

Geochemical Modeling for the WCS Site Model v0.205

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CONTENTS

CONTENTS.....	iv
FIGURES.....	v
TABLES.....	vi
1.0 Overview.....	1
2.0 Parameter Values Summary.....	2
3.0 Geochemical Conditions.....	4
4.0 Solid/Water Partition Coefficients (K_d).....	5
4.1 K_d s in Sand.....	7
4.2 K_d s in Clay.....	7
4.3 K_d s in Cementitious Materials.....	7
4.3.1 Carbon.....	9
4.3.2 Chlorine.....	10
4.3.3 Iodine.....	11
4.3.4 Other Radioelements.....	11
5.0 Aqueous Solubility.....	11
5.1 Solubility in Fresh Water.....	12
5.1.1 Carbon.....	12
5.1.2 Chloride.....	12
5.1.3 Iodine.....	12
5.1.4 Radium.....	13
5.1.5 Technetium.....	13
5.1.6 Uranium.....	13
5.1.7 Other Radioelements.....	14
5.2 Solubility in Cement-Equilibrated Water.....	14
5.2.1 Carbon.....	14
5.2.2 Chloride.....	14
5.2.3 Iodine.....	14
5.2.4 Radium.....	14
5.2.5 Technetium.....	15
5.2.6 Uranium.....	15
5.2.7 Other Radioelements.....	15
6.0 Air/Water Partition Coefficients (K_H).....	15
7.0 Ionic and Molecular Diffusion Coefficients in Water.....	16
8.0 Diffusion Coefficients in Air.....	18
9.0 References.....	19

FIGURES

Figure 1. Evolution of pH in weathering cement. Reproduction of Figure 3.2 in Serne et al. (2009).....	8
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TABLES

Table 1. Summary of input distributions for soil/water partition coefficients (K_d) for the WCS Site Model	2
Table 2. Summary of input distributions for aqueous solubility (mol/L) for the WCS Site Model	3
Table 3. Summary of input distributions for Henry's Law constants (K_H) for volatile radioelements in the WCS Site Model.....	3
Table 4. Summary of input values for free-air diffusion coefficients for volatile radioelements in the WCS Site Model.....	4
Table 5. List of radioelements included in the WCS Site Model	4
Table 6. Diffusion coefficients for selected cations and anions	17

1.0 Overview

Geochemical modeling is a part of performance assessment (PA) modeling that contributes to the fate and transport of contaminants in the natural and engineered environment. Without geochemical considerations, contaminants, when released into the environment from an engineered facility, migrate unrestricted in water and/or air. Unrestricted movement through the system may or may not be conservative for any given contaminant transport or human exposure pathway. The geochemical processes are modeled fairly simply in the model, to provide a mechanism for geochemical processes to occur without undue complexity. Probability distributions are developed for many of the geochemical parameters in order to provide realistic values and to characterize the uncertainty of the system.

The PA modeling for the WCS radioactive waste disposal site at Andrews, Texas, accounts for these geochemical processes: partitioning between solid and water phases via adsorption, solubility in fresh water and in cement water, partitioning between air and water phases, and diffusion in water and air. These processes are included in the WCS Site Model, and are incorporated within the GoldSim modeling platform's contaminant transport module. These geochemical processes are independent of an element's radioactivity, so their representation is on a per-radioelement basis, not a per-radionuclide basis.

Adsorption is a bonding of ions or compounds from the water onto the surface of solid phases. The minerals that compose a soil or other subsurface solids often have surfaces with charges or partial charges that attract molecules in solution. Clay surfaces typically have more surface charge, which encourages more adsorption than on sand, which has no surface charge. Many complex mechanisms can be used to model adsorption, but the most common is a linear relationship expressed by the soil/water partition coefficient K_d , which is simply the proportion of the mass of an element adsorbed onto the solid phase to the mass in solution.

Solubility is a chemical construct which defines the concentration of an element in water in equilibrium with solid minerals. The solubility limit is that solubility that results in precipitation of a chemical out of solution—the maximum concentration attainable for a given element. The main role of solubility and adsorption in the WCS Site Model is to estimate the concentration of an element in the water phase and thus the amount of that element available to move through the system. In general, the solubility of any element depends on water composition, temperature, and which solid minerals are present. The simplified version of solubility modeling in the WCS Site Model does not take these variables into account, but rather assumes a constant value for solubility limits for each radioelement.

Diffusion is the movement of an element within air or water by its own kinetic motion, independent of the movement of the fluid. Molecules move in water or air from regions of higher concentrations to those with lower concentrations, moderated by diffusion coefficients and concentration gradients. Diffusion is modeled as a classic Fickian process.

This document describes these processes in more detail and how specific parameter values and distributions were chosen for the WCS Site Model.

2.0 Parameter Values Summary

Individual model parameters and associated input values used in the geochemical modeling of the WCS Site Model are identified in the *WCS Site Model Parameters.docx* and its companion workbook, *WCS Site Model Parameters.xlsx*. In this document, a more comprehensive record for each parameter is provided, including the source of the values and notes explaining the basis.

For distributions, the following notation is used:

- $N(\mu, \sigma, [min, max])$ represents a normal distribution with mean μ and standard deviation σ , optionally truncated at min and max ,
- $LN(GM, GSD)$ represents a log-normal distribution with geometric mean GM and geometric standard deviation GSD ,
- $LU(min, max)$ represents a log-uniform distribution with minimum value min and maximum value max ,
- $LTri(min, expected, max)$ represents a log-triangular distribution with minimum value min , an expected value $expected$, and maximum value max , and
- $discrete(x)$ represents a discrete distribution that always samples x .

