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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 **microbes**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

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

copy with Attachments to:

MS 1320	Hans W. Papenguth, 6748
MS 1320	W. George Perkins, 6748
DOE/CAO	Robert A. Stroud

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.
SWCF-A:WPO# 35856: Mobile-Colloidal-Actinide Source Term. 4. Microbes

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

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

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):* PROPMIC and CAPMIC.

IV. *Material:* Microbes and the actinides Th, U, Np, Pu, and Am.

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

VI. *Units:* For proportionality constants (PROPMIC), the units are "moles microbe-bound actinide per moles of dissolved actinide." For the maximum concentration of each actinide associated with mobile microbes (CAPMIC), the units are "moles microbe-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 CAPMIC values are supplied for Th, U, Np, and Pu. CAPMIC values for Am are not available (refer to Attachment A, page 6). Constant PROPMIC values are supplied for all five actinide elements listed above.

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

C. *Median:* Not applicable.

D. *Standard Deviation:* Not applicable.

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

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

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

VIII. *Data Collection and Interpretation Information.*

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

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

1. *Data Collection or Test Method:* Experiments were conducted at 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. 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:* Data on actinide bioaccumulation by microbes is reported in actinide concentration or counts per unit volume. Data on actinide toxicity effects is reported in actinide concentration or counts per unit volume and cell population in cells per unit volume or in optical density.

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 BNL and LANL (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. LANL (contract number AP-2272) was audited by SNL (EA96-11) and by DOE/CAO (S-96-08). BNL (contract number AP-2273) is scheduled to be audited by SNL (EA96-19) in May 1996. DOE/CAO conducted a surveillance of BNL (S-96-08).

   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. LANL conducted work under an approved QAPP prepared especially for their program (WIPP Colloid and Bacterial Transport Project, CST-CBT-QAP1-001/0). BNL conducted work under an approved QAPP prepared especially for their program (Examination of the Role of Microorganisms in Colloidal Transport of Actinides under WIPP Repository Relevant Test Conditions). 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 BNL and LANL 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., 1996, Rationale for Definition of Parameter Values for Microbes.

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# 35856: Mobile-Colloidal Actinide Source Term. 4. Microbes.
SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Attachment A:

Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Microbes.

Attachment A.
Rationale for Definition of Parameter Values for Microbes

Hans W. Papenguth

Introduction

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

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

The focus of this document is on the quantification of the actinide concentration mobilized by microbes. In terms of the WIPP performance assessment (PA) calculations, the rationale for selecting the values corresponding to the following parameter designators is discussed:

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

Potentially important colloidal sized microorganisms include bacteria, fungi, yeast, and protozoa. Fungi and yeast are not important for the WIPP Site because of the anticipated anoxic environment of the repository. For the WIPP Site, the focus is on the halophilic and halotolerant microbes that have been identified at the Site (Brush, 1990; Francis and Gillow, 1994). Microbes are important to consider in performance assessments of the WIPP because they may significantly affect the characteristics of the waste stored at the WIPP, and also participate in transport of actinides in the event of human intrusion. Microbes are known to actively bioaccumulate actinides intracellularly as well as act as substrates for passive extracellular sorption.

At the WIPP Site, concentrations of naturally occurring microbes are on the order of 10^4 to 10^7 cells per milliliter (Francis and Gillow, 1994, Table 1). In the presence of nutrients provided by WIPP waste constituents, including nitrates, sulfates, and cellulosic materials such as protective clothing and wood, the population of microbes is likely to increase. Lysis, a natural phenomenon whereby cells die and release their cell constituents to the solution, also provides a source of nutrients to microbes.

When introduced to nutrient, microbes typically follow a predictable growth curve (defined by the number population of microbes plotted as a function of time), consisting of an initial period of inactivity ("very early log phase") ranging up to several days, followed by a sharp increase in growth ("early log phase"). That level of growth is sustained for one or more days ("log phase") during which time microbial metabolites, including carboxylic acids, enzymes, and exocellular polymers, are generated. The growth rate eventually begins to decline ("late log phase") due to the effects of those metabolites, limitations in nutrients or substrates, or population dynamics, and reaches a steady-state population ("stationary phase"). Viable microbes may aggregate to form clusters.

Experimental

Several types of experiments were conducted to evaluate the impact of microbes in support of the WIPP Colloid Research Program (refer to descriptions in Papenguth and Behl, 1996): (1) evaluation of indigenous concentrations of microbes; (2) quantification of mobile concentrations under nutrient- and substrate-rich conditions; (3) quantification and characterization of actinide bioaccumulation by microbes; and (4) evaluation of toxicity effects of actinide elements on microbe growth.

