523407

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 7 May 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Parameter Record Package for Colloidal Actinide Source Term Parameters

Attached is the Parameter Record Package for the WIPP PA parameters describing actinide concentrations associated with mobile **actinide intrinsic colloids**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy with Attachments to:

MS 1320 Hans W. Papenguth, 6748
MS 1320 W. George Perkins, 6748

DOE/CAO Robert A. Stroud

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.
SWCF-A:WPO# 35852: Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids

copy without Attachments to:

MS 1320 E. James Nowak, 6831
MS 1324 Susan A. Howarth, 6115
MS 1328 Hong-Nian Jow, 6741
MS 1328 Amy S. Johnson, 6741
MS 1328 Martin S. Tierney, 6741
MS 1328 Mary-Alena Martell, 6749
MS 1341 John T. Holmes, 6748

Information Only

Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 2. Actinide Intrinsic Colloids

The parameter values in this package are based on data which were collected under the guidance of the Principal Investigator for the Waste Isolation Pilot Plant (WIPP) Colloid Research Program, Hans W. Papenguth, for input to the WIPP Data Entry Form and for use in WIPP Performance Assessment (PA) calculations.

I. *Parameter No. (id):* Not applicable.

II. *Data/Parameter:* Not applicable.

III. *Parameter id (idpram):* CONCINT.

IV. *Material:* Intrinsic colloids of actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am.

VI. *Units:* Concentrations of actinide intrinsic colloids (CONCINT) are in units of "moles colloidal actinide per liter of dispersion."

VII. *Distribution Information.*

A. *Category:* The development of parameter values and their distributions is described in Attachment A. Summaries of the parameter values are presented in Attachments C, E, and F. Constant CONCINT values are supplied for all five actinide elements listed above.

B. *Mean:* See Attachments A, C, E, and F.

C. *Median:* Not applicable.

D. *Standard Deviation:* Not applicable.

E. *Maximum:* See Attachments A, C, E, and F.

F. *Minimum:* See Attachments A, C, E, and F.

G. *Number of data points:* Not applicable.

VIII. *Data Collection and Interpretation Information.*

A. *Data Source Information:* WIPP observational data and literature.

B. *Data Collection (for WIPP observational data).*

1. *Data Collection or Test Method:* Experiments were conducted at Lawrence Livermore National Laboratory (LLNL; contract number AG-4965; Cynthia E. A. Palmer, LLNL PI). Descriptions of experiments conducted at LLNL are included in Attachment A.

2. *Assumptions Made During Testing:* See Attachment A.

Information Only

3. *Standard Error of Measurement of Tests Performed:* See Attachment A.

4. *Form of Raw Data:* Data on actinide concentration associated with actinide intrinsic colloids is reported in molarity.

5. *References Related to Data Collection:* See Attachment A.

6. *QA Status of Data:*

   a. *Are all of the data qualified?* Yes.

   b. *Were data qualified by QAP 20-3?* No. Data packages will be submitted for work conducted at LLNL (see VIII,B,1 above for contract numbers), under File code WBS 1.1.10.2.1.

   c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes. LLNL (contract number AG-4965) was audited twice by SNL (94-04; EA95-13). DOE/CAO conducted a surveillance (S-96-08). LLNL is scheduled to be audited by SNL (EA96-22) in May 1996.

   d. *Were the data collected under an SNL approved QA program?* Yes. Data were collected under SNL WIPP QAPD, Rev. P, effective October 1, 1992, and SNL WIPP QAPD, Rev. R, effective July 31, 1995. LLNL conducted work under an approved QAPP prepared especially for their program (WIPP Actinide Source Term Test Program Quality Assurance Program Plan (LLNL WIPP-LLNL-NCD-ETG-CS-QAPP, Rev. 0-CN1). Data were collected under a test plan for the WIPP Colloid Research Program (Papenguth and Behl, 1996). Detailed descriptions of the experiments and interpretation listed herein will be published in a SAND report. Documents related to data collection at LLNL will be archived in the Sandia WIPP Central Files (SWCF; File code WBS 1.1.10.2.1).

C. *Interpretation of Data.*

1. *Was the interpretation made by reference to previous work.* No.

2. *Was the interpretation made by using newly performed calculations?* Yes.

3. *Form of Interpreted Data.* List of interpreted values.

4. *Assumptions Made During Interpretation.* See Attachment A.

5. *Name of Code(s)/Software used to Interpret Data:* Not applicable.

6. *QA Status of Code(s) used to Interpret Data:* Not applicable.

   a. *Was the code qualified under QAP 19-1?* Not applicable.

   b. *Was the code qualified under QAP 9-1?* Not applicable.

7. *References Related to Data Interpretation:* See XI below and Attachment A.

Information Only

8. *For interpretations made by using a newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B.* The data analysis is controlled by Analysis Plan for the Colloid Research Program, AP-004 (Behl and Papenguth, 1996).

9. *For routine calculations (not using code) did you follow requirements of QAP 9-5?* Yes.

IX. *Correlation with other Parameters:* None.

X. *Limitations or qualifications for usage of data by Performance Assessment (PA):* None.

XI. *References cited above:*

Behl, Y.K., and Papenguth, H.W., 1996, Analysis Plan for the WIPP Colloid Research Program WBS #1.1.10.2.1, SNL Analysis Plan AP-004.