For all radioelements in sand and clay materials, and for all others not listed in Table 1 for cementitious materials, the K_d values for the WCS Site Model are taken from Table 1-1 of Appendix 5 of WCS (2011).

Table 1. Summary of input distributions for soil/water partition coefficients (K_d) for the WCS Site Model

element	soil/water partition coefficients (K_d) in cementitious materials (mL/g)	Comments/reference
C	$LN(500, 6.18)$	See section 4.3
Cl	$LN(10, 4.06)$	See section 4.3
I	$LN(14.1, 7.48)$	See section 4.3

Aqueous solubility values are summarized in Table 2 for those radioelements that were examined for the WCS Site Model. All other radioelements are assumed to have no solubility limits, for now.

Table 2. Summary of input distributions for aqueous solubility (mol/L) for the WCS Site Model

element	aqueous solubility (mol/L)		Comments / reference
	fresh (meteoric) water	cement-equilibrated water	
C	LU(1e-7, 1e-4)	LU(1e-7, 1e-4)	See sections 5.1 and 5.2
Cl	LU(1e-5, 1)	LU(1e-5, 1)	See sections 5.1 and 5.2
I	-1	-1	See sections 5.1 and 5.2
Ra	LTri(1e-9, 1e-7, 1e-5)	LTri(1e-9, 1e-7, 1e-5)	See sections 5.1 and 5.2
Tc	-1	LN(1.0263e-7, 3.7518)	See sections 5.1 and 5.2
U	LU(1e-6, 1e-3)	LU(1e-6, 1e-3)	See sections 5.1 and 5.2

The air/water partition coefficients, or Henry's Law constants, (K_H) are discussed in Section 6.0, and are summarized in Table 3. Values to be used in deterministic simulations are specified because with the truncation, the median of the distribution may not be the median of the non-truncated distribution. The median value is what is used for deterministic simulations for most parameters.

Table 3. Summary of input distributions for Henry's Law constants (K_H) for volatile radioelements in the WCS Site Model

element	Henry's Law constant (K_H) (dimensionless)		Comments / reference
	distribution	deterministic value	
H	N(1.7×10^{-5} , 1×10^{-9} , Small, Large)	1.7×10^{-5}	See section 6.0
C	N(1.2, 0.001, Small, Large)	1.2	See section 6.0
Ar	N(29.5, 0.001, Small, Large)	29.5	See section 6.0
Kr	N(16.1, 0.001, Small, Large)	16.1	See section 6.0
I	N(0.013, 0.00001, Small, Large)	0.013	See section 6.0
Rn	N(4.6, 0.001, Small, Large)	4.6	See section 6.0

The input distribution for the diffusion coefficient in water for all radioelements is

$$N(10^{-5} \text{ cm}^2/\text{s}, 10^{-8} \text{ cm}^2/\text{s}, \text{Small}, \text{Large})$$

or

$$N(10^{-9} \text{ m}^2/\text{s}, 10^{-12} \text{ m}^2/\text{s}, \text{Small}, \text{Large})$$

truncated at the very small value Small, and the very large value Large, both of which are defined in the WCS Site Model. Discussion of this distribution is discussed in Section 7.0.

Free-air diffusion coefficients for volatile radioelements are well-known, and therefore have no uncertainty in the model. These values are summarized in Table 4, and discussed in Section 8.0.

Table 4. Summary of input values for free-air diffusion coefficients for volatile radioelements in the WCS Site Model

element	free air diffusivity at 20°C (cm ² /s)	Comments / reference
H	0.25	As HTO; CRC (1995)
C	0.16	As CO ₂ -air; CRC (2004)
Ar	0.148	As Ar-air; CRC (2004)
Kr	0.14	Derived from equation 11-4.4 (Reid et al., 1987) and diffusion volume from Table 11-1 (ibid).
I	0.09	
Rn	0.11	Rogers and Nielson (1991)

3.0 Geochemical Conditions

The WCS Disposal Facility is located in extreme western Andrews County, Texas, excavated into a near-surface rise in the Dockum Group, a dense red bed clay many hundreds of feet thick. Waste is disposed within two layers of concrete containment, with the addition of grout used for stabilization. In the waste disposal zone, pore waters are expected to be in equilibrium with these ubiquitous cementitious materials. Covering the waste is a collection of engineered layers, including native red bed clays, sands and soils, and additional concrete.

The geochemistry of the site is dominated by three distinct porous material types, grouped into three modeled materials: sands, clays, and cementitious materials. For each of these material types, the WCS Site Model assigns a value or distribution of values for a solid/water partition coefficient (K_d) for each modeled radioelement. The complete list of modeled chemical radioelements is provided in Table 5.

Table 5. List of radioelements included in the WCS Site Model

Ac	Bk	Cs	Ir	Ni	Pt	Si	Ti
Ag	C	Eu	K	Np	Pu	Sm	Tl
Al	Ca	Fe	Kr	Os	Ra	Sn	Tm
Am	Cd	Gd	La	Pa	Rh	Sr	U
Ar	Cf	H	Mn	Pb	Rn	Ta	V
Ba	Cl	Hf	Mo	Pd	Ru	Tb	Zr
Be	Cm	Ho	Na	Pm	Sb	Tc	
Bi	Co	I	Nb	Po	Se	Th	

Source: *WCS Site Model Parameters.xlsx*, sheet "Element Properties", column A

The pore water that occurs in these materials is assumed to be of two types. Within the sands and clays of the cover and below the waste, the water is assumed to be of meteoric origin (i.e. atmospheric water, from precipitation) and of neutral pH. In the region of the waste, however, where there are copious amounts of concrete and grout, the water is assumed to be in equilibrium with these cementitious materials and specifically with portlandite, a hydrated calcium hydroxide mineral. The presence of portlandite is expected to maintain a pore water pH of 12 to 12.5, which will have an effect on K_d as well as aqueous solubility. The two types of water—fresh (meteoric) water as well as water in equilibrium with cementitious materials—are conceived to have potentially different aqueous solubilities, as well as K_d s, based on the expected chemical speciation and oxidation state of the radioelements. WCS is considering the addition of flue dust or other such amendment to the concrete to support the formation of reduced species of elements such as technetium. For technetium, the reduced form is less mobile than the oxidized form of the element.

