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**Recommended Geochemical Input Values for the Special Analyses of the
Slit/Engineered Trenches and Intermediate Level Vault**

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July 23, 2004

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ACRONYMS

CDP	Cellulose Degradation Products
DOC	Dissolved Organic Carbon
Kd	Distribution Coefficient
SRS	Savannah River Site

1.0 ABSTRACT

Selected geochemical input values are provided for the Slit and Engineered Trenches Special Analysis and the Intermediate Level Vault Special Analysis. Only input values for parameters that have new information related to them or that have recently been recognized as being important to the special analysis are discussed. These parameters are 1) plutonium geochemistry (conceptual model and input values), and 2) Kd values for select radionuclides. Due to the differences in the geochemical environment expected at these two disposal locations, the Kd values are expected to differ. The Intermediate Level Vault will create a relatively high pH environment (pH ~10), whereas the Slit and Engineered Trenches will create an environment high in organic matter.

2.0 OBJECTIVE

The objective of this report is to provide geochemical input values for the Slit/Engineered Trenches Special Analysis and the Intermediate Level Vault Special Analysis. Special analyses are calculations conducted to provide information used to determine the amount of radioactive waste that can be safely disposed at a given site. The intent of this document is to provide technical justification for the selection of some, but not all the geochemical input values used in the special analysis. Input values for parameters that have new information related to them or that have recently been recognized as being important to the special analysis are discussed. These parameters are:

- 1) plutonium geochemistry (conceptual model and input values),
- 2) Bi, Ca, Cl, K, Mo and Se Kd values as a function of cellulose degradation products (CDPs) or pH for the Slit/Engineered Trench Special Analysis, and
- 3) Al, Bi, Co, Eu, K, Kr, Mo, Pu(III/IV), Pu(V/VI), Rn, and Se for the Intermediate Level Vault Special Analysis.

3.0 PLUTONIUM GEOCHEMISTRY CONCEPTUAL MODEL FOR THE SLIT/ENGINEERED TRENCH SPECIAL ANALYSIS

There have been several recent reports on Pu geochemistry in the SRS subsurface environment that have direct applicability to these special analyses (Kaplan and Wilhite 2001; Kaplan et al. 2001; Powell et al. 2002; Kaplan et al. 2003; Kaplan et al. 2004a; Kaplan et al. 2004b).

The conceptual model for Pu geochemistry and colloid-facilitated transport was first proposed by Cook (2002). Plutonium is assumed to exist in three forms: Pu(III/IV), Pu(V/VI), and Pu_{colloids}. Pu(III/IV), Pu in the +3 and +4 oxidation states, has one set of geochemical parameters, Pu(V/VI), another set of parameters, and Pu_{colloids}, Pu in the colloidal form, a third

set of parameters. Based on laboratory work using SRS sediments (as well as other sediments), Pu(III/IV) is much less mobile than Pu(V/VI) (Kaplan et al. 2001; Powell et al. 2002; Kaplan et al. 2003; Kaplan et al. 2004a; Kaplan et al. 2004b). Pu(III/IV) is also much more abundant than Pu(V/VI) in the SRS subsurface environment because of natural mineralogy, redox, and pH conditions.

One of the key factors controlling Pu(III/IV) and Pu(V/VI) sorption is assumed to be concentration of cellulose degradation products (CDPs; e.g., wood, paper, and cardboard). CDPs decrease the tendency of Pu to sorb to sediments by 1) reducing the system pH, and 2) promoting the formation of weakly binding Pu-dissolved organic matter (DOC) complexes. To date, no Pu Kd measurements as a function of CDPs concentrations have been made. However, Serkiz (2000) reported a strong correlation between pH and CDP concentrations. The input Kd values were selected from experiments in which pH was varied (Powell et al. 2002). The intent was use the pH variable as a proxy for DOC concentration. One limitation of this approach is that only the pH effect of DOC and not the effect of DOC-Pu complexes is captured by this approach to selecting Kd values, thereby producing a potentially non-conservative estimate. To minimize this potential problem, the minimum Kd value for a specific pH condition was selected. The waste source term is assumed to have an infinite amount of cellulose to form CDP, i.e., CDP is produced throughout the modeling period. More details about the CDP-radionuclide interaction model and its assumptions are presented by Serkiz (2000).

