#416348

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 **mineral fragment type 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
MS 1324 Richard Aguilar, 6851

DOE/CAO Robert A. Stroud

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.
SWCF-A:WPO# 35850: Mobile-Colloidal Actinide Source Term. 1. Mineral Fragment 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 1. Mineral Fragment Type 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):* CONCMIN.

IV. *Material:* Mineral fragment type colloidal particles and the actinides Th, U, Np, Pu, and Am.

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

VI. *Units:* For CONCMIN, the units are "moles colloidal mineral-fragment-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. Triangular distributions are supplied for CONCMIN values for each of the five actinide elements (idmtrl). 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.

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 SNL (Hans W. Papenguth and co-workers). Descriptions of experiments conducted at those institutions are described 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:* Measurements of residual concentrations of colloidal particles are reported in number population.

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, under File code WBS 1.1.10.2.1.

   c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes.

   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 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.

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 Aguilar, Richard, 1996, Rationale for Definition of Parameter Values for Mineral Fragment Type Colloidal Particles.

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# 35850: Mobile-Colloidal Actinide Source Term. 1. Mineral Fragment Colloids.

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

Attachment A:

Papenguth, Hans W., and Aguilar, Richard, 1996, Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids.

Attachment A.
Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids

Hans W. Papenguth and Richard Aguilar

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 mineral fragment type 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:	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids.
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Mineral fragment type colloidal particles may be present in naturally occurring groundwaters, and they may be released from the host rock due to disruption of fragile aggregates by changes in ionic strength or hydrodynamic forces, dissolution of a more soluble surrounding matrix, mechanical grinding of mineral surfaces, or mechanical disruption of secondary minerals present at mineral surfaces. Under certain conditions, such as extreme changes in ionic strength of the groundwater or by physical disruption due to natural or human-induced events, mineral fragment type colloidal particles could also be produced within the Culebra. In an intrusion scenario at the WIPP, mixing of repository brines with Culebra brines is likely to result in mineral precipitation which may include coprecipitation of actinide-bearing mineral fragment type colloidal particles. Within the repository, mineral fragment type colloidal particles may form from corrosion of iron-bearing waste and the steel packaging materials. In addition, Portland cement based matrixes will be attacked and will produce mineral fragment type colloidal particles. Bentonite, which may be a constituent of drilling mud is itself a potential source of mineral fragment type colloidal material that should be considered for actinide transport.

In terms of colloidal actinide transport, mineral fragment type colloids act as carriers, in that actinide ions sorb onto the surfaces of the colloids. Because each mineral substrate has a different affinity for actinides, quantification of actinide concentrations associated with the wide range of mineralogies likely to be present at the WIPP is insurmountable. Instead, we elected to use a bounding approach based on residual concentrations of colloidal particles in WIPP-relevant brines coupled with estimates of reasonable maximum concentrations of actinides which could be sorbed onto the colloid surfaces. That approach requires three pieces of information: (1) the number population of mineral fragment type colloidal particles in the aqueous phase; (2) the geometric surface area of individual colloidal particles; and (3) the site-binding capacity of the mineral surface. 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

Hydrophobic colloidal particles, such as mineral fragments, are kinetically stabilized and destabilized by electrostatic forces (refer to detailed discussion in Papenguth and Behl, 1996, Sections 2.5.1 and 2.6). In an aqueous dispersant, hydrophobic colloidal particles are attracted to one another by van der Waals forces. That electrostatic attraction is countered by repulsive forces generated by a cloud of counterions surrounding each particle. In a kinetically stable colloidal dispersion colloidal particles are usually repelled from one another before they get close enough to become agglomerated. However, as the ionic strength of the dispersion is increased, the thickness of the cloud of counterions is compressed, allowing closer particle-particle

interaction. The net effect is that as colloidal particles come into proximity with one another in the dispersion, a greater chance for sticking exists, and so the rate of agglomeration increases. That phenomenon is very effective at removing colloidal particles from suspension even at fairly low ionic strengths over periods of hours to days.