In addition to interaction between aqueous and solid phases, several radioelements disposed at the WCS Disposal Facility are present to some degree in the gas phase. These elements partition themselves between the gas phase and water according to Henry's Law. Henry's Law states that the amount of specific gas dissolved in water is proportional to the partial pressure of that gas in equilibrium with water (i.e., the partial pressure of the gas above the liquid when the gas and liquid are in equilibrium).

The movement of radioelements is also governed to a large degree in the WCS Site Model by diffusion, both in air and water. In fact, these are arguably the most significant contaminant transport processes at work at the site, since infiltration rates are so low (see the *Groundwater Modeling* white paper for details).

The WCS Site Model simultaneously considers the following geochemical processes, in addition to water advection, biotically-induced transport by plants and animals (see the *Biological Modeling* white paper), radioactive decay and ingrowth and others:

- soil/water partitioning,
- aqueous solubility,
- air/water partitioning,
- diffusion in water, and
- diffusion in gases.

Each of these topics is covered in the following sections.

4.0 Solid/Water Partition Coefficients (K_d)

The transport of dissolved radionuclides is retarded by sorption onto the solid phase of associated minerals and soils within each of the zones considered in the WCS Site Model. Sorption consists of several physicochemical processes including ion exchange, adsorption, and chemisorption.

Sorption onto solid porous media is represented in the model with K_d values. While the geochemistry of contaminant transport is complex, a representative and standard approach was

taken for the purposes of the PA. The current section focuses on the description of sorption and the derivation of parameters for K_d distributions.

Solid/water partition coefficients, or K_d s, are based on a simple equilibrium sorption model, and are a simplification of the wide range of geochemical processes discussed above. Despite the simplicity of the K_d models, they are commonly used in PAs because of their ease of implementation. The K_d model assumes that a given constituent dissolved in the water (e.g., uranium) has some propensity to sorb to the solid phase of a porous medium, while maintaining an aqueous concentration. The definition of the solid/water distribution coefficient, with units of mL/g is:

$$K_d = \frac{\text{mass of constituent sorbed on a unit mass of solid (g/g)}}{\text{mass of constituent within a unit volume of water (g/mL)}}$$

The sorption is assumed to be instantaneously reversible and independent of concentration. That is, no dynamics are accounted for, and the ratio is always simply linear—a constituent's concentration in water is always the same ratio with respect to its sorbed concentration onto the solid, and sorption is instantaneous. This is the commonly used linear isotherm assumption.

Applying the K_d model outside of the range of concentrations used to obtain the values can lead to over- or under-estimation of sorption. To account for ranges of geochemical conditions and the potential deviation from the assumptions underlying the linear sorption model which may result in variation in K_d values, the WCS Site Model includes stochastic (uncertain) parameter distributions for some sorption values. Nominal K_d values were selected using the general scientific literature. K_d values have been chosen for three individual materials: sand, clay, and a generic cementitious material.

The process for selecting K_d values for the modeled elements entailed an extensive literature search to identify sorption values used in other transport models, and in particular from locations that have similar solid phase properties and geochemical conditions. The sorption values used by WCS (WCS 2007, WCS 2011, Serne et al. 2009), DOE (Cochran et al. 2001, Scism 2006, Serne 2007, Krupka et al. 2005, Rood and Magnuson 2009, Kaplan 2010, Krupka and Serne 1998), Bradbury and Sarott (1994), Sheppard and Thibault (1990), Sheppard et al. (2009), and Wang et al. (2009) were evaluated. In addition, the EPA three volume series *Understanding Variation In Partition Coefficient, K_d , Values* (EPA, 1999b, 1999c, 2004) was referenced extensively in this process. The reader is advised to consult that EPA series as it was used for the derivation of many K_d values and much of that information is not repeated here.

This section provides a description of the derivation of the partition coefficient for radioelements in the transport model that had an isotope or progeny that significantly contribute to dose. Data were taken from literature searches, with values chosen from locations with similar geochemistry and soil/mineral conditions as the Andrews County facility. For elements that were not part of this set, the single values used in the Oct 2011 WCS GoldSim PA model are used (WCS 2011). Development of improved distributions for these less significant elements will be developed in the future.

A specific investigation was performed for carbon, chlorine, and iodine following the Oct 2011 PA model. For K_d s in sand and red bed clay, the current data support the updated PA model

values of 0 mL/g. The probability distributions under investigation are based on experimental site-specific data that consist only of negative K_d values in these media, and on literature review information and data that include 0 and small positive numbers for these K_d s. Consequently, based on the site-specific data and literature review information and data available, the use of K_d s in sand and clay of 0 mL/g is well supported as a deterministic choice in the WCS Site Model.

4.1 K_d s in Sand

All radioelements adopted the same values for sandy materials that were used in previous LA modeling, as tabulated for the “Saturated zone” in Table 1-1 of Appendix 5 of WCS (2011).