Papenguth, H.W., and Behl, Y.K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

XII. *Attachments:*

Attachment A: Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids.

Attachment B: Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Attachment C: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Attachment D: Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Attachment E: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Attachment F: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

XIII. *Distribution*

SWCF-A:WPO# 35852: Mobile-Colloidal Actinide Source Term. 2. Actinide Intrinsic Colloids.

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Information Only

Attachment A:

Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids.

Information Only

Attachment A.
Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids

Hans W. Papenguth

Introduction

The actinide source term at the WIPP is defined as the sum of contributions from dissolved actinide species and mobile colloidal actinide species. The dissolved actinide source term has been defined elsewhere (Novak, 1996; Novak and Moore, 1996; Siegel, 1996). It is important to note that colloidal actinides which are not suspended in the aqueous phase (i.e., not mobile) are not included in the colloidal actinide source term. Colloidal actinides may become immobilized by several mechanisms, including precipitation followed by coagulation and gravitational settling (humic substances and actinide intrinsic colloids), adhesion to fixed substrates (microbes), and flocculation or coagulation of colloidal particles followed by gravitational settling (mineral fragments). Sorption of colloidal actinides onto fixed substrates will also reduce the mobile colloidal actinide source term, but no credit is currently being taken for reduction by that means.

To facilitate quantification of the colloidal actinide source term, as well as an efficient experimental approach, the source term has been divided into four components according to colloid types. On the basis of (1) the behavior of colloidal particles in high ionic strength electrolytes, (2) the way in which colloidal particles interact with actinide ions, and (3) the transport behaviors of colloidal particles, four colloidal particle types are recognized (Papenguth and Behl, 1996): mineral fragments, actinide intrinsic colloids, humic substances, and microbes.

In this document, we focus on the quantification of the actinide concentration mobilized by actinide intrinsic colloidal particles. In terms of the WIPP performance assessment (PA) calculations, we discuss the rationale for selecting the values corresponding to the following parameter designators:

idpram:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids.
idmtrl:	Th	thorium [i.e., Th(IV)];
	U	uranium [i.e., U(IV) and U(VI)];
	Np	neptunium [i.e., Np(IV) and Np(V)];
	Pu	plutonium [i.e., Pu(III) and Pu(IV)]; and
	Am	americium [i.e., Am(III)].

Information Only

Actinide intrinsic colloids (also known as true colloids, real colloids, type I colloids, and Eigenkolloide) form by condensation reactions of hydrolyzed actinide ions and consist solely of actinide cations linked by anions. There are several stages in the development of actinide intrinsic colloids at which they have significantly different behaviors. When immature, actinide intrinsic colloids display physicochemical properties that are similar to ionized humic substances. With age, they become more similar to mineral-fragment type colloidal particles.

The experimental approach used was strongly influenced by reviews of published literature on actinide intrinsic colloids. Pertinent literature is discussed below (see also Papenguth and Behl, 1996).

Intrinsic Colloids of Plutonium

The most well-known and well-studied actinide intrinsic colloid is the Pu(IV) intrinsic colloid, which has been used as a basis of comparison for investigating intrinsic colloids of other actinides. Most of the knowledge about the Pu(IV) intrinsic colloid comes from research at high Pu concentrations in highly acidic solutions, which was conducted to help improve the efficiency of processing techniques. The Pu(IV) intrinsic colloid is notorious in its propensity to polymerize to form a gel-like material, which can even plug process lines.

A conclusive demonstration of the mechanisms of formation of the Pu(IV) intrinsic colloid has not yet been made, but there is a preponderance of evidence that suggests that polymerization is strongly linked to hydrolysis, and that the initial polymerization, or condensation, produces a macromolecule that becomes progressively more crystalline with time. The final mature colloid has a composition between $Pu(OH)_{4\ (amorphous)}$ and $PuO_{2\ (crystalline)}$, although the latter compound may be only partly crystalline and both may include interstitial water molecules.

The most convincing and consistent explanation for the chemistry of the Pu(IV) intrinsic colloid is presented by Johnson and Toth (1978) of Oak Ridge National Laboratory. Those authors developed a conceptual model to explain the solution chemistry of a variety of metal cations and a variety of oxidation states. The conceptual model involves processes referred to as "olation" and "oxolation" in which metal cations become bridged with hydroxyl groups, which in turn undergo irreversible elimination of water and concurrent formation of oxygen bridges. Johnson and Toth demonstrate that the model is consistent with the observed behavior of the Pu(IV) intrinsic colloid.

