523406

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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 **humic substances**. 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
MS 1341	Robert C. Moore, 6748
DOE/CAO	Robert A. Stroud

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.
SWCF-A:WPO# 35855: Mobile-Colloidal-Actinide Source Term. 3. Humic Substances

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
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MS 1341	John T. Holmes, 6748

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Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 3. Humic Substances

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):* PROPHUM, PHUMCIM, PHUMSIM, and CAPHUM.

IV. *Material:* Humic substances, which include fulvic acid, aliphatic humic acid, and aromatic humic acid, and the actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am (for PROPHUM and CAPHUM); PHUMOX3, PHUMOX4, PHUMOX5, and PHUMOX6 (for PHUMCIM and PHUMSIM).

VI. *Units:* For proportionality constants (PROPHUM, PHUMCIM and PHUMSIM), the units are "moles colloidal humic-bound actinide per moles of dissolved actinide." For the maximum concentration of each actinide associated with mobile humic colloids (CAPHUM), the units are "moles colloidal humic-bound 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 CAPHUM values are supplied for all five of the actinide elements listed. Constant PROPHUM values are supplied for Th, Np, and Pu. Constant PHUMCIM and PHUMSIM values are supplied for PHUMOX4. Triangular distributions are supplied for PROPHUM values for U and Am. Triangular distributions are supplied for PHUMCIM and PHUMSIM values for PHUMOX3, PHUMOX5, and PHUMOX6. In the event that those triangular distributions of parameter values cannot be sampled in the PA calculations, the maximum value should be selected. The decision of whether to use the distribution or the constant value is to be made by the PA Department.

B. *Mean:* See Attachments A, C, E, and F. (Note that for triangular distributions, the apices of the triangle are defined by the minimum value, the most likely value, and the maximum value; refer to Attachments).

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.

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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 Florida State University (FSU; contract number AH-5590; Greg R. Choppin, FSU PI), at Colorado School of Mines (CSM; contract number AR-9240; Bruce D. Honeyman, CSM PI), and at SNL (Hans W. Papenguth and co-workers). Descriptions of experiments conducted at those institutions are included in Attachment A.

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

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

4. *Form of Raw Data:* Solubilities of humic substances were reported in units of mg/L. Complexation of actinides by humic substances were described in terms of stability constants. Humic substance site binding density was reported in units of milliequivalents of OH^- per gram of humic substance.

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 FSU, CSM, and at SNL (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. Florida State University (contract number AH-5590) was audited by SNL (94-03 and EA95-02) and is scheduled to be audited again in May 1996 (EA96-15). Colorado School of Mines (contract number AR-9240) is working under the SNL WIPP QA Program.

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. 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 SNL, Florida State University, and the Colorado School of Mines 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.

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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.

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:* Parameter values describing the concentration of actinides associated with mobile humic substances are linked to solubility of the dissolved actinides, with a maximum value which cannot be exceeded.

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., and Moore, Robert C., 1996, Rationale for Definition of Parameter Values for Humic Substances.

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.

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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# 35855: Mobile-Colloidal Actinide Source Term. 3. Humic Substances.

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

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Attachment A:

Papenguth, Hans W., and Moore, Robert C., 1996, Rationale for Definition of Parameter Values for Humic Substances.

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Attachment A.
Rationale for Definition of Parameter Values for Humic Substances

Hans W. Papenguth and Robert C. Moore

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 humic substances. In terms of the WIPP performance assessment (PA) calculations, we discuss the rationale for selecting the values corresponding to the following parameter designators:

idpram:	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids;
	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); and

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	CAPHUM	maximum (cap) concentration of actinide associated with mobile humic 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)];
	Am	americium [i.e., Am(III)];
	PHUMOX3	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3 [i.e., Pu(III) and Am(III)];
	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4 [i.e., Th(IV), U(IV), Np(IV), and Pu(IV)];
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5 [i.e., Np(V)]; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6 [i.e., U(VI)].