4.2 K_d s in Clay

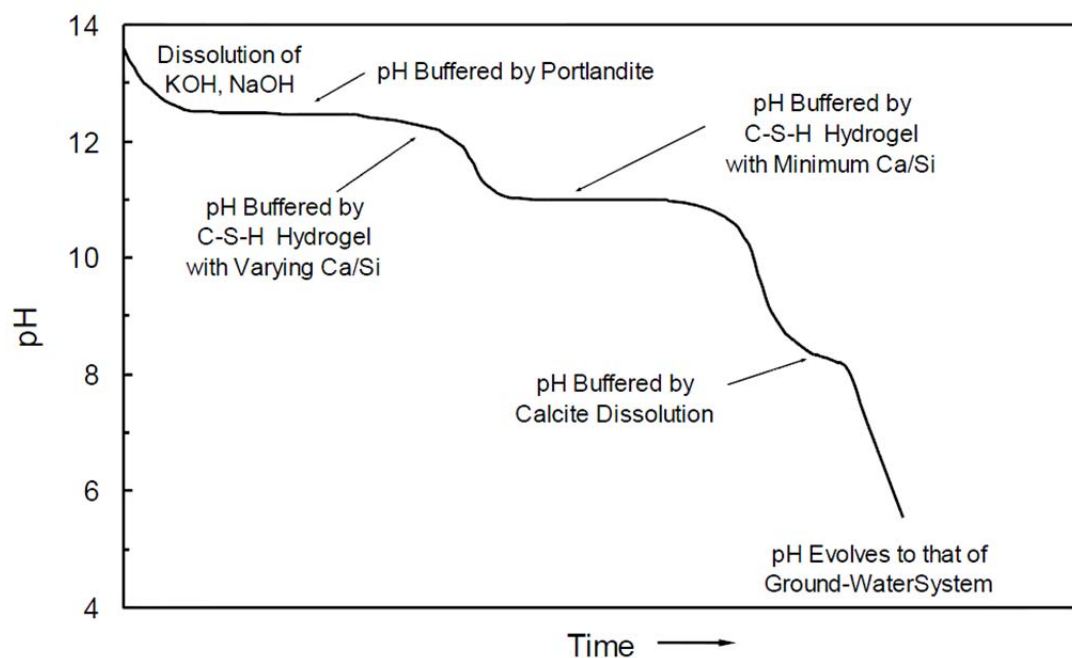
All radioelements adopted the same values for clayey materials that were used in previous LA modeling, as tabulated for the “Red bed” in Table 1-1 of Appendix 5 of WCS (2011).

4.3 K_d s in Cementitious Materials

Chemical stability is largely independent of structural stability. Even if a mass of concrete, such as an MCC waste container, or a mass of grout, such as the fill surrounding waste drums inside the MCC, fails mechanically, it continues to control the chemical environment. Cracking, spalling, and general structural degradation will not change the mass of portlandite and other hydroxides in the cement. Until these minerals are leached out, they continue to act as buffers to pH—their primary role here in moderating K_d chemistry.

The high pH concrete-dominated waste conditions at the WCS facility are expected to be very similar to the young concrete conditions described in Krupka et al. (2004), Kaplan (2010), and Wang et al. (2009). These sources, along with the WCS site-specific study by Serne et al. (2009), provide summaries of estimated K_d values for radionuclides in concrete vault environments. Extensive research on the K_d s in cementitious materials has also been conducted at the Savannah River Site (SRS), as exemplified in the PA for the F Area Tank Farm (SRS, 2010).

A cement weathering model is described by Bradbury and Sarott (1995), Krupka and Serne (1998, which is NUREG/CR-6377), Wang et al. (2009), and SRS (2010), with the change in pore water pH during weathering generally represented in Figure 3.2 of Serne et al. (2009), reproduced here:



Evolution of Cement Pore Water pH as Cement Weathers from Contact with Infiltrating Water and Air

Figure 1. Evolution of pH in weathering cement. Reproduction of Figure 3.2 in Serne et al. (2009)

Cementitious materials will consume water via a hydration reaction, and will interact with infiltrating water with the surrounding environment. In the early phases of this weathering of cement, termed “State I” by Wang et al. (2009), the pH drops rapidly as the Na and K hydroxides are leached out. Once the pH is buffered by portlandite (calcium hydroxide, $\text{Ca}(\text{OH})_2$), the system enters what Wang et al. call “State II”, where the pH will likely range from 11 to 13.3 pH units, with a value of pH 12.5 the most likely (Serne et al. 2009, Wieland and Van Loon 2003). Wang et al. (2009) estimate that the transition from State I to State II occurs after about 5 pore volumes of fresh water has passed through the material (p. 13 in Wang et al., 2009). Given this transition, it is assumed that the cementitious materials at WCS spend the bulk of their time in State II, buffered by portlandite.

This young concrete environment, saturated with respect to portlandite, is identified in the first pH “plateau” of the Serne et al. (2009) figure. The transition from this stage of cement weathering to the next plateau occurs when infiltrating water has removed the portlandite, and corresponds to what is called the transition from State II to State III in Wang et al. (2009). The quantities of portlandite contained in the cement are so large and water flow rates so small, however, that this transition takes a very long time. The volume of infiltrating water required to achieve this transition is estimated as 2063 water-filled pore volumes by researchers investigating the use of cementitious materials in the closure of the tank farms at the SRS (SRS 2010).

In the WCS Site Model, it is assumed that the cementitious materials behave as in Wang et al. (2009). The WCS Site Model uses the equation:

$$\text{time to transition} = \text{WaterMassForTransition} \times \text{MCCConcretePerArea} / \text{WaterMassFlux_Waste}$$

where

WaterMassForTransition is the mass of water required to make the transition from one state of concrete to the next state,

MCCConcretePerArea is the average thickness of concrete across the site, and

WaterMassFlux_Waste is the infiltration rate of water, expressed in terms of the mass of water.