Information Only

Hydrolysis reactions for metal cations such as plutonium may be written as follows:

first: $Pu^{4+}_{(aq)} + H_2O \leftrightarrow PuOH^{3+}_{(aq)} + H^+$ (1)

second: $PuOH^{3+}_{(aq)} + H_2O \leftrightarrow Pu(OH)^{2+}_{2\,(aq)} + H^+$ (2)

third: $Pu(OH)^{2+}_{2\,(aq)} + H_2O \leftrightarrow Pu(OH)^{+}_{3\,(aq)} + H^+$ (3)

fourth: $Pu(OH)^{+}_{3\,(aq)} + H_2O \leftrightarrow Pu(OH)^{0}_{4\,(aq)} + H^+$ (4)

Johnson and Toth point out, however, that in interpreting the formation of the Pu(IV) intrinsic colloid, it makes better sense to include the implied waters of hydration that surround metal cations in solution. Hydrolysis equations (1) through (4) can be rewritten as follows, where n equals 4:

first: $[Pu(H_2O)_m]^{n+} \leftrightarrow [Pu(OH)(H_2O)_{m-1}]^{n-1} + H^+$ (5)

second: $[Pu(H_2O)_{m-1}]^{n-1} \leftrightarrow [Pu(OH)(H_2O)_{m-2}]^{n-2} + H^+$ (6)

third: $[Pu(H_2O)_{m-2}]^{n-2} \leftrightarrow [Pu(OH)(H_2O)_{m-3}]^{n-3} + H^+$ (7)

fourth: $[Pu(H_2O)_{m-3}]^{n-3} \leftrightarrow [Pu(OH)(H_2O)_{m-4}]^{n-4} + H^+$ (8)

From the literature, it is clear that polymerization occurs nearly immediately after the first hydrolysis occurs (5). Johnson and Toth suggest the following reaction involving polymerization of two hydrolyzed species by loss of water (oxolation):

$$2\{[(H_2O)_{d-2}Pu(OH)(H_2O)]^{+(y-1)}\} \leftrightarrow [(H_2O)_{d-2}Pu(OH)(OH)Pu(H_2O)_{d-2}]^{+2(y-1)} + 2H_2O \quad (9)$$

Aging or maturation of polymer then occurs by loss of water (olation) as follows:

$$Pu(OH)(OH)Pu(OH)(OH)Pu(OH)(OH)\cdots] \rightarrow [Pu(O)Pu(O)Pu(O)\cdots]_n + 3nH_2O \quad (10)$$

Maiti et al. (1989) and Laul et al. (1985) describe similar reactions, but it appears as though they believe that the third hydrolysis reaction occurs, because they use the $Pu(OH)^{+}_{3\,(aq)}$ ion in their proposed polymerization reaction. Use of that ion does not appear to be consistent with observations by many workers that polymerization occurs immediately after the first hydrolysis reaction.

As the actinide polyelectrolytes mature through the olation process to become closer in composition to an actinide-oxide mineral, they will be kinetically destabilized by the high ionic strengths of the WIPP brines, and will not be mobile. Further, the solubilities of the mature solid phase cannot be exceeded. In fairly long-term experiments, Nitsche et al. (1992, 1994) showed

Information Only

that the concentration of Pu(IV) intrinsic colloid stabilized at about 10^{-8} M. It is not known whether the form was Pu(IV) polyelectrolyte or Pu(IV) mineral fragment type colloid.

Intrinsic Colloids of other Actinides

Reference is made to a variety of intrinsic colloids of other actinides, but no systematic investigations of their formation and behaviors appear to have been made. Plutonium is apparently unique in its propensity to form an intrinsic colloid. No mention is made in the literature of maturation of polyelectrolytes of other actinides to form mineral fragment type colloidal particles as plutonium does.

In general, the tendency of actinides to hydrolyze and to polymerize to form intrinsic colloids follows the order:

$$An^{4+} >> An(VI)O_2^{2+} > An^{3+} > An(V)O_2^{+} \qquad (11)$$

where An represents an actinide element (Cleveland, 1979a,b; Choppin, 1983; Kim, 1992; Lieser et al., 1991, p. 119). The order of oxidation states in the equation above results from the ionic charge to ionic radius ratios. The tendency for hydrolysis of $An(VI)O_2^{2+}$ is greater than for An^{3+} because the effective charge on the central cation on the linear $[O\text{-}An\text{-}O]^{2+}$ ion is 3.3±0.1, slightly greater than 3. This trend generally holds true for the actinide elements in general, because of the very small changes in ionic radii among the actinide elements (this is the oxidation state analogy; refer to Novak, 1996). There are differences in the behaviors of the actinides from element to element that stem from very subtle changes in the charge to radius ratio and the nature of the configuration of the f molecular orbital.

Considering Pu as an example, hydrolysis becomes significant for Pu^{4+}, $Pu(VI)O_2^{2+}$, Pu^{3+}, and $Pu(V)O_2^{+}$ at pH values of <1, 4-5, 6-8, and 9-10, respectively (Choppin, 1983). On the basis of the hydrolysis trend, it is not likely that An(III) and An(V) actinides will form actinide intrinsic colloids. That group includes Pu^{3+}, Am^{3+}, $Pu(V)O_2^{+}$, and $Np(V)O_2^{+}$. There are suggestions in the literature, however, that Am^{3+} may form an intrinsic colloid, which is surprising because it does not undergo hydrolysis until relatively high pH values. Thorium does not follow the trend described by equation (11) because its large size makes it resistant to hydrolysis (Cotton and Wilkinson, 1988). Nevertheless, thermodynamic data suggest that in almost all environments (near neutral or higher pH) thorium exists as $Th(OH)^0_{4(aq)}$. Moreover, thorium has been reported to form a polymer (Kraus, 1956; Johnson and Toth, 1978), although as discussed below, should be referred to as an oligomer.