Humic substances are defined as high-molecular-weight organic compounds generally present as anions in natural waters. Humic substances may consist of humic acids, which may be aliphatic or aromatic, or fulvic acids. The difference between humic acids and fulvic acids is largely an operational distinction; humic acids can be precipitated at pH values below about 2, whereas fulvic acids are soluble over the entire pH range. Fulvic acids generally have lower molecular weights than humic acids. The dominant functional group which may react with dissolved actinides are carboxyl groups, but phenolic hydroxyl and alcoholic hydroxyl groups also contribute to complexation. At the WIPP, humic substances may be introduced to the repository as a constituent of soil-bearing waste or may be a constituent of the organic carbon component of Castile, Salado, or Culebra groundwaters. Probably more importantly, humic substances may form from condensation reactions between microbial metabolites (e.g., carboxylic acids), cellulosic degradation products, and the extracellular polymers associated with microbes. Because of the general lack of knowledge in the scientific community regarding the formation and humic substances form, we have not attempted to directly quantify the amounts of humic substances likely to be introduced to the WIPP or that would form in situ. Instead, we have elected to bound the contribution of humic-bound actinides through quantification of humic-actinide complexation behavior coupled with quantification of solubilities of humic substances in WIPP-relevant brines. Regardless of the source of humic substances, the total concentration is

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limited by the solubility of humic substances in WIPP brines. The chemical nature of humic substances generated in situ cannot be predicted either, but can be bounded by the three types of humic substances.

To determine the concentration of actinides associated with humic substances, four pieces of information are required: (1) the concentration of reactive humic substance in the aqueous phase (i.e., humic solubility); (2) the binding capacity of the humic substance; (3) actinide uptake (i.e., actinide complexation constants); and (4) concentrations of actinide ions in the aqueous phase (i.e., actinide solubility). The quantification of actinide solubilities (4) is described in Novak (1996) and results are summarized in Siegel (1996). In the remainder of this document, we focus on the determination of items (1) through (3), the interpretation of that information, and the development of parameter values suitable for PA calculations.

Experimental

In general, humic substances encompass a broad variety of high-molecular-weight organic compounds. The range of their chemical behaviors, however, is covered by consideration of three types: aliphatic humic acid (generally terrestrial); aromatic humic acid (generally marine); and fulvic acid. In our work, the following humic substances were used:

FA-Suw:	fulvic acid isolated from the Suwannee River purchased from the International Humic Substances Society, Golden, Colorado;
HA_{al}-LBr:	aliphatic humic acid isolated from sediments collected from Lake Bradford, Florida, prepared by Florida State University;
HA_{al}-Ald:	aliphatic humic acid purchased from Aldrich Chemical Co., purified by Florida State University;
HA_{ar}-Gor:	aromatic humic acid isolated from groundwaters near Gorleben, Germany, obtained from Professor J.-I. Kim, Institut für Radiochemie, München; and
HA_{ar}-Suw:	aromatic humic acid isolated from the Suwannee River purchased from the International Humic Substances Society, Golden, Colorado.

Solubilities of humic substances were measured at SNL (Hans W. Papenguth and coworkers) and at the Colorado School of Mines (CSM; contract number AR-9240; Bruce D. Honeyman, CSM PI). At SNL, solubilities were measured in experiments which were conducted over periods of several weeks. The concentrations of humic substances remaining in the fluid column was determined using a scanning fluorometer, carbon coulometer, and UV/Visible light spectrophotometer, in WIPP-relevant brine simulants with FA-Suw, HA_{al}-LBr, HA_{al}-Ald, and HA_{ar}-Suw. In addition to spectroscopic data, visible inspection proved valuable. In over saturation experiments, humic substances were dissolved in deionized water under basic pH

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conditions to enhance dissolution and then added as a spike to a brine solution. In undersaturation experiments, humic substances were added directly to brine solutions and allowed to dissolve until an equilibrium was reached. In either case, an equilibrium was reached between dissolved (i.e., ionic) and precipitated humic substances. The precipitated humic substances coagulated and settled by gravity. The kinetics of precipitation were sufficiently slow that several weeks were required for equilibrium to be reached. Brine solutions consisted of a NaCl matrix with various concentrations of Ca^{2+} and Mg^{2+}. The concentration of Na^{+} in the brine had little effect on solubility except at very high concentrations, but the concentration of the divalent cations had a significant impact on humic substance solubilities. Consequently, experiments were conducted with a NaCl background electrolyte concentration with concentrations of Ca and Mg ranging from 10 mM each (representative of natural WIPP brines) to 500 mM each (representative of CaO or MgO backfill scenarios). At SNL, solubilities between approximately 1.5 mg/L and 2.0 mg/L were observed in systems containing 10 mM or greater Ca^{2+} and Mg^{2+}. For the calculations described below, the higher solubility value of 2.0 mg/L was used.