The colloid model is simplistic and reflects a first attempt at accounting for this potential vector of transporting Pu. The model is devoid of mechanism and is based on a field experiment conducted in a nearby site on the SRS, F-Area (Kaplan et al. 1994). It is anticipated that as more information about Pu colloidal transport is made available, this model will be modified as part of the performance assessment maintenance program. $Pu_{colloids}$ concentration in the flow path is assumed to exist at a concentration similar to that measured in F-Area (Kaplan et al. 1994) and to move at the same rate as water, i.e., to have a Kd value of 0 mL/g. All Pu in the source exists as Pu(III/IV) because Pu(IV) is the oxidation state it was disposed as and because of the natural tendency of Pu to convert to Pu(IV) (Kaplan et al. 2004a). CDPs do not influence $Pu_{colloids}$ Kd values (because they already have a Kd value of 0 mL/g). More details about the Pu geochemistry model and its assumptions are presented in Section 3.4 and in Cook (2002).

3.1 Proton Sorption to Sediment and Background pH

Prior to modeling Pu transport, pH or proton concentrations in the sediment need to be modeled so that the appropriate pH-dependent Kd value can be selected for each node in the reactive-transport model. A Freundlich-sorption isotherm will be used to describe proton sorption to the E-Area sediment, using the approach first proposed by Brewer and Sochor (2002) and data generated from SRS sediment by Kaplan (2003). The non-linear (Eq. 1) and linear (Eq. 2) forms of the Freundlich-sorption isotherm are as follows:

$$S = kC^n \quad (1)$$

$$\log[S] = \log[k] + n\log[C] \quad (2)$$

where

- S = sorbed phase concentration,
- k = Freundlich absorption constant,
- C = aqueous phase concentration, and
- n = Freundlich exponent.

Brewer and Sochor (2002; page 52) reported that the value for n is 0.38 and the value for k is $396 \text{ L}^{0.38} \mu\text{g}^{0.62}/\text{kg}$.

To establish background pH levels, Hiergesell (2004) used historic groundwater monitoring data from wells in the flow path of a hypothetical plume from the Slit/Engineered Trench Facility in E-Area. The flow path was established by using groundwater flow simulations. Three wells were identified as existing in the hypothetical plume, BG 96, BGX 6D, and HMD 4D. All field pH values for each of these wells were extracted from the SRS ERDMS database (Table 1). Based on this data, an assignment of a site background pH of 5.5 is appropriate. Assuming a lower background pH yields a conservative estimate because most metals and radionuclides have enhanced transport under acidic conditions.

Table 1. pH levels in 3 wells located in a hypothetical plume emanating from the Slit/Engineered Trench Facility in E-Area; data used to estimate background pH at E-Area.

Well	Mean pH	Median pH	# of Measurements
BG 96	5.4	5.5	15
BGX 6D	6.2	6.2	24
HMD 4D	5.7	5.7	23

3.2 Pu(III/IV) Geochemistry

- Pu(III/IV) adsorbs to the sediment in a linear and reversible manner, as described by the Kd construct (Eq. 3).

$$\text{Pu(III/IV)}_{aq} + S_s \rightleftharpoons \text{Pu(III/IV)}S_s; \text{ where } S_s = \text{sediment} \quad (3)$$

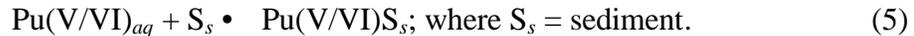
- Kd values vary as a function of pH (more specifically, as a function of CDP concentrations; see Section 3.0).
- Once adsorbed to the sediment, the Pu(III/IV) slowly oxidizes to Pu(V/VI). Oxidation of Pu(III/IV) to Pu(V/VI) occurs through a reversible, first-order kinetic process:



3.3 Pu(V/VI) Geochemistry

Pu(V/VI) geochemistry is treated similar to Pu(III/IV), namely it adsorbs and then undergoes a redox reaction, reduction.