To estimate the time of transition for the WCS Andrews County facility, the following values in the above equation are used:

- WaterMassForTransition = 350 kg/m³ (Wang et al. (2009) State I to State II transition)
- MCCConcretePerArea = concrete volume / disposal area = ~6.9 m for CWF, ~4.8 for FWF
- WaterMassFlux_Waste = 0.0 kg/m²/yr (from HYDRUS modeling)

Since the infiltration rate is zero, the resulting time to transition is infinite. The cementitious materials used in the waste disposal system in Andrews County are therefore expected to remain in a “young” condition (the first pH plateau in the figure) for an extremely long time.

For K_d s in cementitious materials there are no WCS site-specific data available. Serne et al. (2009) did perform tests using a cement-equilibrated leachate in WCS soils, but the results were inconclusive, and these are different conditions from those of a cementitious porous medium at any rate. Literature values have therefore been used to develop probability distributions for K_d in cementitious materials for C, Cl, and I. These input distributions are presented in the following sections.

4.3.1 Carbon

The carbon K_d value is a difficult empirical value to derive under the high-pH conditions that would exist in a cementitious environment. Under such conditions inorganic carbon will be solubility-limited, and will precipitate as calcite (calcium carbonate, CaCO₃). Wang et al. (2009) identify the final “State IV” where the all cement has been replaced by calcite. Precipitation is a different physical process from sorption. Tests show, however, that there is considerable precipitation of inorganic ¹⁴C when spiked into simulated cement leachate, and this is difficult to differentiate from a high K_d (Serne et al. 2009).

In the site-specific study by Serne et al. (2009), adding inorganic ¹⁴C to the simulated cement leachate led to the vast majority of the radioactivity disappearing from the solution as a precipitate (e.g. calcite). It is important to recognize that the study by Serne et al. (2009) is not equivalent to conditions in cementitious materials themselves, but is rather a simulated high-pH water mixed with the sandstone or clay that is found below the waste repository. Nevertheless,

the study shows that inorganic carbon is solubility-limited and therefore has little potential to transport while in a high-pH environment when calcium is available, as it is in cementitious materials.

Wang et al. (2009) present a very detailed analysis on the forms of ^{14}C produced in nuclear reactors and their subsequent fate before being shipped to typical LLW burial grounds. They estimate that at least two-thirds of the ^{14}C will arrive at burial facilities as inorganic carbon (HCO_3^- and H_2CO_3). The remainder is carbon tightly bound within activated metals, which after very slow corrosion also will yield mainly inorganic ^{14}C as the mobile species. In young cement-dominated environments (above pH 10), the divalent carbonate anion dominates in any solution, and its solubility is controlled by calcite. When portlandite controls the dissolved calcium concentration, the precipitation of calcite lowers the carbonate concentrations in solution to values below $8 \times 10^{-6} \text{ M}$ (8 μM), a very low concentration compared to mM (millimolar) quantities often found in natural pore- and ground-waters (Krupka et al. 2004).

For portlandite-buffered cementitious materials, Wang et al. (2009) present in Table 57 of that report a best estimate carbon K_d value of 5000 mL/g, with a range of 2000 to 20,000 mL/g. Note that Wang et al. (2009) present results as R_d , which are experimentally-derived values. In section 2.4 of that document, they state that “Therefore, R_d is a general term to be used instead of K_d suggesting that equilibrium may not be achieved, the sorption process may not be linear and reversible. For use in SA [Safety Analysis (equivalent to performance assessment)], where retardation factors ... are used, assuming reversible and linear sorption, R_d values will be used to represent K_d values.”

Krupka et al. (2004, Tables 5.3 and 5.4, Zone 1b – Near Field/Cementitious Secondary Waste) recommend that cement-based solids used in subsurface disposal facilities either as structures (i.e. containers) or waste solidification agents (i.e. grouted wastes) be assigned carbon K_d values of 20 mL/g for young cements, with a range from 10 to 1000 mL/g. These K_d values were obtained from the aforementioned published studies and all values and ranges presented are considered in developing a distribution for carbon K_d .

The input distribution for the K_d of carbon in cementitious materials is derived as a log-normal distribution. In order to arrive at a distribution that fits the disparate information from Krupka et al. (2004) and Wang et al. (2009), a median (50th percentile) value is set at 500 mL/g, and a 95th percentile at 10,000 mL/g. The preliminary recommended distribution for carbon K_d in cementitious materials is thereby a log-normal distribution, with a geometric mean of 500 mL/g, and a geometric standard deviation of 6.18 mL/g. The median value of 500 mL/g is recommended for use in deterministic modeling.

4.3.2 Chlorine

Wang et al. (2009) provide detailed reviews of chlorine adsorption and possible solubility constraints for chlorine in all stages of cement aging and under both high and low chloride concentration conditions. Since at this point we do not know what chloride concentrations to expect in the WCS waste cell environment, we use both conditions to inform the distribution. Under low chloride concentrations, portlandite-buffered (State II) cement would have a recommended chlorine K_d value of 50 L/kg (50 mL/g) for, with a range from 10 to 200 mL/g.

For high chloride conditions, the recommended K_d value of 1 mL/g, with a range from 0.2 to 10 mL/g (Table 17 in Wang et al., 2009). Krupka et al. (2004) recommend that young cement be attributed a chlorine K_d value of 8 mL/g, with a range from 0.8 to 25 mL/g, again from Table 5.3 in that document.

The K_d distribution for chlorine is fit using a log-normal distribution, using a median value of 10 mL/g, based on the recommended values of 1, 8, and 50 mL/g. A reasonable maximum value (95th percentile) used for the fit is 100 mL/g, based on the maxima of 10, 25, and 2000 mL/g.