At the CSM, three humic substances (FA-Suw, HA_{al}-LBr, and HA_{ar}-Suw) were labeled with ^{14}C so that concentrations in WIPP-relevant brines could be tracked with liquid scintillation counting. That technique was anticipated to provide better analytical results because it is free from spectral interference problems of spectroscopic techniques. Because of slow precipitation kinetics, the duration of the experiment of only one week was not sufficient for equilibrium to be reached. Consequently, we elected to use the SNL results, which were conducted over a period of several weeks.

Site-binding capacity values were determined by titration at Florida State University for two humic substances (HA_{al}-LBr and HA_{al}-Ald). Those values were supplemented with values for a variety of humic substances compiled from published literature. In general, site-binding capacities for humic substances are between 3 and 6 meq OH^{-}/g, but in isolated cases are as low as about 1.5 and as high as about 9.5 meq OH^{-}/g. For the calculations described below, we used values of 4.65, 5.38, and 5.56 meq OH-/g for aliphatic humic acid, aromatic humic acid, and fulvic acid, respectively. The aliphatic humic acid value was determined from HA_{al}-LBr at FSU. The aromatic humic acid value was from Gorleben (Gohy-573). The fulvic acid value represents the mean of 11 published values for fulvic acids collected in Europe (Ephraim et al., 1995).

Actinide complexation factors for Am(III) and U(VI) binding on three humic substances (FA-Suw, HA_{al}-LBr, and HA_{ar}-Gor) were measured at Florida State University (FSU; contract number AH-5590; Greg R. Choppin, FSU PI). Complexation measurements were made at measured pH_{obs} values of approximately 4.8 and 6, conditions at which the humic substances are highly deprotonated, and actinides U and Am have not undergone hydrolysis reactions. Those conditions were chosen to maximize complexation between the humic substances and those

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actinide elements. Measurements were made in NaCl media with ionic strengths of approximately 3 and 6 molal. Those experiments were completed prior to the WIPP Project establishing the position that MgO backfill would be emplaced to scrub CO_2 and fix pcH at about 9.3. The experiments conducted at FSU represent worst-case scenarios designed to provide high-end estimates of actinide uptake by humic substances. Actinide complexation by humic substances generally decreases at basic pH values because of the reduction in actinide-complex charges due to hydrolysis reactions. In addition, the high concentrations of Mg^{2+} in solution due to the presence of MgO backfill will compete with actinides for binding sites on humic substances and reduce the actinide uptake. FSU reported the first and second stability constants defined as follows (square brackets represent concentration):

$$An + HS \leftrightarrow AnHS; \qquad b_{1;An} = \frac{[AnHS]}{[An]\,[HS]} \tag{1}$$

$$An + 2(HS) \leftrightarrow An(HS)_2; \qquad b_{2;An} = \frac{[An(HS)_2]}{[An]\,[HS]^2} \tag{2}$$

where:

HS	=	humic substance (eq OH^-/L, i.e., site-binding capacity incorporated)
An	=	actinide element
$b_{1;An}$	=	first stability constant, for 1:1 An:humic binding
$b_{2;An}$	=	second stability constant, for 1:2 An:humic binding

For the calculations described below, complexation constants were selected from the most relevant experimental conditions, which were pH_{obs} 6 and 6 molal NaCl. The following stability constants reported by FSU were used (reported as log values):

humic substance	Am^{3+}; b_1	Am^{3+}; b_2	$U(VI)O_2^{2+}$; b_1	$U(VI)O_2^{2+}$; b_2
HA_{al}-LBr	6.09±0.05	10.46±0.12	5.91±0.16	10.43±0.19
HA_{ar}-Gor	6.02±0.04	10.41±0.10	5.35±0.15	8.98±0.26
FA-Suw	4.6±0.3	8.95±0.45	not measured	not measured

The FSU results show that there is little difference in Am(III) and $U(VI)O_2^{2+}$ uptake by aliphatic and aromatic humic acids, but that uptake by fulvic acid is significantly less. The FSU results also show that an increase of NaCl ionic strength from 3 to 6 has little effect on actinide uptake. Those observations aid in justifying the use of published stability constants for other actinide elements experimentally determined at lower ionic strengths and for other humic substances. On

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the basis of the similarities in stability constants for Am(III) and $U(VI)O_2^{2+}$ for the humic acids, we have used the Am(III) stability constant for FA-Suw for $U(VI)O_2^{2+}$ on FA-Suw.