- Sorption is described by Kd values that quantify the reaction in equation 5:



- Kd values vary as a function of pH (more specifically, as a function of CDP concentrations; see Section 3.0).
- Once adsorbed to the sediment, the Pu(V/VI) quickly reduces to Pu(III/IV). Reduction of Pu(V/VI) to Pu(III/IV) occurs through a reversible, first-order kinetic process:



3.4 Pu_{colloids} Geochemistry

3.4.1 General Description

Modeling colloid facilitated transport of Pu in the SRS subsurface environment is greatly hindered by the paucity of data on the subject. Kaplan et al. (1994) measured Pu associated with a filterable fraction in groundwater recovered in F-Area, adjacent to E-Area. Measurements made from this study form the basis for the proposed conceptual model. This conceptual model is devoid of mechanism and is greatly simplified. As such, there is a great deal of uncertainty associated with the calculated results. However, we felt that it is important to start accounting for the possibility of this transport mechanism in the Special Analyses, with the intent of improving on the model as part of the performance assessment maintenance program as more experimental data becomes available (discussed in more detail in Section 8.0). The assumption that colloid facilitated transport occurs in the modeled system is conservative with respect to the groundwater risk calculation because it provides an additional vector for transporting Pu to the 100-m well. Details regarding how colloid facilitated transport of Pu is conceptualized in this model are presented below.

3.4.2 Detailed Description

Plutonium associated with a filterable fraction, was measured in F-Area (Kaplan et al. 1993). This data was used to form the basis for estimating colloidal Pu, $Pu_{colloid}$, in E-Area. Kaplan et al. (1993) reported total Pu concentrations in the F-Area Seepage Basin and $Pu_{colloids}$ concentrations in three wells located 30 m, 320 m and 550 m from the seepage basin. Because of considerable differences in pH and other geochemical parameters between E- and F-Area, the data at the 30-m and 320-m wells were not considered further. For simplicity, the ratio between the concentration of $Pu_{colloids}$ at the 550-m well to the concentration of Pu in vadose zone samples at the seepage basin is assumed to apply to solid waste disposed in trenches inside the E-Area.

The ratio between the Pu concentrations on colloids at a 550-m well and the liquid in the source zone was found to be $1.1E-3$ in the field. It will be assumed that an estimated 550-m well concentration for the $Pu_{colloids}$ in E-Area should be calculated by multiplying the non-colloidal model's average initial concentration of the Pu in the liquid in the source zone by $1.1E-3$ to match field observations at the other site.

The PA uses a hypothetical 100-m well to establish risk. $Pu_{colloids}$ concentrations may be expected to be greater at 100 m than 550 m from a well. To account for the shorter distance to the 100-m well, the model's 550-m well concentration should be multiplied by $550/100$ to produce an estimate of the Pu colloid concentration in the 100-m well.

Plutonium concentrations reported by Kaplan et al. (1994) in the source well included colloids and non-colloids, while the concentrations at the distant wells consisted almost entirely of colloids. To best capture the value in the existing data, the ratio of the Pu colloid amount at the distant well to the Pu total amount at the source well will be directly added to modeling results for non-colloid Pu isotopes. As a conservative approach, that ratio will be applied to each and every Pu isotope. Although water from the source will not reach the 100-m well for several years, the ratio will be applied from time zero.

As the total source amount decays, the amount of the $Pu_{colloids}$ at the well will similarly decay. Progeny will be produced and included in the potential effects on a receptor. For example, if the ratio of $Pu_{colloids}$ concentration at the 100-m well to the source is $1E-3$ and the initial quantity of source term for Pu-238 is 1000 Ci, then 1 Ci ($1000 \text{ Ci} * 1E-3$) of Pu-238 would initially be at the well. After one half-life, the quantity of Pu-238 at the source would be reduced by one-half by decay as well as by leaching and diffusion. However, if only the decay is considered, then the quantity of Pu-238 at the source would be one-half or 500 Ci and the quantity of Pu-238 at the well as colloids would be reduced by half to 0.5 Ci. Progeny at the well are assumed to be generated and that they do not migrate away from the well.