The kinetic stability of the mineral-fragment-type colloids in WIPP-relevant brines was evaluated in coagulation series experiments. Colloidal dispersions of mineral fragments were prepared by mechanical disaggregation of representative mineral, rock samples, and other materials or by chemical precipitation from laboratory reagents. Brine simulants were prepared which covered the ranges of ionic strengths observed in WIPP brines. The brines were sequentially diluted with deionized water by factors of 10 and adjusted to acidic, neutral, and basic pH conditions to evaluate the effects of ionic strength and pH on kinetic stability. At the ionic strength referred to as the critical coagulation concentration (c.c.c.), colloidal particles will rapidly coagulate, forming agglomerates large enough to settle by gravitational forces. The number population of colloidal particles remaining in suspension in the various dispersions was measured over time to assess their stability as a function of solution ionic strength and time.

Colloidal dispersions were prepared for the following minerals or materials: bentonite, kaolinite, montmorillonite, vermiculite, illite, anhydrite, calcium carbonate, magnesite, hematite (mechanically disaggregated), hematite (chemical precipitate), limonite, goethite, magnetite, quartz, siderite, brucite, strontianite, diatomaceous earth, pyrite, and cellulosic materials (Masslinn paper towels and Scott paper towels). The brine solutions used included a Salado-like brine simulant (SPC brine) and a Culebra brine simulant (H-17). For c.c.c. experiments, sequential dilutions of those brines were made which spanned approximately five orders-of-magnitude. Brine simulants consisting of 0.5M NaCl or $CaCl_2$ were also used. For the residual concentration measurements which were used as the basis for the PA deliverables described herein, the one order-of-magnitude dilution (i.e., 10 percent of original strength) of the Salado-like brine and the Culebra brine simulants were used. That reduction in ionic strength provides a degree of conservatism in the results.

C.c.c. experiments for the various concentrations of WIPP brine simulants were conducted under acidic (observed pH generally ranging from 3 to 4), neutral (pH 6 to 8), and basic (pH 9 to 12) conditions. Following the introduction of an aliquot of dispersed colloidal particles to a series of test tubes containing the sequentially diluted brine, colloidal particle concentrations remaining near the top of the fluid columns (residual concentration) were measured as a function of time. The degree of coagulation and settling was quantified using an inductively coupled argon-plasma atomic emission spectrophotometer (ICP-AES), nephelometry, and direct particle counting.

Most of the experiments conducted relating to the kinetic stability of mineral fragment colloidal particles were qualitative to semi-quantitative, and were focused on evaluating whether a c.c.c.

existed. For the final experiments, however, we used a state-of-the-art particle spectrometer designed for semiconductor fabrication plants, which require extremely pure processing water, and use a similar instrument to ascertain purity. Our final experiments were conducted over an extended period of time using that more sensitive analytical technique to determine the number and size of colloids in the brine suspensions. Those experiments were conducted in a similar fashion to previous experiments for bentonite (Aldrich Chemical Co.), goethite, and hematite (mechanically disaggregated), but in a relatively dilute (and therefore conservative) brine simulant consisting of 0.1 M NaCl. Residual particle concentrations made with the particle spectrometer compared favorably with measurements made with spectroscopic techniques made at similar experiment times. Generally after the first day of the c.c.c. experiments, the majority (greater than 99 percent) of the colloidal particles had already settled out of suspension. With the more sensitive particle spectrometer, however, residual concentrations of colloidal particles were observed to continue to decrease. For experiments analyzed by spectroscopic or light-scattering techniques, final residual colloid number populations remaining suspended in the test vessels were determined by multiplying the initial colloid number populations determined at the start of our experiments by the fraction of suspended colloids remaining at the final reading. Using the particle spectrometer, final number populations were measured directly.

Discussion

Parameter values (CONCMIN) describing the amount of actinide element bound by mineral fragment type colloidal particles were determined from the information described above, combined with estimates of adsorption site densities.

Actinides sorbed to the surfaces of colloidal particles can be estimated using ranges of values for adsorption site densities taken from published surface complexation modeling research. The actinide concentration contained by a single mineral fragment type colloidal particle is calculated by considering the geometrical surface area of a spherical particle:

$$[An]_p = \frac{\pi D^2 N_s}{N_A} \qquad (1)$$

where:

$[An]_p$	=	concentration of an adsorbed actinide element (moles/particle)
D	=	spherical colloidal particle diameter (nm)
N_s	=	adsorption site density (sites/nm^2)
N_A	=	Avogadro constant

An adsorption site density of 1 site/nm^2 was used for N_s in the above equation, a value which we believe is conservative. With that site density, 10 nm and 1 μm diameter particles could have a

maximum of about 10^{-22} and 10^{-18} moles actinide per particle, respectively. To obtain an estimate of the maximum actinide concentrations that could be associated with the colloids, the estimates of residual colloid number populations (particles per liter of dispersion) were multiplied by the estimated maximum actinide transport capacity described by equation (1). Our use of a uniform adsorption site density is a conservative approach, because the actual sorption on mineral surfaces should be described by some kind of isotherm which will result in less than 100 percent coverage.