Stability constants for Th(IV) with several humic and fulvic acids were reported by Nash and Choppin (1979). In NaCl media at pH values between 3.95 and 5.03, those authors reported log stability constants between 9.7 and 13.2. Under basic conditions expected in the WIPP repository, it is likely that complexation of Th(IV) will be markedly less, because the dominant Th(IV)-bearing aqueous species will be $Th(OH)_4^0$ (Novak and Moore, 1996). As far as we know, no investigations of Th-complex binding on humic substances have been made. For the calculations described herein, we have elected to use published results from Baskaran et al. (1992) describing the distribution of Th(IV) in sea water. From that work, a ratio of dissolved versus colloidal Th(IV) of 6.349 was calculated, assuming that the solubility of colloidal organic material in sea water is equivalent to our measured value of humic substances in WIPP-relevant brines (i.e., 2.0 mg/L). The nature of the humic substances is likely to be dominated by aromatic humic acid, but may also contain fulvic acid.

For the calculations described herein, we use a log stability constant for $Np(V)O_2^+$ of 3.67 measured at pH 9 for a Gorleben humic acid (Gohy-573; Kim and Sekine, 1991). Results presented in Rao and Choppin (1995) for Lake Bradford humic acid and a Gorleben humic acid (Gohy-573) show little effect of pH on Np(V) stability constants, presumably because of the lack of hydrolysis of reactions for Np(V) over the pH range those authors studied. The Gorleben humic acid is aromatic in nature.

No published stability constants were found for plutonium. For the calculations described herein, we use an oxidation state analogy for the plutonium oxidation species, which we believe is conservative. Allard et al. (1980) have shown that at pH 9, Pu(IV) undergoes hydrolysis reactions to a greater extent than Th(IV), which should result in reduced complexation of Pu(IV).

We also used an oxidation state analogy to develop parameter values for elements expected to have multiple oxidation states in the WIPP repository. Oxidation speciation of the actinide elements was evaluated as part of the dissolved actinide source term program. Weiner (1996) has concluded that in the WIPP repository, the following species will be present: Th(IV); U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV); and Am(III). The relative concentrations of oxidation species of a particular element are designated by their respective solubility values. The substitutions made following the oxidation state analogy are summarized in the following table:

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required binding constant	substitute	source of data
Th(IV)	Th(IV)	Baskaran et al. (1992)
U(IV)	Th(IV)	Baskaran et al. (1992)
U(VI)	U(VI)	WIPP-specific data, FSU
Np(IV)	Th(IV)	Baskaran et al. (1992)
Np(V)	Np(V)	Kim and Sekine (1991)
Pu(III)	Am(III)	WIPP-specific data, FSU
Pu(IV)	Th(IV)	Baskaran et al. (1992)
Am(III)	Am(III)	WIPP-specific data, FSU

To compensate for the effects of competition for actinide complexation by the high concentrations of calcium and magnesium in repository brines in the presence of MgO backfill, stability constants for Ca^{2+} and Mg^{2+} were used in simultaneously solved equations (described below). Stability constants for Ca^{2+} and Mg^{2+} at basic pH values are not available, but several published reports provide values in the acidic range. Choppin and Shanbhag reported log stability constants of 2.25 to 3.32 for Ca^{2+} in 0.1m $NaClO_4$ at pH 3.9 and 5.0 for an aliphatic humic acid (Aldrich humic acid). Schnitzer and Skinner (1966) reported log binding constants ranging from 2.2 to 3.72 for Ca^{2+} in low ionic strength solutions over a pH range of 3.5 to 5.0 for fulvic acid. For Mg^{2+}, Schnitzer and Skinner (1966) reported log stability constants ranging from 1.23 to approximately 2.0 under the same experimental conditions. For our calculations, we used a log stability constant of 2.0 for the sum of Ca^{2+} and Mg^{2+} concentrations, which we believe is a conservative value.

Binding of Ca^{2+} and Mg^{2+} to humic substances is described in the same way as equation (1) above:

$$(Ca+Mg) + HS \leftrightarrow (CaMg)HS; \qquad b_{1;Ca,Mg} = \frac{[(Ca+Mg)HS]}{[Ca+Mg]\,[HS]} \tag{3}$$

where:

$b_{1;CaMg}$ = first stability constant, for 1:1 (Ca+Mg):humic binding (note that no second stability constants exists for divalent cation binding)

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Interpretation of Experimental and Literature Results

Proportionality constants (PROPHUM, PHUMCIM, and PHUMSIM) describing the amount of actinide element bound to humic substances were determined from the data listed above, coupled with dissolved actinide concentrations. In addition, maximum theoretical concentrations of actinides that could be associated with humic substances (CAPHUM) were calculated from the data above.