To incorporate the above assumptions, the $Pu_{colloid}$ construct will be simulated as follows. Some of these recommendations are specifically designed to be compatible to the PORFLOW code used in the special analyses.

- Pu concentration fraction of the source to field measurements (Kaplan et al. 1994) is assigned as $WellFrac_{colloids}$.
- The source for the non-colloids modeled for the groundwater pathway is assigned as $Source_{all}$.
- The quantity of Pu colloids at the 100-m well is the product of these two factors:
 $Well_{colloid} = Source_{all} * WellFrac_{colloids}$.
- The quantity of Pu in $Well_{colloids}$ is simply decayed in place, thereby reducing the parent and generating progeny.
- Transport of $Pu_{colloid}$ is not retarded by the aquifer sediment, i.e., $Pu_{colloids}$ Kd value is 0 mL/g.
- $Pu_{colloid}$ does not have any assigned redox status, and as such its concentration is not influenced by the other two Pu fractions, Pu(III/IV) and Pu(V/VI).
- CDPs do not influence $Pu_{colloids}$ mobility or speciation.
- Pu associated with the colloids does not decay into daughter products. This is conservative with respect to the groundwater pathway risk calculation because the $Pu_{colloid}$ has a Kd of 0 mL/g. Many of the daughter products would likely desorb from colloids and would take on the much higher Kd value of a dissolved solute.

For ancestors of Pu that generate Pu, the same method will be applied with two exceptions. First, the starting quantity at the well will be for the $Source_{all}$ ancestor multiplied by the $WellFrac_{colloids}$. Second, none of the quantity of ancestors of Pu will be excluded from the effects that could potentially affect a receptor, because it is the Pu colloids being analyzed, not the ancestors.

In summary, $Pu_{colloid}$ will not be directly modeled for solid waste disposed in E-Area trenches to determine their concentrations at a 100-m well. Rather the effects of the colloids will be captured by separately calculating the 100-m well concentration for the colloids using the ratios presented above. The well concentration for the colloids can then be summed with the well concentration from the non-colloids to predict a total well concentration. Additional data and information about colloid generation at the E-Area site is necessary before a more direct approach to modeling Pu transport by colloids is possible (discussed in Section 8.0).

4.0 PLUTONIUM GEOCHEMISTRY CONCEPTUAL MODEL FOR THE INTERMEDIATE LEVEL VAULT SPECIAL ANALYSIS

The assumptions underlying how Pu geochemistry will be modeled in the Intermediate Level Vault Special Analysis are identical to those for the Slit/Engineered Trench Special Analysis (Section 3.0), except for two important differences. The first difference is that Pu sorption will not be influenced by CDPs, because little or no cellulose containing material will be disposed at the Intermediate Level Vault Facility. Thus, Pu Kd values appropriate for a pH 5.5 sediment (background; Section 3.1) will be used in the far field. The second difference is that $Pu_{colloids}$ will not be included. Insufficient conceptual and quantitative data is presently available to include this transport process in the model. As part of the performance assessment maintenance program, additional research needs to be directed at this issue (Section 8.0)

5.0 RECOMMENDED PLUTONIUM INPUT VALUES

Table 2. Recommended Input Values, Comments, and References for Plutonium Redox-Reaction Rates and Colloidal Transport (Conservative for Groundwater Pathway for Sandy Textured Sediment)