The preliminary recommended distribution for chlorine K_d in cementitious materials is a log-normal distribution, with a geometric mean of 10 mL/g, and a geometric standard deviation of 4.06 mL/g. The median value of 10 mL/g is recommended for use in deterministic modeling.

4.3.3 Iodine

For portlandite-buffered cementitious materials, Wang et al. (2009) present in Table 19 a best estimate iodine K_d value of 10 mL/g, with a range of 0 to 1000 mL/g. Krupka et al. (2004) presents values of 20 mL/g with a range of 10 to 150 mL/g. Interestingly, Wang et al.'s expected value is the most conservative value presented by Krupka et al. For iodine in high-pH environments, however, the lower reported K_d values in the literature are deemed less appropriate than the middle of the reported range, based on discussions from Krupka et al. (2004) and Wang et al. (2009).

The K_d distribution for iodine is fit using a log-normal distribution, using the geometric mean of the recommended values of 8 mg/L and 20 mL/g to determine a median value of 14.1 mL/g. A reasonable maximum (95th percentile) value used for the fit is 387 mL/g, a geometric mean of the maxima 150 and 1000 mL/g.

The preliminary recommended distribution for iodine K_d in cementitious materials is a log-normal distribution, with a geometric mean of 14.1 mL/g, and a geometric standard deviation of 7.48 mL/g. The median value of 14.1 mL/g is recommended for use in deterministic modeling.

4.3.4 Other Radioelements

All other radioelements adopted the same values for cementitious materials that were used in previous LA modeling, as tabulated for the "Waste" in Table 1-1 of Appendix 5 of WCS (2011).

5.0 Aqueous Solubility

In keeping with the assumptions of the License Application and the Oct 2011 WCS GoldSim Model, solubility is modeled only for those radioelements shown to be significant contributors to dose. In GoldSim, the lack of any solubility limit is indicated by setting the solubility to the value "-1" (any units), and this indication has been made for most radioelements in the WCS Site Model.

Solubility of some elements was examined more closely for the latest version of the PA model. These elements are: C, Cl, I, Ra, Tc, and U. These are the elements most likely to be under

saturated conditions in the waste layer and possibly in the layers immediately outside the waste layer.

Solubility distributions were chosen for two different water chemistries: meteoric water (neutral pH and low TDS) and cementitious water (pH of around 12 - 12.5 and saturated with portlandite, a calcium hydroxide mineral). Because of the low water contents throughout most of the disposal layers, oxidized conditions generally were assumed. The exception to this assumption was that for technetium in cement, a distribution was given because of the likelihood of cement to be under more reducing conditions if flue dust or iron shavings were added to the cement mixture. It is not clear how long the reducing conditions would last, although they could potentially last for a long time. Recent studies (e.g., Apted 2012) have investigated additions of flue dust or iron shavings to cement to create a localized reducing environment for immobilizing or slowing down the transport of contaminants that are highly sensitive to redox conditions, such as technetium. The effects of adding flue dust or iron filings to grouts will be investigated further under PA maintenance.

5.1 Solubility in Fresh Water

5.1.1 Carbon

Carbon is expected to be found in the waste in potentially several different forms, including metallic carbon and potentially organic carbon. For this version of the PA model, it is assumed that all carbon is inorganic, for simplification. According to Lindsay (1979), inorganic carbon solubility is often controlled by equilibrium with the partial pressure of CO₂ in the soil. Typically, this partial pressure is found to be somewhere around atmospheric pressure to 10 times atmospheric pressure, with the higher pressure due to soil microbial activity. Thus it follows from Lindsay 1979 that the solubility of neutral pH soils is around 10⁻⁷ to 10⁻⁴ mol/L.

The final input distribution for carbon solubility in fresh water is LU(min = 10⁻⁷ mol/L, max = 10⁻⁴ mol/L).

5.1.2 Chloride

Chlorine is highly soluble and 1 mol/L was considered a reasonable solubility approximation for the Yucca Mountain TSPA (LANL 1997). This is also used for a high value in the WCS PA for both neutral and basic pH values. Silver may be present in small amounts, since Ag-108m is a reported radionuclide. This would limit the solubility to 10⁻⁵ mol/L, which is the solubility of silver chloride. This value is used as the low value for Cl-36 solubility.

The final input distribution for chlorine solubility in fresh water is LU(min = 10⁻⁵ mol/L, max = 1 mol/L).

5.1.3 Iodine

Iodine can form a number of oxidation states, but within the Eh and pH conditions expected at the Andrews County facility, iodine is expected to exist in the -1 oxidation form, I⁻. This is consistent with the modeling provided by EPA (2004). In addition to dissolving and sorbing reactions, iodine can also volatilize to the gas phase either as I₂ (molecular iodine) or hydrogen

iodide and organic (e.g. methyl) iodides. Iodine is not likely to form minerals due to the highly oxidizing conditions. After literature review and further consideration of site conditions, iodine remains infinitely soluble in the PA model, with a solubility value of -1 mol/L.

Below, for technetium a closer look was given at the potential to include iron filings or flue dust to provide a more reducing environment. Until more details about the potential long-term effect of these amendments to cement are investigated, infinite solubility is assumed for iodine.

The final input distribution for iodine solubility in fresh water is -1, implying no solubility limit.

5.1.4 Radium

In nature, radium only exists in the II oxidation state and is generally present as an uncomplexed Ra^{2+} ion in the pH range of 3 to 10 (EPA 2004). Radium behaves similarly to barium and forms a co-precipitate in the presence of sulfate $[(\text{Ba,Ra})\text{SO}_4]$. This co-precipitate would likely control the solubility at the WCS site if radium were reach saturation levels. At Yucca Mountain, the radium solubility used in the TSPA ranged from 10^{-9} to 10^{-5} mol/L, with an expected value of 10^{-7} mol/L (LANL 1997). This assessment assumed: 1) well water sampled was similar to groundwater at Yucca Mountain, 2) oxidizing conditions, and 3) solubilities would be determined by the far-field environment. For the WCS Site Model, this same 10^{-9} M to 10^{-5} M range is used for both meteoric and cementitious waters.