Interpreted Results

Final residual colloid number populations quantified by spectrophotometry or nephelometry showed that mineral fragment type colloidal particles are kinetically destabilized by brines similar in composition to those present at the WIPP Site. Colloid number population values were, with a few exceptions, reduced to less than 5 percent of the initial values within 1 day. Conservative estimates of maximum actinide concentrations associated with those residual colloid populations are on the order of 10^{-7} to 10^{-9} moles actinide per liter of dispersion.

The final experiments, which utilized the particle spectrometer to measure the quantity of colloids remaining in suspension offered the most sensitive estimates. Moreover, those experiments were conducted for substantially longer periods of time than the semi-quantitative c.c.c. experiments. Those experimental results are the following:

Mineral	Time of final reading (days)	Estimated actinide concentration (moles/L dispersion)
hematite	12.8	1.6×10^{-8}
goethite	12.9	9.5×10^{-10}
bentonite	12.8	1.6×10^{-10}
geometric mean		1.3×10^{-9}

We believe that the experimental results using the particle spectrometer, although only reflecting three distinct colloids (hematite, goethite, and bentonite), are representative of other mineral fragment type colloidal particles in terms of their behavior in brine solutions. The geometric mean was assumed to be a more representative average of the final colloid concentrations than the arithmetic mean because of the very small final colloid concentrations (which, for this particular case, is also conservative).

Mineral fragment type colloidal particles are unique among the four colloidal particle types addressed for WIPP, because their concentrations are not generally linked to solubility, as are actinide intrinsic colloids and humic substances, or to a maximum supportable population in the case of microbes. Consequently, in an intrusion scenario at the WIPP, as dissolved actinide elements are introduced to the Culebra, it is possible that those dissolved actinides could sorb onto a separate population of indigenous mineral fragments, producing a supplemental source term. To account for that possibility, we recommend multiplying the geometric mean value listed above by a factor of two, producing a final "most-likely value" of 2.6×10^{-9} moles actinide per liter of dispersion.

To capture uncertainty, mainly stemming from knowledge of the adsorption site density value, we recommend a triangular distribution with "minimum values" and "maximum values" spanning one order of magnitude about the geometric mean.

Summary

Interpreted values for CONCMIN are summarized in Attachments C, E, and F. In those values, we have incorporated conservatism in two ways. First, we have increased the experimental results by a factor of two to account for the possibility that the indigenous mineral fragment colloidal particles in the Culebra could sorb dissolved actinides (see Attachment F). Second, we have essentially multiplied the total concentration of actinides carried by mineral fragment colloidal particles by a factor of five, because we have assumed a separate population of colloidal particles for each actinide element. No consideration of competition for sorption sites is incorporated into our calculation approach. We believe that the value used for adsorption site density is conservative, but reasonable. The triangular distribution of one-order-of-magnitude about the "most-likely value" essentially captures our uncertainty in site density values. If the WIPP PA Department elects to not use the triangular distribution in their calculations, we recommend that the "maximum values" be used as constant values.

References

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.

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.

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.

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.

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

Attachment C:

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

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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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

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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

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

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).

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

Attachment E:

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

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

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:

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MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

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

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).						

Attachment F:

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

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 1341	Ruth F. Weiner, 6747
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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	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

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).

WPO 42248

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 20 November 1996

to: Distribution

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6832)

subject: Addendum to Colloidal Actinide Source Term Parameter Record Packages

This document provides clarification of the derivation of the colloidal actinide source term parameters used in the 1996 Performance Assessment (PA) calculations supporting the Compliance Certification Application (CCA). The objectives of this document are to: (1) provide clarification on the algorithms and numerical values used to develop PA parameters; (2) provide indexing (a "road map") between the Parameter Record Packages and the Data Record Packages related to the development of the colloidal actinide source term parameters; and (3) document the technical reviews of the data analysis conducted to develop the parameter values. This document is a supplement to existing components of the Parameter Record Packages that have been previously submitted to the Sandia WIPP Central Files - Albuquerque (SWCF-A; WPO# 35850, 35852, 35855, and 35856).