Parameter	Value	Units	Comment	Ref.
Reduction Rate: Pu(V/VI) \rightarrow Pu(III/IV)	1E-3	1/hr	Best-fit value to data was calculated from a data set generated from a study involving a lysimeter containing SRS sediment and Pu(IV). The reduction rate was $1E-3 \text{ hr}^{-1}$ (See Figure 3 in Reference 2). The lysimeter was exposed to natural rainfall for 11 years and this rate constant was estimated by applying a reactive transport code to a Pu-sediment concentration vs. depth data set. The first order reduction rate constant measured from a laboratory experiment was $1.1E-1 \text{ hr}^{-1}$, a faster rate, which was likely the result of better mixing obtained during the beaker-size laboratory study (See Figure S4 in Ref. 2). The slower reduction rate was selected in an effort to be conservative, i.e., the rate that Pu(V/VI) converts to the less mobile Pu(III/IV) will be slow.	1
Oxidation Rate: Pu(III/IV) \rightarrow Pu(V/VI)	1.5E-8	1/hr	There are 2 estimates for this parameter using SRS sediment. One estimate was calculated from the same lysimeter data involving a Pu(IV) spike discussed above. An oxidation rate was fitted to the data set: $1E-8 \text{ 1/hr}$. A laboratory measurement of this parameter, designed to provide highly accelerated oxidizing conditions, was $1e-6 \text{ 1/hr}$. The highly oxidizing conditions created during the laboratory study could not be achieved in the SRS subsurface. The conservative oxidation rate was estimated by increasing the lysimeter oxidation rate by 50%, thereby increasing the rate that oxidation converts the less mobile form of Pu, Pu(III/IV), to Pu(V/VI).	1
Pu _{colloids} concentration;	4.5E-3	wt-% of Inven- tory	This is the percent of Pu assumed to exist in the colloidal fraction. Pu was detected in F-area as a colloidal (filterable) fraction about 550m from the seepage basins, the point source: $[\text{Pu}]_{550\text{m}}/[\text{Pu}]_{0\text{m}} \times 100 = \text{Pu}_{\text{colloid}}$ concentration. This value was 0.0029% in a well 30 m from the point source, 0.0045% at a well 320 m from the point source, 0.0011% in a well 550 m from the point source, and <0.0002% in a well 1020 m from the point source. The largest value was selected.	2
Pu _{colloid} Kd	0	mL/g	Conservative estimate assuming all the colloidal Pu is highly mobile and is not held up (retarded) by the subsurface sediment.	2

1. Kaplan et al. (2004); Figure 3.

2. Kaplan et al. (1994); Table 3.

Table 3. Pu(III/IV) and Pu(V/VI) and Pu_{colloids} Kd Values as a Function of pH (Conservative for Groundwater Pathway for Sandy Textured Sediment)

DOC (mg C/L)	pH ^(a)	Pu(III/IV) Kd (mL/g) ^(b)	Pu(V/VI) Kd (mL/g) ^(b)	Pu _{colloids} Kd (mL/g)
1000	4.5	220	8	0
100	4.75	270	8	0
30	5.0	310	8	0
10	5.25	350	9	0
1	5.5	370	15	0
<1	5.75	390	21	0
<1	6.0	1000	70	0
<1	pH 5.5 for Clayey Sediment ^(c)	6500	50	0

^(a) Following the pH–DOC correlation described in by Serkiz (2000).

^(b) Pu(III/IV) and Pu(V/VI) data taken from Powell et al. (2002): Subsurface Sandy Sediment, Figure 13 on page 33; and Appendix B on page 46. These Kd values were the lowest of 4 SRS sediments tested. The other 3 sediments generally had Kd values an order of magnitude greater than the Pu(IV) presented in this table.

^(c) Pu(III/IV) and Pu(V/VI) data taken from Powell et al. (2002): Subsurface Clayey Sediment, Figure 13 on page 33; and Appendix B on page 47. These Kd values are for use in a clay layer included in the Special Analysis that is sufficiently deep that the concentration of dissolved organic matter will be assumed to be negligible, thus the pH in the clay layer is assumed to be 5.5.

6.0 RECOMMENDED K_d VALUES FOR USE IN THE SPECIAL ANALYSIS OF THE SLIT/ENGINEERED LLW TRENCHES

Table 4. Select Conservative (Low) K_d Values as a Function of pH for a Sand-textured Sediment For Use in the Special Analysis of the Slit/Engineered LLW Trenches.

pH ^(a)	Bi K _d ^(f) (mL/g)	Ca K _d ^(b) (mL/g)	Cl K _d (mL/g)	K K _d ^(e) (mL/g)	Mo K _d ^(d) (mL/g)	Se K _d ^(c) (mL/g)
4.5	2	0.1	0	2	3	36
4.75	4	0.1	0	2	3	36
5.0	13	0.2	0	3	3	36
5.25	80	4	0	3	3	36
5.5	450	10	0	3	3	36
5.75	--	10	0	4	3	36
6.0	--	10	0	4	3	36

^(a) Following the conceptual model proposed by Serkiz (2000), pH values are used as a proxy for dissolved organic carbon.