The final input distribution for radium solubility in fresh water is LTri(*min* = 10^{-9} mol/L, *expected* = 10^{-7} mol/L, *max* = 10^{-5} mol/L).

5.1.5 Technetium

Technetium can exist in multiple oxidation states, but VII is dominant under oxidizing conditions (EPA 2004, Langmuir 1997, Wildung et al. 2004). In oxidizing conditions the species is the oxyanion TcO_4^- which is highly soluble and is not known to form complexes. Under slightly reducing conditions technetium exists as an uncharged hydroxide. Under stronger reducing conditions technetium can form a very insoluble solid. For the WCS Site Model, with the oxidizing conditions at the waste site, Tc is assigned infinite solubility for meteoric water.

The final input distribution for technetium solubility in fresh water is -1, implying no solubility limit.

5.1.6 Uranium

The uranium waste received by WCS will mostly be in the uranium oxide form U_3O_8 with lesser amounts (e.g., the Savannah River DU) in the UO_3 form. The U.S. DOE has characterized U_3O_8 as insoluble (DOE 1999; DOE 2001). It is not easy to discern exactly what solid phase will control the solubility of uranium. U(VI) oxide, schoepite, is commonly used as the solubility-controlling solid to predict uranium solubilities for models (DOE 2011). There are other uranium solids that may control its solubility, such as uranophane, soddyite, calcium uranate, becquerelite, or sodium uranate (DOE 2011). In the WCS Site Model, we use schoepite to model uranium solubility in fresh waters, which ranges from 10^{-6} to 10^{-3} mol/L (Jang et al. 2006). However, studies have shown that actual uranium solution concentrations in cement leachates

are significantly lower than those for schoepite. Future versions of the model could include a refinement for U solubility, such that something less conservative than schoepite is assumed to control U solubility.

The final input distribution for chlorine solubility in fresh water is LU($min = 10^{-6}$ mol/L, $max = 10^{-3}$ mol/L).

5.1.7 Other Radioelements

The interim input distribution for solubility for all other radioelements in fresh water is -1, implying no solubility limit. This is consistent with previous modeling submitted with the LA, but may change under PA maintenance.

5.2 Solubility in Cement-Equilibrated Water

As noted in the discussion above about stages of cement degradation, the principal consideration in evaluating water chemistry in cements is that of pH. Solubility for a given chemical element is controlled by chemical speciation, which depends on oxidation states, but this is more a function of reduction/oxidation mechanisms than it is on pH. So, for many radioelements, there is no essential difference in aqueous solubility limits between meteoric and cement-equilibrated water, and solubilities remain unchanged. However, in the case of technetium, the presence of additives to the cement may influence its oxidation state. This radioelement, therefore, has different solubility limits depending on the water type.

5.2.1 Carbon

The cement likely contains carbon in the form of carbonate, which may make carbon less soluble than for meteoric water. The addition of flue dust may also affect carbon solubility. Since there is some ambiguity, for the current PA model, carbon solubility in cement is given as the same as that in meteoric water.

The final input distribution for carbon solubility in cement-equilibrated water is the same as for fresh water: LU($min = 10^{-7}$ mol/L, $max = 10^{-4}$ mol/L).

5.2.2 Chloride

The final input distribution for chlorine solubility in cement-equilibrated water is the same as for fresh water: LU($min = 10^{-5}$ mol/L, $max = 1$ mol/L).

5.2.3 Iodine

The final input distribution for iodine solubility in cement-equilibrated water is the same as for fresh water: -1, implying no solubility limit.

5.2.4 Radium

The final input distribution for radium solubility in cement-equilibrated water is the same as for fresh water: LTri($min = 10^{-9}$ mol/L, $expected = 10^{-7}$ mol/L, $max = 10^{-5}$ mol/L).

5.2.5 Technetium

Since technetium is highly sensitive to changes in redox conditions, and since it can play a large role in doses at the surface because of diffusion of technetium upward in the model, it was appropriate to take a closer look at Tc solubility and put forth a refined input distribution for Tc in cementitious waters. At pH 12, and assuming the addition of iron filings or flue dust can provide a sustained reduced environment immediately around the disposed waste, Tc solubility can be based on TcO_2 . A likely value of 10^{-7} with error bars of approximately an order of magnitude was based on Apted (2012). From this figure, estimates of the 5th, 50th, and 95th percentiles of a log-normal distribution were assumed to be: 9.01×10^{-9} , 1×10^{-7} , and 9.01×10^{-7} mol/L, respectively. A log-normal distribution was fit to these solubility values, with a resulting geometric mean of 1.0263×10^{-7} mol/L and geometric standard deviation of 3.7518.

The final input distribution for carbon solubility in cement-equilibrated water is LN(GM = 1.0263×10^{-7} mol/L, GSD = 3.7518).

5.2.6 Uranium

The final input distribution for uranium solubility in cement-equilibrated water is the same as for fresh water: LU(*min* = 10^{-6} mol/L, *max* = 10^{-3} mol/L).

5.2.7 Other Radioelements

The interim input distribution for solubility for all other radioelements in cement-equilibrated water is -1, implying no solubility limit. This is consistent with previous modeling submitted with the LA, but may change under PA maintenance.