The concentration of an actinide element of a given oxidation state was calculated by simultaneous solution of equations (1) and (3), combined with a mass-balance expression:

$$[HS_{tot}] = [AnHS] + [(CaMg)HS] + [HS] \quad (4)$$

where:

$[HS_{tot}]$	=	total concentration of humic substance
$[HS]$	=	concentration of uncomplexed humic substance
$[AnHS]$	=	concentration of humic complexed with an actinide element
$[(CaMg)HS]$	=	concentration of humic complexed with divalent cations

Equation (2) describing the effect of two humic substances binding with one actinide ion was disregarded for these calculations, because its contribution to the total humic-bound actinide concentrations was negligible.

Rearranging equations (1) and (3) provides:

$$[AnHS] = b_{1;An}\,[An]\,[HS] \quad (5)$$

$$[(CaMg)HS] = b_{1;CaMg}\,[Ca+Mg]\,[HS] \quad (6)$$

Substituting equations (5) and (6) into equation (4) results in:

$$[HS_{tot}] = b_{1;An}\,[An]\,[HS] + b_{1;Ca,Mg}\,[Ca+Mg]\,[HS] + [HS] \quad (7)$$

Rearranging equation (7) provides:

$$[HS] = \frac{[HS_{tot}]}{b_{1;An}\,[An] + b_{1;CaMg}\,[Ca+Mg] + 1} \quad (8)$$

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Equations (5), (6), and (8) were used to calculate humic-bound actinide concentrations ([AnHS]). The resulting AnHS concentration values were then summed for actinide elements with multiple oxidation states, and then divided by the dissolved concentration of the respective actinide element. The final forms of the parameter values PROPHUM, PHUMCIM, and PHUMSIM are proportionality constants in units of "moles humic-bound colloidal actinide per mole of dissolved actinide." In WIPP PA calculations, the proportionality values may be multiplied by the dissolved actinide concentration expressed in molarity or molality, depending on what the desired final unit should be. Note, however, that dissolved actinide element concentration to be used in that calculation must not include complexes containing commercial organic complexants (e.g., EDTA).

Depending on the intrusion scenario, the WIPP repository may be dominated by Castile brine or by intergranular Salado brine, resulting in different actinide solubilities. In addition to brine type, commercial organic complexants such as EDTA affect actinide solubilities. Finally, actinide solubilities are dependent on the mineral assemblage (either brucite plus magnesite, or portlandite plus calcite) buffering the system. On the basis of those scenarios, Siegel (1996) provided solubility parameters for the following eight brine compositions:

idpram	brine	invariant point	organic complexants
SOLSIM	Salado	$Mg(OH)_2$-$MgCO_3$-CO_2	absent
SOLSIC	Salado	$Ca(OH)_2$-$CaCO_3$-CO_2	absent
SOLCIM	Castile	$Mg(OH)_2$-$MgCO_3$-CO_2	absent
SOLCIC	Castile	$Ca(OH)_2$-$CaCO_3$-CO_2	absent
SOLSOM	Salado	$Mg(OH)_2$-$MgCO_3$-CO_2	present
SOLSOC	Salado	$Ca(OH)_2$-$CaCO_3$-CO_2	present
SOLCOM	Castile	$Mg(OH)_2$-$MgCO_3$-CO_2	present
SOLCOC	Castile	$Ca(OH)_2$-$CaCO_3$-CO_2	present

In determining the concentration of humic-bound actinides, we assume that dissolved actinides complexed with commercial organic complexants are not available for interaction with humic substances. Therefore the brines listed above with organic complexants present can be disregarded herein. Wang (1996) conducted calculations which demonstrate that the brines buffered by portlandite plus calcite will not be present in the WIPP repository. Therefore, those brines can be disregarded. For determination of humic-bound actinide concentrations, therefore, we are left with two brine types, designated by SOLSIM and SOLCIM above. The solubilities of actinides of oxidation states III, IV, V, and VI in those brines were provided by Siegel (1996) (solubility values are listed in molality):

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IDPRAM:	IDMTRL: SOLMOD3	IDMTRL: SOLMOD4	IDMTRL: SOLMOD5	IDMTRL: SOLMOD6
SOLSIM	4.4e-6	5.0e-6	2.6e-6	1.0e-5
SOLCIM	4.1e-7	6.8e-9	2.5e-6	1.0e-5

In our calculations described herein, those values were used. Concentrations of Ca^{2+} and Mg^{2+} in those two brines were obtained from Novak and Moore (1996).