The PA parameter values for the colloidal actinide source term used in the 1996 PA calculations in support of the CCA are listed in a memorandum to Christine T. Stockman from Hans W. Papenguth (Colloidal Actinide Source Term Parameters, Revision 2, dated 22 April 96). A photocopy of that memorandum, as well as related correspondence and request letters, is included in each of the Parameter Record Packages (WPO# 35850, 35852, 35855, and 35856).

The experimental work conducted to provide data for the development of the WIPP colloidal actinide source term values was guided by a Test Plan for that work (Papenguth and Behl, 1996). The analysis of the data was conducted under following an Analysis Plan (Behl and Papenguth, 1996). Analysis of the data and the development of parameter values is described in documents residing in the Parameter Record Packages (Papenguth, 1996a,b; Papenguth and Aguilar, 1996; and Papenguth and Moore, 1996; those documents are included as Attachment A in Packages WPO# 35852, 35853, 35850, and 35855, respectively). A technical review of those data analysis documents was conducted by Dr. W. George Perkins (copies of the signed Review Sheets are attached to this document; the complete reviews are located in the SWCF-A). The computer code COLUMN, described in the Analysis Plan (Behl and Papenguth, 1996), was <u>not used</u> in the development of the colloidal actinide source term parameter values.

HWP 11/21/96

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page 1

1. Mineral Fragment Colloids (WPO# 35850)

The names of the parameters and materials are the following:

idpram:	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Experiments were conducted at SNL (Hans W. Papenguth and co-workers).

Experiment data is compiled in Scientific Notebooks, Reports, Tables, and Figures in Data Record Package WPO# 10121; the interpretation and analysis is described in Parameter Record Package WPO# 35850 (see Papenguth and Aguilar, 1996).

2. Actinide Intrinsic Colloids (WPO# 35852)

The names of the parameters and materials are the following:

idpram:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids.
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Experiments were conducted at Lawrence Livermore National Laboratory (LLNL; contract number AG-4965; Cynthia E. A. Palmer, LLNL PI).

Experiment data is compiled in Data Record Package WPO# 41898; the interpretation and analysis is described in Parameter Record Package WPO# 35852 (see Papenguth, 1996a).

3a. Humic Substances (WPO# 35855) — Proportionality Constants

The names of the parameters and materials are the following:

idpram:	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (complexes with man-made organic ligands are not important), solubilities were calculated assuming 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 (complexes with man-made organic ligands are not important), solubilities were calculated assuming equilibrium with Mg-bearing minerals (brucite and magnesite).
idmtrl:	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)].

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). Experiment data is compiled in Data Record Packages WPO# 36475, 41970, 10121; the interpretation and analysis is described in Parameter Record Package WPO# 35855 (see Papenguth and Moore, 1996).

The following sections provide clarification of the development of PA parameter values. Note that Tables 2a-f and 3 were included in WPO# 35855, Attachment A (i.e., Papenguth and Moore, 1996) to clarify the derivation of humic proportionality constants (PROPHUM for Th, U, Np, Pu, and Am) calculated by actinide element rather than by oxidation state (refer to Papenguth and Moore, 1996). That set of parameter values was not used in PA calculations, and so it is probably best to simply disregard Tables 2a-f and 3 and rely solely

on Tables 1a and 1b, coupled with the step-by-step clarification below. The humic proportionality constants used in the 1996 PA calculations were derived as follows:

Step 1. Compile elemental concentrations. Actinide, magnesium, and calcium concentrations in Salado and Castile brines were compiled from WIPP Dissolved Actinide Solubility program and listed in Tables 1a and 1b (Papenguth and Moore, 1996). The source of those values can be found in Laboratory Notebooks and Monthly Reports contained in Data Record Packages supporting Parameter Record Package WPO# 35835, but is summarized in Novak and Moore (1996).

Step 2. Compile humic solubilities. The solubility of humic substances themselves (recorded in Scientific Notebooks and/or Reports found in Data Record Packages WPO# 10121 and WPO# 41970) is listed in Tables 1a and 1b (Papenguth and Moore, 1996).

Step 3. Compile site binding densities. The site-binding densities of humic substances are compiled in Tables 1a and 1b (WPO# 35855, Attachment A). Sources of values are described in WPO# 35855 (Papenguth and Moore, 1996, page 4, paragraph 2); see also Scientific Notebooks and Reports in Data Record Package WPO# 36475.

