2}D \pm \cancel{2}\sqrt{D^2 + u^2x^2}}{\cancel{2}u^2}$$

$$= \frac{-D \pm \sqrt{D^2 + u^2x^2}}{u^2}$$

Because it will always be the case that $D > 0$, $x > 0$, and $u > 0$, it follows that $-D - \sqrt{D^2 + u^2x^2} < 0$ (i.e., the travel time would be less than zero). Therefore:

$$t_p = \frac{-D + \sqrt{D^2 + u^2x^2}}{u^2}$$

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Figure A-5. Derivation of the Travel Time Equation (3 sheets)

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SUBJECT Solving Equation 6 for Moisture Content

BY JP McDonald

SHEET NO. 1 of 1 DATE 6/1/2016

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$$K(\theta) = K_s \left(\frac{\theta}{n}\right)^{2b+3}$$

$$\frac{K(\theta)}{K_s} = \left(\frac{\theta}{n}\right)^{2b+3}$$

$$\left[\frac{K(\theta)}{K_s}\right]^{\frac{1}{2b+3}} = \left[\left(\frac{\theta}{n}\right)^{2b+3}\right]^{\frac{1}{2b+3}}$$

$$\frac{\theta}{n} = \left(\frac{K(\theta)}{K_s}\right)^{\frac{1}{2b+3}}$$

$$\theta = n \cdot \left(\frac{K(\theta)}{K_s}\right)^{\frac{1}{2b+3}}$$

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Figure A-6. Equation for Volumetric Moisture Content

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