Calculations are summarized in three tables. Tables 1a and 1b are calculations using equations (5), (6), and (8) to determine humic-bound actinide concentrations ([AnHS]) for one or more humic substance type for Am(III), Th(IV), Np(V), and U(VI). In Tables 2a through 2f, results of Tables 1a and 1b are transferred to facilitate summing humic-bound actinide concentrations for actinide elements with multiple oxidation species. The oxidation state analogy is most heavily drawn on for plutonium, because stability constants for Pu(III) or Pu(IV) are not available.

In Table 3, results of Tables 2a through 2f are summarized according to brine type and humic substance type. Table 3 was used to formulate the final PROPHUM, PHUMCIM, and PHUMSIM parameter values provided to PA. For americium and uranium (i.e., III and VI oxidation states, respectively), for which the greatest amount of information is available, we have calculated a "most-likely value" for humic-bound actinide concentration by taking the largest values for fulvic acid, aromatic humic acid, and aliphatic humic, and calculated the arithmetic mean. We recommend that a triangular distribution be established about that "most-likely value." The "minimum value" and "maximum value" correspond to the largest humic-bound actinide concentrations associated with fulvic acid and aliphatic humic acid, respectively. For thorium, plutonium, and neptunium (i.e., IV, V, and V oxidation states, respectively), for which less information is available, we have used the largest humic-bound actinide value for each as the "most-likely value." No distribution is recommended for those three actinide elements. For uranium and americium, in the event that the distributions of parameter values cannot be sampled in the PA calculations, we recommend that the maximum value be used as a constant value. The decision of whether to use the distribution or the constant value is to be made by the PA Department.

The PROPHUM idpram, used in conjunction with idmtrls Th, U, Np, Pu, or U, is designed to be used to calculate actinide-humic concentration by element. The PHUMCIM and PHUMSIM idpram's, used in conjunction with idmtrls PHUMOX3, PHUMOX4, PHUMOX5, or PHUMOX6, provides the means to calculate actinide-humic concentrations by actinide oxidation state and for different brine intrusion scenarios. The latter approach may be more analogous to the approach used to determine concentrations of dissolved actinide elements in the repository. For example, in an E1 scenario under "reducing conditions" in the WIPP repository, PHUMCIM

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would be used with the following idmtrls to determine actinide-humic concentrations: thorium = PHUMOX4; uranium = PHUMOX4; neptunium = PHUMOX4; plutonium = PHUMOX3; and americium = PHUMOX3. For an E2 scenario under "oxidizing conditions" in the WIPP repository, PHUMSIM would be used with the following idmtrls to determine actinide-humic concentrations: thorium = PHUMOX4; uranium = PHUMOX6; neptunium = PHUMOX5; plutonium = PHUMOX4; and americium = PHUMOX3.

Uncertainties due to analytical precision are small compared to uncertainties in knowledge of the dominant humic substance type, site binding densities, and actinide solubilities. The proportionality factor approach coupled with the plus or minus one order-of-magnitude uncertainty in actinide solubilities results in a plus or minus one order-of-magnitude uncertainty in the concentration of actinides bound by mobile humic substances.

The CAPHUM parameter simply represents the theoretical maximum concentration of actinides that can be bound by a humic substance. Based on a solubility limit concentration of humic substances of 2.0 mg/L, and the highest site-binding capacity (for fulvic acids) of 5.56 meq OH^-/g, the theoretical maximum is 1.1 x 10^{-5} eq/L (refer to Tables 1a and b, column 4). Assuming the conservative case in which actinide species are monovalent, the maximum theoretical concentration of actinides that can be bound by humic substances is 1.1 x 10^{-5} molar. Note that that number is conservative, because it assumes a pool of humic substances is available for each actinide element, when in reality, actinide elements will compete for the same pool of humic substances. CAPHUM is intended to be used in an expression such as the following:

[AnHS] = MIN(AnHS value calculated using PROPHUM, 1.1e-5) (9)

Summary

Interpreted values for PROPHUM, PHUMCIM, PHUMSIM, and CAPHUM are summarized in Attachments C, E, and F.