Step 4. Calculate total binding capacity. Total binding capacities of humic substances calculated in column 5 of Tables 1a and 1b (Papenguth and Moore, 1996).

Step 5. Compile complexation constants. Complexation constants (betas) for humic-actinide and humic-magnesium and -calcium interactions are compiled in Tables 1a and 1b (WPO# 35855, Attachment A). Sources of the values are described in WPO# 35855 (Papenguth and Moore, 1996, page 4, paragraph 3 through page 7); see also Scientific Notebooks and Reports in Data Record Package WPO# 36475.

Step 6. Calculate humic-complexation. Using the complexation constants (betas) for humic-actinide and humic-magnesium and -calcium interactions listed in Tables 1a and 1b together with the total binding capacities of humic substances, calculate the concentrations of (a) free humic substances, (b) actinide-bearing humic substances, and (c) Mg-Ca-bearing humic substances. Results are listed in Tables 1a and 1b (columns 8, 9, and 10 respectively; WPO# 35855, Attachment A). Those calculations were conducted using the expressions listed in WPO# 35855 (Papenguth and Moore, 1996, page 8, equations 8, 5, and 6 were used to calculate values in columns 8, 9, and 10, respectively, in Tables 1a and 1b in Papenguth and Moore, 1996).

Step 7. Cross-check calculations. Check the calculations by summing the concentrations of (a) free humic substances, (b) actinide-bearing humic substances, and (c) Mg-Ca-bearing humic substances and compare to the total binding capacity (i.e., in Tables 1a and 1b of Papenguth and Moore, 1996, sum columns 8, 9, and 10 and compare with column 5).

Step 8. Develop PA parameters. Divide humic-actinide concentrations "[An-HS]" by "dissolved actinide concentrations" listed in Tables 1a and 1b to produce proportionality

constants in terms of "moles colloidal humic-bound actinide per moles dissolved actinide" for each of the four oxidation states. To clarify the resulting proportionality constants, compare values in Tables 1a and 1b with Table A attached to this document.

3b. Humic Substances (WPO# 35855) — Maximum Values

The names of the parameters and materials are the following:

idpram:	CAPHUM	maximum (cap) concentration of actinide associated with mobile humic colloids.
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Development of the "CAPHUM" values (refer to WPO# 35855, Attachment A, page 11, Tables 1a and 1b) were calculated using the solubility of humic substances (Data Record Package WPO# 10121) and the highest value for binding-site density which was determined from fulvic acids (refer to Papenguth and Moore, 1996, page 4, paragraph 2), by multiplication of the solubility and binding site densities (Tables 1a and 1b, columns 3 and 4), followed by units conversion.

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).

Experiment data is compiled in Data Record Packages WPO# 36475, 41970, 10121; the interpretation and analysis is described in Parameter Record Package WPO# 35855 (see Papenguth and Moore, 1996).

4a. Microbes (WPO# 35856) — Proportionality Constants

The names of the parameters and materials are the following:

idpram:	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes.
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Experiments were conducted at Brookhaven National Laboratory (BNL; contract number AP-2273; A. J. Francis, BNL PI) and at Los Alamos National Laboratory (LANL; contract number AP-2272; Inés R. Triay, LANL PI). Work conducted at LANL was done as a collaborative effort under the guidance of the BNL PI.

Experiment data is compiled in Scientific Notebooks, Reports, Tables, and Figures in Data Record Package WPO# 41969; additional supporting data is archived in Data Record Package WPO# 41966; the interpretation and analysis is described in Parameter Record Package WPO# 35856 (see Papenguth, 1996b).

4b. Microbes (WPO# 35856) — Maximum Values

The names of the parameters and materials are the following:

idpram:	CAPMIC	maximum (cap) concentration of actinide associated with mobile microbes; and
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Experiments were conducted at Brookhaven National Laboratory (BNL; contract number AP-2273; A. J. Francis, BNL PI) and at Los Alamos National Laboratory (LANL; contract number AP-2272; Inés R. Triay, LANL PI). Work conducted at LANL was done as a collaborative effort under the guidance of the BNL PI.

Experiment data is compiled in Scientific Notebooks, Reports, Tables, and Figures in Data Record Package WPO# 41969; additional supporting data is archived in Data Record

Package WPO# 41966; the interpretation and analysis is described in Parameter Record Package WPO# 35856 (see Papenguth, 1996b).