^(b) Serkiz (2000); page 16, Table 13. Assumed Ca K_d values are identical to those for Sr reported by Serkiz.

^(c) Thibault et al. (1990); page 90, Table B-28. Assume either SeO₄²⁻ or SeO₃²⁻. Se values range from 36 to 310 mL/g. Sand (pH 5.3) K_d = 70 mL/g; Sand (pH 6.0) K_d = 70 mL/g; Sand (pH 6.3) K_d = 36 mL/g. Increase in K_d as pH decreases is expected for anionic radionuclides; credit for this is not taken by Serkiz (2000) or in this table. Higher Se K_d values are reported by Thibault et al (1990) for sediments with finer texture.

^(d) Thibault et al. (1990); page 79, Table B-28. Assume MoO₄²⁻. Mo K_d values range from 1 to 400 mL/g. Mo K_d values in sand range from 1 to 8 mL/g. Mo K_d values tend to increase as pH decreases; again, credit for this is not taken by Serkiz (2000) or in this table.

^(e) Kaplan and Serkiz (2000); page 26, Table 9. Two K adsorption K_d values were measured in pH 4.2 subsurface SRS sediment: 2 ± 1 and 6 ± 4 mL/g.

^(f) Bi exists as either Bi(III) or Bi(0) across a wide range of pH, pH 2 to 11 (Pourbaix 1974). Importantly it does not form the oxidized, more mobile, +5 form under conditions expected in the SRS subsurface. As such, Bi K_d values provided in this table are those used by Serkiz (2000) for all Ac(III), a +3 element with approximately the same atomic weight as Bi (Bi atomic weight = 209; Ac atomic weight = 227). Assuming Bi exists as Bi(III) and not Bi(0) is conservative for the groundwater pathway because the latter is expected to be less mobile than the former.

7.0 RECOMMENDED KD VALUES FOR USE IN THE SPECIAL ANALYSIS OF THE INTERMEDIATE LEVEL VAULT

Table 5. Select Conservative (Low) Kd Values (mL/g) for Use in the Special Analysis of the Intermediate Level Vault.

	Soil	Grout (non-reducing)	Clay	Concrete (non-reducing)
Co	8 ^(a)	100 ^(l)	96 ^(b)	100 ^(l)
Se	36 ^(c)	0.1 ^(e)	76 ^(d)	0.1 ^(f)
Kr	0	0	0	0
Eu	1900 ^(g)	5000 ^(g)	8400 ^(g)	5000 ^(g)
Rn	0	0	0	0
Pu(III/IV)	370 ^(h)	100 ⁽ⁱ⁾	6500 ^(h)	5000 ⁽ⁱ⁾
Pu(V/VI)	15 ^(h)	100 ⁽ⁱ⁾	50 ^(h)	5000 ⁽ⁱ⁾
K	3 ^(c)	2 ^(f)	5 ^(k)	2 ^(f)
Mo	3 ^(c)	1 ⁽ⁿ⁾	13 ^(m)	1 ⁽ⁿ⁾
Bi	450 ⁽ⁱ⁾	5000 ^(p)	12,000 ^(q)	5000 ^(p)
Al	40 ^(r)	5000 ^(p)	12,000 ^(q)	5000 ^(p)
¹⁴ C (K-Basin Waste)	No estimate	No estimate	No estimate	5000 ⁽ⁱ⁾
⁹⁹ Tc	0.1 ⁽ⁱ⁾	1 ^(o)	0.1 ^(j)	1 ^(o)
⁹⁹ Tc (K-Basin Waste)	No estimate	No estimate	No estimate	0 ^(j)
¹²⁹ I (K-Basin Waste)	No estimate	No estimate	No estimate	2 ^(f)

(a) Hoeffner (1985); E-Area sediment, no pH adjustment, Figure 1; page 22.

(b) Neiheisel (1983); based on SRS E-Area conditions; Table 4 & Figure 6.

(c) Table 4 in this document. Assuming background pH in soil is 5.5.