6.0 Air/Water Partition Coefficients (K_H)

Most volatile solutes exist to varying degrees in both air and water. In the absence of other processes, a solute will partition between air and water phases in a given proportion (for a given temperature), following Henry's Law. The ratio of the concentration of a chemical in water to its concentration in air is known as its Henry's Law constant, which can have many functional forms. The principal airborne radionuclides of interest in the modeling of radioactive wastes disposed at the WCS Andrews Facility are ^3H , ^{14}C , ^{39}Ar , ^{85}Kr , ^{129}I , and the isotopes of radon (^{222}Rn in particular).

Henry's Law constants are provided by Sander (1999, Table 7, p.6) for H as H_2 , I as I_2 (*ibid.*, p.11), Ar, Kr, and Rn (*ibid.*, p.13), and C as CO_2 (*ibid.* p. 57). These constants are defined using a form of Henry's Law that relates the partial pressure of the solute in the gas above the water to the concentration of the water:

$$K_{H,cp} = \frac{c}{p}$$

where

$K_{H,cp}$ is the Henry's Law constant relating c to p , in units of mol/L·atm
 c is the concentration of the solute, in mol/L, and
 p is the partial pressure of the solute in the gas phase, in atm.

This Henry's Law constant must be converted to the dimensionless form—a ratio of the concentration in water to that in gas (air):

$$K_H = \frac{C_{(water)}}{C_{(air)}}$$

This conversion is done using the following equation:

$$K_H = \frac{1}{K_{H,cp} R T_{soil}}$$

where

R is the ideal gas constant (8.314 J/mol-K), and
 T_{soil} is the soil temperature.

The gas constant R is conveniently provided as a defined constant in GoldSim. The K_H values in Table 1 for modeled gases are consistent with previous modeling. Standard deviations for the normal distributions are provided.

7.0 Ionic and Molecular Diffusion Coefficients in Water

The diffusion coefficient (D_m) is required for calculating the movement of solutes due to differences in concentration gradient. Movement by diffusion can occur without advective flow of water. Ionic and molecular diffusion coefficients are derived in theory from the Stokes-Einstein equation:

$$D_m = \frac{R T}{6 \pi \eta_B r_A}$$

where

R is universal gas constant,
 T is temperature,
 η_B is absolute viscosity of the solvent (water), and
 r_A is radius of the assumed spherical solute.

A variety of empirical equations have been derived based on the Stokes-Einstein equation for different scenarios. For a dilute solution of a single salt the diffusion coefficient can be derived

from the Nernst-Haskell equation (Reid et al., 1987). This equation includes the valence of the cation and anions as well as ionic conductances. Specific ionic conductances are required for each cation and anion species. When two or more chemical species are present at different concentrations, interdiffusion (counterdiffusion) must be included to satisfy electroneutrality (Lerman 1979). For a geochemical system as large as that found in radioactive waste disposal facilities this quickly becomes too complex to model, even if ionic conductivities are available for each species.

An additional difficulty in deriving ion-specific diffusion coefficients lies in the large number of potential ions. Over 60 radioelements modeled in the WCS Site Model, and for each element in this list one can expect multiple forms. For example, U has four redox states, and many soluble species for each of these. Assuming oxic conditions, U will be primarily found as $\text{UO}_2(\text{CO}_3)_3^{4-}$, $\text{UO}_2(\text{CO}_3)_2^{2-}$, and UO_2CO_3 , but there are at least eight additional forms of U(+VI) that may be found. Thus the potential number of ions that would need to be included in the model would easily be in the hundreds. Obtaining the parameters for each species that would be required to model the ionic diffusion would be difficult.

Given these issues with developing ion-specific values of D_m , the approach used in modeling diffusion in the WCS Site Model is to use a range of D_m values. This range can be derived from Table 3.1 in Lerman (1979). For conditions near 25°C, the range of D_m for the elements of interest is 4×10^{-6} to 2×10^{-5} cm²/s. For cooler temperatures, which would be expected in the deeper subsurface, the values are somewhat lower. The values for 25°C are reproduced in the Table below.

Based on these values, the diffusion coefficient is represented in the WCS Site Model as a normal distribution with a mean of 1×10^{-9} cm²/s and a standard deviation of 1×10^{-12} cm²/s, and a single default value is used to represent all radioelements.

Table 6. Diffusion coefficients for selected cations and anions

Cation	D_m (10^{-6} cm ² /s)	Anion	D_m (10^{-6} cm ² /s)
K ⁺	19.6	Cl ⁻	20.3
Cs ⁺	20.7	I ⁻	20
Sr ²⁺	7.94	IO ³⁻	10.6
Ba ²⁺	8.48		
Ra ²⁺	8.89		
Co ²⁺	6.99		
Ni ²⁺	6.79		
Cd ²⁺	7.17		
Pb ²⁺	9.45		
UO ₂ ²⁺	4.26		

Cation	D_m ($10^{-6} \text{ cm}^2/\text{s}$)	Anion	D_m ($10^{-6} \text{ cm}^2/\text{s}$)
Al^{3+}	5.59		

Source: Table 3.1 in Lerman (1979)

8.0 Diffusion Coefficients in Air

Several of the modeled radioelements are volatile, and exist in the air (gas) phase, as discussed in Section 6.0 on Henry's Law constants. Volatile species will diffuse in water according to the molecular diffusion coefficient discussed above, and will simultaneously diffuse in air, all while honoring the Henry's Law partitioning ratio. The air phase diffusion coefficient governs the rate at which a particular gaseous radionuclide will diffuse in air, given a concentration gradient. While the WCS Site Model determines the rate of radionuclide transport using internal GoldSim diffusion functions, the free-air diffusivity for each volatile radioelement still must be specified. These coefficients are well-established for these gases, with little uncertainty, and are collected as deterministic values in Table 4, with data sources noted.

9.0 References

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