References:

Behl, Y. K., and Papenguth, H. W., 1996, Analysis Plan for the WIPP Colloid Research Program. AP-004. Albuquerque, NM. Sandia National Laboratories.

Data Record Package WPO# 10121: Kinetic Stability/Settling Experiments.

Data Record Package WPO# 36475: Organic Ligand Complexation Data.

Data Record Package WPO# 41898: Experimental Investigation of Actinide Intrinsic Colloids.

Data Record Package WPO# 41966: Support for Microbe Experiments.

Data Record Package WPO# 41969: Microbe Experiments.

Data Record Package WPO# 41970: Investigation of Solubilities of Labeled Humic Substances.

Novak, C. F., and Moore, R. C., 1996, Estimates of Dissolved Concentrations for +III, +IV, +V, and +VI Actinides in a Salado and a Castile Brine under Anticipated Repository Conditions, memorandum to Malcolm D. Siegel, data 28 March 1996, in Parameter Record Package WPO# 35835: Solubility Parameters for use in CCA NUTS and GRIDFLOW Calculations and Actinide Solubility Tables.

Papenguth, H. W., 1996a, Rational for Definition of Parameter Values for Actinide Intrinsic Colloids, in Attachment A, Parameter Record Package WPO# 35852: Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids.

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Papenguth, H. W., and Moore, R. C., 1996, Rational for Definition of Parameter Values for Humic Substances, in Attachment A, Parameter Record Package WPO# 35855: Mobile-Colloidal-Actinide Source Term. 3. Humic Substances.

Parameter Record Package WPO# 35835: Solubility Parameters for use in CCA NUTS and GRIDFLOW Calculations and Actinide Solubility Tables.

Parameter Record Package WPO# 35850: Mobile-Colloidal Actinide Source Term. 1. Mineral Fragment Colloids.

Parameter Record Package WPO# 35852: Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids.

Parameter Record Package WPO# 35855: Mobile-Colloidal-Actinide Source Term. 3. Humic Substances.

Parameter Record Package WPO# 35856: Mobile-Colloidal-Actinide Source Term. 4. Microbes.

Parameter Record Package WPO# 38173: Colloidal Actinide Retardation Parameters.

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SWCF-A:WBS1.1.10.2.1:PDD:QA:Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids (Parameter Record Package WPO# 35850) (2)

SWCF-A:WBS1.1.10.2.1:PDD:QA:Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids (Parameter Record Package WPO# 35852) (2)

SWCF-A:WBS1.1.10.2.1:PDD:QA:Mobile-Colloidal-Actinide Source Term. 3. Humic Substances (Parameter Record Package WPO# 35855) (2)

SWCF-A:WBS1.1.10.2.1:PDD:QA:Mobile-Colloidal-Actinide Source Term. 4. Microbes (Parameter Record Package WPO# 35856) (2)

SWCF-A:WBS1.1.10.2.1:PDD:QA:Colloidal Actinide Retardation Parameters (Parameter Record Package WPO# 38173) (2)

Table A

idpram	idmtrl	type of humic substance	table number; element (oxidation state)	humic actinide concentration (dividend)	actinide solubility (divisor)	proportionality constant (quotient)	designation in PA parameter values
phumsim	phumox3	Suwannee River fulvic acid	1b; Am(III)	3.51E-08	4.39E-06	8.0E-03	"minimum value"
phumsim	phumox3	Gorleben (aromatic) humic acid	1b; Am(III)	8.27E-07	4.39E-06	1.9E-01	
phumsim	phumox3	Lake Bradford (aliphatic) humic acid	1b; Am(III)	8.29E-07	4.39E-06	1.9E-01	"maximum value"
phumsim	phumox3	mean				1.3E-01	"most likely value"
phumsim	phumox4	fulvic acid	1b; Th(IV)	N.A.	4.98E-06	N.A.	
phumsim	phumox4	(aromatic) humic acid	1b; Th(IV)	N.A.	4.98E-06	N.A.	
phumsim	phumox4	marine (aliphatic) humic acid	1b; Th(IV)	3.16E-05	4.98E-06	6.3E+00	"minimum value" and "maximum value"
phumsim	phumox4	mean				6.3E+00	"most likely value"
phumsim	phumox5	fulvic acid	1b; Np(V)	N.A.	2.64E-06	N.A.	
phumsim	phumox5	Gorleben (aromatic) humic acid	1b; Np(V)	2.41E-09	2.64E-06	9.1E-04	"maximum value"
phumsim	phumox5	Lake Bradford (aliphatic) humic acid	1b; Np(V)	1.41E-10	2.64E-06	5.3E-05	"minimum value"
phumsim	phumox5	mean				4.8E-04	"most likely value"
phumsim	phumox6	Suwannee River fulvic acid	1b; U(VI)	7.96E-08	1.00E-05	8.0E-03	"minimum value"
phumsim	phumox6	Gorleben (aromatic) humic acid	1b; U(VI)	4.19E-07	1.00E-05	4.2E-02	
phumsim	phumox6	Lake Bradford (aliphatic) humic acid	1b; U(VI)	1.19E-06	1.00E-05	1.2E-01	"maximum value"
phumsim	phumox6	mean				5.6E-02	"most likely value"