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Table 1a. Complexation of actinides with humic substances in Castile brine in the presence of magnesium oxide backfill.

	pH	Am(III)	Th(IV)	Np(V)	U(VI)	Mg+Ca
Dissolved Actinide Concentration (molality)	9.24	4.12E-07	6.78E-09	2.53E-06	1.00E-05	5.76E-02

Actinide	Type of humic Substance	humic substance total amount mg/L	humic substance meq OH^-/g	humic substance total capacity eq/L	$\beta_{1;An}$	$\beta_{1;(MgCa)}$	$[HS]_{free}$ molality	[An-HS] molality	[(MgCa)-HS] molality	Check sum: humic substance total cap. eq/L
Am(III)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	1.64E-06	2.69E-08	9.45E-06	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	1.23E+06	1.00E+02	1.28E-06	6.49E-07	7.37E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	1.05E+06	1.00E+02	1.50E-06	6.45E-07	8.62E-06	1.08E-05
Th(IV)	Constant ratio of humic bound actinide conc. to dissolved actinide conc. of 6.34 used in all calculations.									
Np(V)	Lake Bradford Humic Acid	2	4.65	9.30E-06	3.16E+02	1.00E+02	1.38E-06	1.10E-09	7.92E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	4.68E+03	1.00E+02	1.59E-06	1.88E-08	9.17E-06	1.08E-05
U(VI)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	1.55E-06	6.18E-07	8.95E-06	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	8.13E+05	1.00E+02	6.25E-07	5.08E-06	3.60E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	2.24E+05	1.00E+02	1.20E-06	2.68E-06	6.89E-06	1.08E-05

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Table 1b. Complexation of actinides with humic substances in Salado brine in the presence of magnesium oxide backfill.

	pH	Am(III)	Th(IV)	Np(V)	U(VI)	Mg+Ca
Dissolved Actinide Concentration (molality)	8.69	4.39E-06	4.98E-06	2.64E-06	1.00E-05	5.42E-01

Actinide	Type of humic Substance	humic substance total amount mg/L	humic substance meq OH^-/g	humic substance total capacity eq/L	$\beta_{1;An}$	$\beta_{1;(MgCa)}$	$[HS]_{free}$ molality	[An-HS] molality	[(MgCa)-HS] molality	Check sum: humic substance total cap. eq/L
Am(III)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	2.01E-07	3.51E-08	1.09E-05	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	1.23E+06	1.00E+02	1.53E-07	8.29E-07	8.32E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	1.05E+06	1.00E+02	1.80E-07	8.27E-07	9.75E-06	1.08E-05
Th(IV)	Constant ratio of humic bound actinide conc. to dissolved actinide conc. of 6.34 used in all calculations.									
Np(V)	Lake Bradford Humic Acid	2	4.65	9.30E-06	3.16E+02	1.00E+02	1.68E-07	1.41E-10	9.13E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	4.68E+03	1.00E+02	1.95E-07	2.41E-09	1.06E-05	1.08E-05
U(VI)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	2.00E-07	7.96E-08	1.08E-05	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	8.13E+05	1.00E+02	1.47E-07	1.19E-06	7.96E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	2.24E+05	1.00E+02	1.87E-07	4.19E-07	1.02E-05	1.08E-05

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Table 2a. Concentration of dissolved and fulvic acid complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				moles fulvic acid bound actinide/ moles dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	6.2E-02
Fulvic-U concentration		*		6.18E-07	
Np					
dissolved concentration		6.78E-09	2.53E-06		*
Fulvic-Np concentration		*	*		
Pu					
dissolved concentration	4.12E-07	6.78E-09			*
Fulvic-Pu concentration	*	*			
Am					
dissolved concentration	4.12E-07				6.5E-02
Fulvic-Am concentration	2.69E-08				
Th					
dissolved concentration		6.78E-09			*
Fulvic-Th concentration		*			

* no available information

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Table 2b. Concentration of dissolved and fulvic acid complexed actinide for each oxidation state in Salado brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole fulvic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		4.98E-06		1.00E-05	8.0E-03
Fulvic-U concentration		*		7.96E-08	
Np					
dissolved concentration		4.98E-06	2.64E-06		*
Fulvic-Np concentration		*	*		
Pu					
dissolved concentration	4.39E-06	4.98E-06			*
Fulvic-Pu concentration	*	*			
Am					
dissolved concentration	4.39E-06				8.0E-03
Fulvic-Am concentration	3.51E-08				
Th					
dissolved concentration		4.98E-06			*
Fulvic-Th concentration		*			