Information Only

Examples can be found in the literature of polymeric species of many of the actinides of importance to WIPP (see e.g., Baes and Mesmer, 1976; Kim, 1992). It is important, however, to note the sizes of polymers described in the literature. It is well known that as polyvalent metals, the actinides can form polynuclear species, but they are largely lower polymers (i.e., oligomers) such as dimers, trimers, tetramers, and hexamers (see, e.g., Choppin, 1983, p. 46). However, in terms of physical transport behavior, lower polymers will behave no differently than dissolved monomeric species. In contrast, the higher polymers, such as the Pu(IV)-polymer, may reach colloidal sizes (1 nm to 1 μm) and will have different hydrodynamic properties than the sub-colloidal-sized dissolved species. Johnson and Toth (1978) reported a molecular weight of 4000 for a Th polymer. Assuming that it consisted of $Th(OH)_4$, that polymer would consist of about 13 thorium metal ions (i.e., the degree of polymerization number, N). That observation is consistent with Kraus (1956), in which he quotes an N value of about 9 for Th polyelectrolyte.

Empirical evidence published in the literature does not always support the suggestion that Am, as a trivalent cation, will form an intrinsic colloidal particle. Avogadro and de Marsily (1984) suggested that, like Pu, Am is a likely candidate to form an insoluble hydroxide. Buckau et al. (1986) reported the formation of Am(III) intrinsic colloids at near neutral pH conditions, with a particle size greater than 1 nm. In their study of the hydrolysis of Am(III) over a pH range from 3 to 13.5, however, Kim et al. (1984a) found only monomers of Am. Regardless of whether Am(III) intrinsic colloids will form under highly idealized laboratory environments, it would be highly unlikely that they would form in a geologic system, because of the tremendously strong sorption properties of the Am(III) ion.

Experimental

Because of the absence of conclusive evidence in the literature that intrinsic colloids of Th, U, Np, and Am develop to sizes large enough to affect transport behavior, the focus of the experimental program was on Pu. A variety of screening experiments were conducted at Lawrence Livermore National Laboratory (LLNL; contract number AG-4965, Cynthia E. A. Palmer, LLNL PI) to test phenomena described in the published literature, under WIPP-relevant conditions:

- Critical coagulation concentration for mature Pu(IV) mineral fragment type colloid (refer to description of experiment AIC-1 in Papenguth and Behl, 1996);
- formation of Pu(IV) colloid, from oversaturation and undersaturation in the absence of carbon dioxide (AIC-8 and AIC-9, respectively);
- inhibition of Pu(IV) polymerization due to organic complexants (AIC-2);
- depolymerization of Pu-colloid due to organic complexants (AIC-2b);

Information Only

- polyelectrolyte chain termination by non-actinide metal cations (AIC-4); and
- sorption effects of WIPP repository substrates on Pu(IV) colloid (AIC-5).

The last four experiments listed above provide evidence that, under some conditions at the WIPP, the Pu(IV)-colloid is less likely to form or is sorbed. To parameterize the WIPP PA calculations, however, the first two experiments listed above were used. Both sets of experiments (AIC-1, AIC-8/9) can essentially be viewed as solubility experiments. The critical coagulation experiments are solubility experiments conducted from undersaturation conditions, in which the in-growth of free Pu(IV) is observed (and are therefore equivalent to AIC-9). In both sets of experiments (AIC-1, AIC-8/9), the Pu solution concentration is measured as a function of time for as long as 5 weeks, as steady-state concentration is being reached. The two sets of experiments were anticipated to provide information to resolve the question of kinetic versus thermodynamic stability control on the formation and development of the Pu(IV) colloid. That question was not resolved, but the data still provide the necessary information for parameterizing the WIPP PA calculations. The values for the parameters submitted to PA were derived from the following experiments:

number	experiment	starting material	approx. pcH	[NaCl]	duration
AIC-1	c.c.c. (equivalent to undersaturation experiment AIC-9)	Pu(IV)-colloid; aged 1-month: ~2 x 10^{-4} M	4 7 10	0.001 m 0.01 m 0.1 m 0.8 m 3.0 m 5.0 m	3 to 5 weeks
AIC-8	oversaturation	Pu(IV) aquo ion: ~1 x 10^{-4} M	3 7 11	0.05 m 0.5 m 1.0 m 5.0 m	4 weeks

The data from those experiments are plotted in Figure 1 along with regression lines for data collected by Rai et al. (1980) for $Pu(OH)_{4\,(amorphous)}$ and PuO_2 and Rai and Swanson (1981) for Pu(IV)-polymer under acidic pH conditions. The current WIPP Project position is that MgO backfill will be added to control pCO_2. With MgO backfill, the pcH of the repository brine is expected to be about 9.3 (refer to Wang, 1996; also see Novak and Moore, 1996; Siegel, 1996). As shown in Figure 1, the regression line calculated from the LLNL data suggests that at a pcH of 9.3 the solubility of Pu(IV)-polymer is approximately 5 x 10^{-10} M. Because the extrapolated concentration is less than the minimum analytical detection limit (ADL) of 1 x 10^{-9} M, the ADL value was selected for use in WIPP PA calculations. The LLNL results are consistent with the extrapolated relationships based on published results of Rai et al. (1980) and Rai and Swanson (1981).