Table A

idpram	idmtrl	type of humic substance	table number; element(oxidation state)	humic actinide concentration (dividend)	actinide solubility (divisor)	proportionality constant (quotient)	designation in PA parameter values
phumcim	phumox3	Suwannee River fulvic acid	1a; Am(III)	2.69E-08	4.12E-07	6.5E-02	"minimum value"
phumcim	phumox3	Gorleben (aromatic) humic acid	1a; Am(III)	6.45E-07	4.12E-07	1.6E+00	
phumcim	phumox3	Lake Bradford (aliphatic) humic acid	1a; Am(III)	6.49E-07	4.12E-07	1.6E+00	"maximum value"
phumcim	phumox3	mean				1.1E+00	"most likely value"
phumcim	phumox4	fulvic acid	1a; Th(IV)	N.A.	6.78E-09	N.A.	
phumcim	phumox4	(aromatic) humic acid	1a; Th(IV)	N.A.	6.78E-09	N.A.	
phumcim	phumox4	marine (aliphatic) humic acid	1a; Th(IV)	4.30E-08	6.78E-09	6.3E+00	"minimum value" and "maximum value"
phumcim	phumox4	mean				6.3E+00	"most likely value"
phumcim	phumox5	fulvic acid	1a; Np(V)	N.A.	2.53E-06	N.A.	
phumcim	phumox5	Gorleben (aromatic) humic acid	1a; Np(V)	1.88E-08	2.53E-06	7.4E-03	"maximum value"
phumcim	phumox5	Lake Bradford (aliphatic) humic acid	1a; Np(V)	1.10E-09	2.53E-06	4.3E-04	"minimum value"
phumcim	phumox5	mean				3.9E-03	"most likely value"
phumcim	phumox6	Suwannee River fulvic acid	1a; U(VI)	6.18E-07	1.00E-05	6.2E-02	"minimum value"
phumcim	phumox6	Gorleben (aromatic) humic acid	1a; U(VI)	2.68E-06	1.00E-05	2.7E-01	
phumcim	phumox6	Lake Bradford (aliphatic) humic acid	1a; U(VI)	5.08E-06	1.00E-05	5.1E-01	"maximum value"
phumcim	phumox6	mean				2.8E-01	"most likely value"
Notes:							
N.A. = not available							

WPO 35855

To: Hans Papenguth

From: Vann Bynum

Date: September 16, 1997

Subject: Clarification of Humic Solubilities In CCA Appendix SOTERM

The origin and meaning of solubility value utilized for the humic substances solubilities in the Compliance Certification Application Appendix SOTERM[1], page SOTERM-59 may be unclear from the text. This value was derived from an experiment where the humic substance was added to WIPP brines containing varying concentrations of Ca^{2+} and Mg^{2+}. After mixing, any solid phase was allowed to settle and a sample taken from the fluid column and analyzed for total humic substances. No external physical means were employed to separate humic substances potentially present as colloidal species from the sample. Therefore, the measured humic concentration represents the total humics present, which includes any humics which may be present as dissolved species and any humics which may be present as colloidal species.

SWCF-A: 1.1.09.1.1:TD:QA:Colloid Source Term, organic materials, humics:WPO #35855

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[1] DOE (U.S. Department of Energy). 1996. Title 40 CFR 191 Compliance Certification Application. DOE/CAO-1996-2184, Carlsbad Area Office, Carlsbad, NM.