* no available information

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Table 2c. Concentration of dissolved and Gorleben humic acid (aromatic) complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	2.7E-01
Humic-U concentration		4.30E-08		2.68E-06	
Np					
dissolved concentration		6.78E-09	2.53E-06		2.4E-02
Humic-Np concentration		4.30E-08	1.88E-08		
Pu					
dissolved concentration	4.12E-07	6.78E-09			1.6E+00
Humic-Pu concentration	6.45E-07	4.30E-08			
Am					
dissolved concentration	4.12E-07				1.6E+00
Humic-Am concentration	6.45E-07				
Th					
dissolved concentration		6.78E-09			6.3E+00
Humic-Th concentration		4.30E-08			

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Table 2d. Concentration of dissolved and Gorleben humic acid (aromatic) complexed actinide for each oxidation state in Salado brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		4.98E-06		1.00E-05	2.1E+00
Humic-U concentration		3.16E-05		4.19E-07	
Np					
dissolved concentration		4.98E-06	2.64E-06		4.1E+00
Humic-Np concentration		3.16E-05	2.41E-09		
Pu					
dissolved concentration	4.39E-06	4.98E-06			3.5E+00
Humic-Pu concentration	8.27E-07	3.16E-05			
Am					
dissolved concentration	4.39E-06				1.9E-01
Humic-Am concentration	8.27E-07				
Th					
dissolved concentration		4.98E-06			6.3E+00
Humic-Th concentration		3.16E-05			

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Table 2e. Concentration of dissolved and Lake Bradford humic acid (aliphatic) complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	5.1E-01
Humic-U concentration		4.30E-08		5.08E-06	
Np					
dissolved concentration		6.78E-09	2.53E-06		1.7E-02
Humic-Np concentration		4.30E-08	1.10E-09		
Pu					
dissolved concentration	4.12E-07	6.78E-09			1.7E+00
Humic-Pu concentration	6.49E-07	4.30E-08			
Am					
dissolved concentration	4.12E-07				1.6E+00
Humic-Am concentration	6.49E-07				
Th					
dissolved concentration		6.78E-09			6.3E+00
Humic-Th concentration		4.30E-08			

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Table 2f. Concentration of dissolved and Lake Bradford humic acid (aliphatic) complexed actinide for each oxidation state in Salado brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		4.98E-06		1.00E-05	2.2E+00
Humic-U concentration		3.16E-05		1.19E-06	
Np					
dissolved concentration		4.98E-06	2.64E-06		4.1E+00
Humic-Np concentration		3.16E-05	1.41E-10		
Pu					
dissolved concentration	4.39E-06	4.98E-06			3.5E+00
Humic-Pu concentration	8.29E-07	3.16E-05			
Am					
dissolved concentration	4.39E-06				1.9E-01
Humic-Am concentration	8.29E-07				
Th					
dissolved concentration		4.98E-06			6.3E+00
Humic-Th concentration		3.16E-05			

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Table 3. Summary of humic substance actinide complexation in Castile and Salado brines in the presence of magnesium oxide backfill.

Actinide	Brine/ Backfill	Ratio of humic bound actinide to dissolved actinide concentration		
		Suwannee River Fulvic Acid	Gorleben Humic Acid	Lake Bradford Humic Acid
U	Castile/Mg	6.2E-02	2.7E-01	5.1E-01
	Salado/Mg	8.0E-03	2.1E+00	2.2E+00
Pu	Castile/Mg	*	1.6E+00	1.7E+00
	Salado/Mg	*	3.5E+00	3.5E+00
Am	Castile/Mg	6.5E-02	1.6E+00	1.6E+00
	Salado/Mg	8.0E-03	1.9E-01	1.9E-01
Th	Castile/Mg	*	6.3E+00	6.3E+00
	Salado/Mg	*	6.3E+00	6.3E+00
Np	Castile/Mg	*	2.4E-02	1.7E-02
	Salado/Mg	*	4.1E+00	4.1E+00

* no available information

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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.

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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

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Attachment C:

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

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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

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copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
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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

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Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

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

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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).						

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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.

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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

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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;

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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

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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.

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DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

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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).						

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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

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Attachment F:

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

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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.

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MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

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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

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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).						

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