Information Only

Interpreted Results

Parameter values (CONCINT) describing the amount of actinide element bound by actinide intrinsic colloidal particles were determined from the information described above. For the Pu(IV)-polymer, the minimum ADL was selected. In the absence of conclusive evidence that intrinsic colloids of other actinides form, or form polymers rather than oligomers, the concentration of Th-, U-, Np-, and Am-intrinsic colloids was set to zero.

Geochemical conditions in the Culebra are not conducive to the formation of a new supplementary population of actinide intrinsic colloids. In particular, the concentration of actinide ions is reduced. Therefore, the source term for actinide intrinsic colloids only reflects what would form in the WIPP repository.

Summary

Interpreted values for CONCINT are summarized in Attachments C, E, and F.

References

Avogadro, A., and G. de Marsily. 1984. "The Role of Colloids in Nuclear Waste Disposal," *Scientific Basis for Nuclear Waste Management VII, Materials Research Society Symposia Proceedings, Boston, MA, November 14-17, 1983*. Ed. G.L. McVay. New York, NY: North-Holland. Vol. 26, 495-505.

Baes, C.F., Jr., and R.E. Mesmer. 1976. *The Hydrolysis of Cations*. New York, NY: Wiley Interscience.

Buckau, G., R. Stumpe, and J.I. Kim. 1986. "Americium Colloid Generation in Groundwaters and Its Speciation by Laser-Induced Photoacoustic Spectroscopy," *Journal of the Less-Common Metals*. Vol. 122, 555-562.

Choppin, G.R. 1983. "Solution Chemistry of the Actinides," *Radiochimica Acta*. Vol. 32, no. 1-3, 43-53.

Cleveland, J.M. 1979a. *The Chemistry of Plutonium*. La Grange Park, IL: American Nuclear Society.

Cleveland, J.M. 1979b. "Critical Review of Plutonium Equilibria of Environmental Concern," *Chemical Modeling in Aqueous Systems: Speciation, Sorption, Solubility, and Kinetics, 176th Meeting of the American Chemical Society, Miami Beach, FL, September 11-13, 1978*. Ed. E.A. Jenne. Washington, DC: American Chemical Society. 321-338.

Cotton, F.A., and G. Wilkinson. 1988. *Advanced Inorganic Chemistry*. 5th ed. New York, NY: John Wiley & Sons.

Information Only

Johnson, G.L., and L.M. Toth. 1978. *Plutonium(IV) and Thorium(IV) Hydrous Polymer Chemistry*. ORNL/TM-6365. Oak Ridge, TN: Oak Ridge National Laboratory, Chemistry Division.

Katz, J.J., L.R. Morss, and G.T. Seaborg. 1986. "Summary and Comparative Aspects of the Actinide Elements," *The Chemistry of the Actinide Elements*. 2nd ed. Eds. J.J. Katz, G.T. Seaborg, and L.R. Morss. New York, NY: Chapman and Hall. Vol. 2, 1121-1195.

Kim, J.I. 1992. "Actinide Colloid Generation in Groundwater," *Radiochimica Acta*. Vol. 52/53, pt. 1, 71-81.

Kim, J.I., M. Bernkopf, Ch. Lierse, and F. Koppold. 1984a. "Hydrolysis Reactions of Am(III) and Pu(VI) Ions in Near-Neutral Solutions," *Geochemical Behavior of Disposed Radioactive Waste*. Eds. G.S. Barney, J.D. Navratil, and W.W. Schulz. ACS Symposium Series 246. Washington, DC: American Chemical Society. 115-134.

Kraus, K.A. 1956. "Hydrolytic Behavior of the Heavy Elements," *Proceedings of the International Conference on the Peaceful Uses of Atomic Energy, Geneva, August 8-20, 1955*. New York, NY: United Nations. Vol. 7, 245-257.

Laul, J.C., M.R. Smith, and N. Hubbard. 1985. "Behavior of Natural Uranium, Thorium and Radium Isotopes in the Wolfcamp Brine Aquifers, Palo Duro Basin, Texas," *Scientific Basis for Nuclear Waste Management, Materials Research Society Symposia Proceedings, Boston, MA, November 26-29, 1984*. Eds. C.M. Jantzen, J.A. Stone, and R.C. Ewing. Pittsburgh, PA: Materials Research Society. Vol. 44, 475-482.

Lieser, K.H., R. Hill, U. Mühlenweg, R.N. Singh, T. Shu-De, and Th. Steinkopff. 1991. "Actinides in the Environment," *Journal of Radioanalytical and Nuclear Chemistry, Articles*. Vol. 147, no. 1, 117-131.

Maiti, T.C., M.R. Smith, and J.C. Laul. 1989. "Colloid Formation Study of U, Th, Ra, Pb, Po, Sr, Rb, and Cs in Briny (High Ionic Strength) Groundwaters: Analog Study for Waste Disposal," *Nuclear Technology*. Vol. 84, no. 1, 82-87.