(d) Thibault et al. (1990); Page 90, Kd values for clay sediments between pH 5 – 6 were reported as 76, 140, 80, 246, and 170 mL/g.

(e) Bradbury and Sarott (1995). I and Tc are reported by Bradbury and Sarott. Assumed K Kd values were identical to Cs Kd values reported by Bradbury and Sarott.

(g) Assumed Kd values for Eu are identical to those for Am. Values reported here are taken from McDowell-Boyer et al. (2000), Table 4.1-4, page 4-16. The accuracy of the Am Kd values was not evaluated.

(h) Table 3 in this document. Assuming background pH in soil is 5.5.

(i) McDowell-Boyer et al. (2000), Table 4.1-4, page 4-16. The accuracy of the Kd values reported in this reference was not evaluated.

(j) Kaplan (2003); TcO_4^- Kd values in SRS sediment varied from 0.2 at pH 3 to -0.1 at pH >5 (negative Kd values, an anion exclusion, is possible for anions.

This indicates that the anion is repulsed from by the sediment's negative charge to move faster than the average groundwater velocity.)

- ^(k) Thibault et al. (1990); Table 2 on page 7 and Table 9 on page 14.
- ^(l) Bradbury and Sarott (1995); assumed Co sorption behavior was similar to that of reported by Bradbury and Sarott for Ni. Both elements are divalent cation that share a number of inorganic chemistry behavior.
- ^(m) Thibault et al. (1990), page 79, Table B-20. They report seven K_d values for “silt-clay” textured sediments ranging from 13 to 400 mL/g, medium = 40 mL/g.
- ⁽ⁿ⁾ Bradbury and Sarott (1995), page 42, Table 4. Assumed Mo is an anion and used lowest K_d reported by Bradbury and Sarott for anions, that for Tc.
- ^(o) Bradbury and Sarott (1995), page 42, Table 4.
- ^(p) Bradbury and Sarott (1995), page 42, Table 4. Assumed Am(III) as analogue.
- ^(q) Thibault et al. (1990), page 11, Table 6. Used Ce(III) as an analogue, selected minimum value of reported range.
- ^(r) Thibault et al. (1990), page 9, Table 4. Used Ce(III) as an analogue, selected minimum value of reported range.
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8.0 ADDITIONAL DATA NEEDS

There are two important research topics that could reduce uncertainty and improve accuracy in future performance assessment and special analysis calculations: 1) colloid facilitated transport, and 2) the influence of cellulose degradation products on radionuclide sorption to sediments. Theory underlying colloid facilitated transport of contaminants is fairly advanced (Tien 1989). However, there are few examples of successful applications of this theory to natural conditions (Tien 1989). This is due to a number of factors, including the need for site specific data. To better understand and to reduce uncertainty associated with the Pu_{colloid} calculation in the special analysis, site specific colloid-removal efficiency values (λ ; a kinetic term describing colloid removal by a porous media) must be measured. As K_d values are contaminant and sediment specific, so is λ ; it is sediment and colloid specific. Another related subject that requires additional research is whether concrete structures, such as the Intermediate Level Vault, create colloids that can move through SRS sediments and act as a vector for radionuclide transport. Initial research indicated that immediately after concrete was placed in a column of sediment, colloid concentrations in the leachate were high, but that they returned to negligible concentrations within a short time period, less than a dozen pore volumes (equivalent to a couple of weeks of subsurface flow in E-area) (Serkiz et al. 2000).

The second important research area for future performance assessments and special analyses is the impact of cellulose degradation products on radionuclide K_d values. As described in this document (Section 3.0), it is being addressed in a rather indirect manner. Serkiz (2000) had information about the influence of pH on select radionuclide K_d values. He also measured a correlation between total organic carbon in the aqueous phase and sediment pH. He then combined these two results to produce estimates of the influence of CDPs on K_d values. More direct measurements are needed. Such measurements have been initiated with a wide range of elements, including Ce, Cs, Eu, Ni, K, Rh, Sr, Th, and Zr. It is anticipated that the results from this work will greatly reduce uncertainty and improve accuracy of future calculations.

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