Nitsche, H., K. Roberts, R. Xi, T. Prussin, K. Becraft, I. Al Mahamid, H.B. Silber, S.A. Carpenter, R.C. Gatti, and C.F. Novak. 1994. "Long Term Plutonium Solubility and Speciation Studies in a Synthetic Brine," *Radiochimica Acta, Special Issue: Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere, Proceedings of the Fourth International Conference, Charleston, SC, December 12-17, 1993*. Munich: R. Oldenbourg Verlag. Vol. 66/67, 3-8.

Nitsche, H., K. Roberts, R.C. Gatti, T. Prussin, K. Becraft, S.C. Leung, S.A. Carpenter, and C.F. Novak. 1992. *Plutonium Solubility and Speciation Studies in a Simulant of Air Intake Shaft Water from the Culebra Dolomite at the Waste Isolation Pilot Plant*. SAND92-0659. Albuquerque, NM: Sandia National Laboratories.

Novak, C. F., 1996, The Waste Isolation Pilot Plant (WIPP) Actinide Source Term Program: Test Plan for the Conceptual Model and the Dissolved Concentration Submodel, Albuquerque, New Mexico, Sandia National Laboratories, SAND95-1895 (submitted).

Novak, C. F., and Moore, R. C., 1996, Estimates of dissolved Concentration for +III, +IV, +V, and +VI Actinides in a Salado and a Castile Brine under Anticipated Repository Condtions. SNL Technical memorandum dated 28 March 1996 to Malcolm D. Siegel.

Information Only

Papenguth, H. W., and Behl, Y. K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

Rai, D., and J.L. Swanson. 1981. "Properties of Plutonium(IV) Polymer of Environmental Importance," *Nuclear Technology*. Vol. 54, no. 1, 107-111.

Rai, D., R.J. Serne, and Moore. 1980. "Solubility of Plutonium Compounds and their Behavior in Soils," *Soil Science Society of America Journal*. Vol. 44, 490-.

Siegel, M. D., 1996, Solubility parameters for use in the CCA NUTS and GRIDFLOW calculations. SNL Technical memorandum dated 29 March 1996 to Martin S. Tierney.

Wang, Y., 1996, Estimate of Repository pH and f_{CO2} Distribution for the Long-Term WIPP Performance Assessment (PA). SNL Technical memorandum dated 29 March 1996 to Martin S. Tierney and Christine T. Stockman.

Information Only

Figure 1.

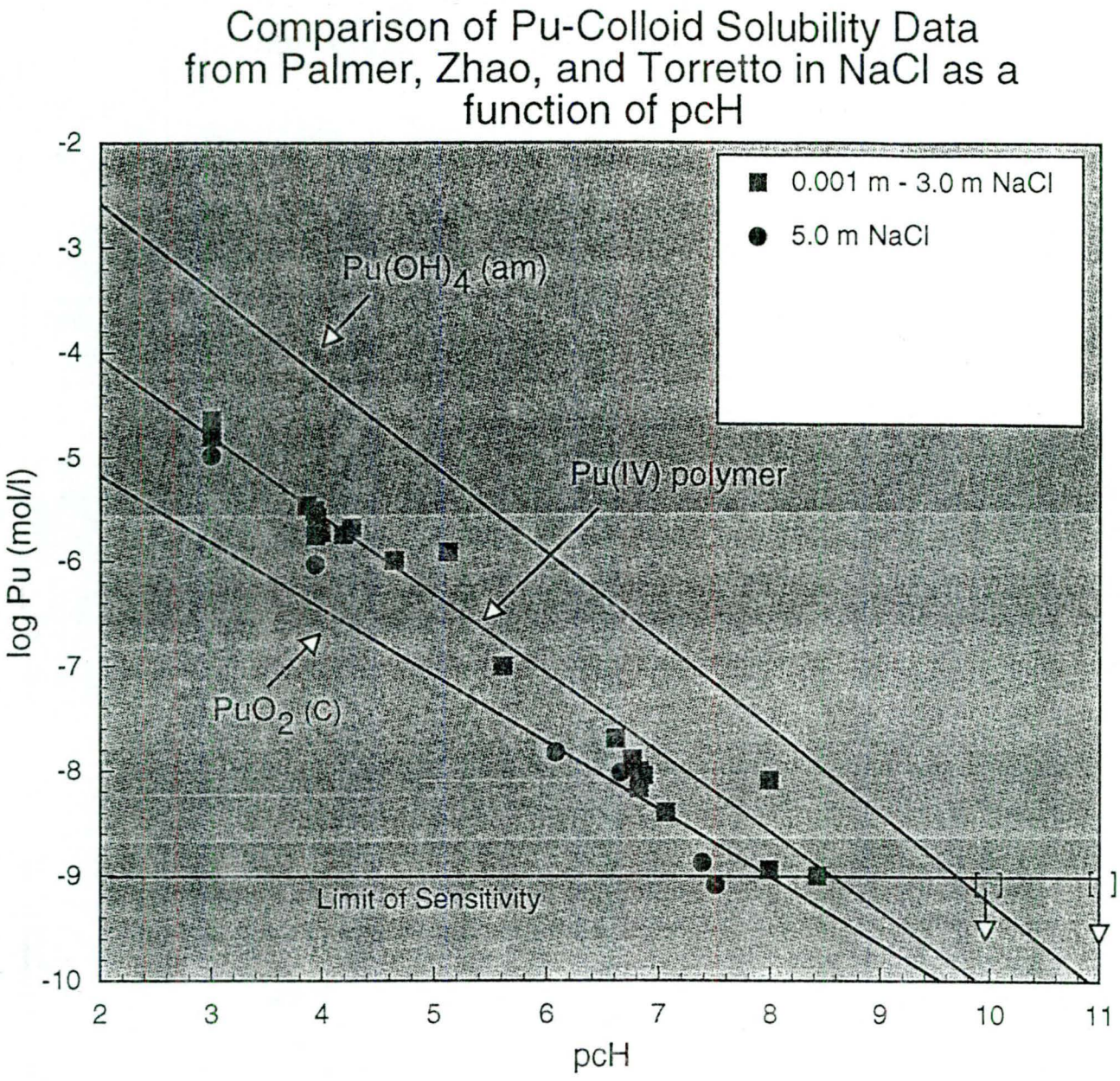

Figure 1: Solubility of Pu(IV)-polymer as a function of pcH+. Open brackets with arrows pointing down indicate that Pu concentration is below the Limit of Sensitivity. Note: Solubility lines for $Pu(OH)_4$ and PuO_2 are extrapolated from Rai, Serne, and Moore, *Soil Sci. Soc. Am. J.*, **44**, 490, (1980). Solubility line for Pu(IV) polymer is extrapolated from Rai and Swanson, *Nuc. Tech.*, **54**, 107, (1981)

Information Only

Attachment B:

Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Information Only

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/29/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

In order to properly model the transport of radionuclides within the Salado formation, we will need information about the possible transport of these radionuclide on colloids. In this memo we request the maximum mobilized radionuclide concentration and/or the proportionality constant defining the moles mobilized on colloid per moles in solution, for each transported element and colloid type. We are planning to transport Am, Pu, U, and Th, and may also transport Cm, Np, Ra, and Sr. If we transport Ra and Sr, we are planning to model them as very soluble, and not sorbed, so I believe modeling of colloids for them will not be necessary. For Cm solubility, we will be using the Am(III) model. If you believe that Cm colloids also behave similarly to Am colloids, we could extend the chemical analogy to the colloid behavior. If you agree with these simplifications then we will need the parameters for Am, Pu, U, Th and Np only.

Suggested names for database entry:
IDMTRL: Am, Pu, U, Th, Np

IDPRAM:

CONCINT	for concentration of actinide on mobilized intrinsic colloid
CONCMIN	for concentration of actinide on mobilized mineral fragments
CAPHUM	for maximum concentration of actinide on humic colloids
CAPMIC	for maximum concentration of actinide on microbe colloids
PROPHUM	for moles actinide mobilized on humic colloids per moles dissolved
PROPMIC	for moles actinide mobilized on microbe colloids per moles dissolved

You will need to provide a distribution for each material-parameter pair, but that distribution may be "CONSTANT" for most of the numbers. Eight sampling slots have been reserved for the most important of these parameters that have non-constant distributions.

cc:

Mary-Alena Martell	Amy S. Johnson	J. T. Schneider
Hong-Nian Jow	Martin S. Tierney	Richard V. Bynum
E. James Nowak	W. George Perkins	Ali A. Shinta
James L. Ramsey		

SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Information Only

Attachment C:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Information Only

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:

CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
CAPHUM	maximum concentration of actinide associated with mobile humic colloids
CAPMIC	maximum concentration of actinide associated with mobile microbes
PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

Information Only

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1320	E. James Nowak, 6831 EJN
MS 1320	R. Vann Bynum, 6831
MS 1341	John T. Holmes, 6748
MS 1341	Laurence H. Brush, 6748
MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748 wgp
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt O. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851

SWCF-A:WBS1.1.10.2.1

Information Only

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Information Only

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CAPHUM	Th	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
CAPHUM	U	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
CAPHUM	Np	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
CAPHUM	Pu	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
CAPHUM	Am	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the sum of actinide oxidation species for each actinide element (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used for humic-bound U or Am, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).

Information Only

Attachment D:

Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Information Only

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 4/2/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

YiFeng Wang has revised his recommendation to use 2 invariant points in the PA calculation. He now recommends that we use the $Mg(OH)_2 + MgCO_3$ invariant point for all calculations. If this invalidates the assumptions that you used to prepare colloid concentration or proportion parameters please indicate as soon as possible which parameters are affected, and as soon as possible after that provide a memo documenting the new values.

cc:
Mary-Alena Martell
Amy S. Johnson
Hong-Nian Jow
Martin S. Tierney
J. T. Schneider
Richard V. Bynum
E. James Nowak
W. George Perkins
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Exceptional Service in the National Interest

Information Only

Attachment E:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Information Only

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 18 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 1

This memorandum summarizes the revised best estimates for the mobile colloidal-actinide source term for input to the WIPP Compliance Certification Application. Values presented herein supersede the values provided to you on 29 March 1996 (Papenguth, 1996) in response to your memorandum of 29 March 1996 (Stockman, 1996a). The present memorandum addresses your request for modifications stated in your memorandum dated 2 April 1996 (Stockman, 1996b).

In the attached table, I have summarized the complete set of parameters and values for the mobile colloidal-actinide source term. Revised values for maximum actinide concentration values for humic substances and constants describing actinide concentrations associated with mineral-fragment-type colloidal particles are included. New values (i.e., corresponding to new idpram's and idmtrl's) for proportionality constants describing actinide concentrations associated with humic substances are also included.

The revisions described herein for humic substances reflect a shift in approach from proportionality constants describing actinide-humic concentration by element, to proportionality constants describing actinide-humic concentration by actinide oxidation state. That change affects treatment of actinide elements that will have multiple oxidation states in the WIPP repository [e.g., U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV)]. A second modification in approach, is that I now provide values for two cases: (1) a Castile brine in equilibrium with brucite and magnesite; and (2) a Salado brine in equilibrium with brucite and magnesite. For humic substances, the following material-parameter combinations apply:

IDMTRL: PHUMOX3 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3;

Information Only

PHUMOX4 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4;

PHUMOX5 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5; and

PHUMOX6 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6.

IDPRAM: PHUMCIM proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);

PHUMSIM proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite).

The revisions made for actinide concentration associated with mineral-fragment-type colloidal particles were made to include the potential contribution of actinide-mineral colloids formed in the Culebra. To accomplish that, the original repository source term values (Papenguth, 1996) have been doubled. That approach is not necessary for humic substances or actinide intrinsic colloids [i.e., Pu(IV)-polymer], because their concentrations are limited by solubilities. Concentrations of actinides associated with microbes are limited by the steady-state population of microbes in the repository, which will not increase when introduced to the Culebra.

The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

Information Only

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, SNL technical memorandum dated 29 March 1996 to Christine T. Stockman.

Stockman, C.T., 1996a, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 29 March 1996 to Hans W. Papenguth.

Stockman, C.T., 1996b, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 2 April 1996 to Hans W. Papenguth.

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1320	E. James Nowak, 6831
MS 1320	R. Vann Bynum, 6831
MS 1341	John T. Holmes, 6748
MS 1341	Laurence H. Brush, 6748
MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt W. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Information Only

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
revised (new)	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Information Only

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
revised	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
revised	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
revised	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
revised	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7
	Notes:							
	general	The colloidal actinide source term is added to the dissolved actinide source term.						
	general	None of the parameters are correlated.						
	1	If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.						
	2	Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.						
	3	Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).						
	4	If a distribution is not used, use the maximum concentration as a constant value.						
	5	The maximum ("cap") values are in units comparable to molarity rather than molality.						
	6	CAPHUM is compared to the concentration of the respective humic-bound actinide element.						
	7	CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).						

Information Only

Attachment F:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

Information Only

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 22 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 2

In my rush to complete and distribute Revision 1 (Papenguth, 1996), I made mistakes on the minimum and maximum values for actinide concentrations associated with mineral-fragment-type colloidal particles. The attached Table contains the correct values.

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL technical memorandum dated 18 April 1996 to Christine T. Stockman.

Information Only

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1320	E. James Nowak, 6831
MS 1320	R. Vann Bynum, 6831
MS 1341	John T. Holmes, 6748
MS 1341	Laurence H. Brush, 6748
MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt W. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Information Only

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Information Only

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7
	Notes:							
	general	The colloidal actinide source term is added to the dissolved actinide source term.						
	general	None of the parameters are correlated.						
	1	If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.						
	2	Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.						
	3	Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).						
	4	If a distribution is not used, use the maximum concentration as a constant value.						
	5	The maximum ("cap") values are in units comparable to molarity rather than molality.						
	6	CAPHUM is compared to the concentration of the respective humic-bound actinide element.						
	7	CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).						

Information Only

29 March 1996

Parameter Packages for Hans W. Papenguth (WBS 1.1.10.2.1):

#	Package Name
1	Parameter Record Package for Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
2	Parameter Record Package for Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
3	Parameter Record Package for Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
4	Parameter Record Package for Mobile-Colloidal-Actinide Source Term. 4. Microbes

Information Only

Sandia National Laboratories — WASTE ISOLATION PILOT PLANT

Document Review and Comment

Form Number: 430 **Effective: 7/31/95**

Procedure: QAP 6-3
Revision: 1
Page 1 of 1

This form may be used for test plans, procedures, reports, design packages, abstracts, and Technical Operating Procedures

Title: Parameter Record Package for Mobile-Colloidal Actinide Source Term. Part 4. Microbes

☒ Pre-Publication ☐ Post-Publication

Reviewer's Comments				Author/Designer's Response			Reviewer's Respoi	
Item No.	Ref. Loc.	Mandatory F	Comment	Accept	Reject	Reasoning	Accept	Reject
1	All		Make spelling and grammar changes indicated on pages	✓				
			indicated by editing marks					
2	Attach-	Y	Include Attachments B through F	✓				
	ments							

Reviewed By: W. George Parkins Date: 1 May 96

Response Prepared By: Hans W. Papenguth Date: 6 May 96
Author/Designer Name

Response Concurrence:
W. George Parkins Date: 8 May 96
Reviewer Name

To Be Completed on First Page Only

SWCF File Code: _____
WRS#

Information Only