Experiments were conducted at Brookhaven National Laboratory (BNL; contract number AP-2273; A. J. Francis, BNL PI) and as a collaborative effort between BNL and Los Alamos National Laboratory (LANL; contract number AP-2272; Inés R. Triay, LANL PI). Evaluation of indigenous concentrations was a collaborative effort between BNL and LANL. Quantification of mobile concentrations was conducted at BNL. The bioaccumulation and toxicity work was conducted at BNL or LANL depending on actinide element. Thorium and uranium were investigated at BNL. The other actinide elements of interest, neptunium, plutonium, and americium, were investigated at LANL under the guidance of BNL personnel.

Experiments to determine the mobile concentrations of microbes remaining suspended in the fluid column were conducted similarly to experiments previously conducted in support of the WIPP Gas Generation Program (Brush, 1990; Francis and Gillow, 1994). Bacterial cultures were introduced to a solution containing nutrient and substrate, and sealed. Bacteria population was monitored over periods of several weeks or more using measurements of optical density or by direct counting of aliquots of fixed cells. An important change in protocol from previous experiments, however, is that instead of filtering the entire contents of the vessels, only the mobile cells remaining suspended in the fluid column were counted. Results of the experiments showed that the mobile concentration of microbes was a couple orders-of-magnitude less than the total concentration of microbes. The existence of indigenous microbes in Salado groundwaters has been demonstrated in previous work (Francis and Gillow, 1994). As part of the WIPP Colloid Research Program, samples of Culebra groundwater were carefully collected from the H-19 hydropad, processed, and characterized for indigenous microbes. Concentrations of naturally occurring microbes were on the order of 10^5 cells per milliliter, determined using direct counting methods.

The evaluation of indigenous concentrations of microbes and quantification of mobile concentrations provided important supporting evidence for quantifying the microbial actinide source term and for evaluating microbe-facilitated transport of actinides in the Culebra. However, the basis for developing the actual parameter values to be used in PA calculations was established with bioaccumulation and toxicity experiments, referred to herein as filtration experiments. Those experiments were conducted by combining microbe cultures with various concentrations and complexes of ^{232}Th, ^{238}U, ^{237}Np, ^{239}Pu, or ^{243}Am. The actinide reagents used were thorium nitrate, thorium EDTA, uranyl(VI) nitrate, uranyl(VI) citrate, neptunyl(V) EDTA, plutonyl(V) perchlorate, plutonyl(V) EDTA, and americium EDTA. For those experiments, a pure bacterial culture (WIPP-1A) and a mixed bacterial culture (BAB) were used. Most of the experiments were conducted with the WIPP-1A culture, because of the fast growth of that pure culture. The WIPP-1A mixed culture typically reaches steady-state concentration within several days, whereas the BAB pure culture requires several weeks. Because of the rapid response of the WIPP-1A culture, most of the experiments in support of the WIPP Colloid Research Program were conducted with that culture to expedite the research program. A complementary set of experiments were repeated with the BAB mixed culture, to evaluate the representativeness of the pure culture. Experiments were conducted over periods of 11 to 15 days for the WIPP-1A microbe culture, and up to 21 days for the BAB culture. Each experiment consisted of a subset of two or three replicate test vessels, which were sampled during the overall test interval, to provide time sequence data. In addition, replicate test vessels which were not inoculated with microbes were included in each experiment to provide a control. Sequential filtration with 0.03 µm, 0.4 µm, and 10 µm filter pore sizes was conducted on each vessel. The following size fractions were obtained:

fluid column sample	particle size	actinide association with:
not filtered	all	all forms listed below
0.22 µm syringe filter, filtrate	< 0.22 µm	dissolved; lysed microbes
10 µm filter, filter rententate	> 10 µm	clumped microbes
10 µm filter, filtrate	< 10 µm	dissolved; dispersed microbes; lysed microbes
0.4 µm filter, filter rententate	= 0.4 to 10 µm	dispersed microbes
0.4 µm filter, filtrate	< 0.4 µm	dissolved; lysed microbes
0.03 µm filter, filter rententate	= 0.03 to 0.4 µm	lysed microbes
0.03 µm filter, filtrate	< 0.03 µm	dissolved; lysed microbes

In addition to the potential actinide associations listed above, there was some evidence of the formation of inorganic precipitates in some of the experiments. The nutrient used in many experiments was phosphate (1 g PO_4^{3-}/L), which is known to coprecipitate actinide cations. The inoculated control samples provided the means to evaluate the extent of that experimental artifact. The control samples also provided the means to assess the extent of sorption of actinides onto test vessels, sampling, and filtration equipment. All sequential filters were composed of the same material, which simplifies assessment of sorption on the filtration equipment.

The toxicity experiments were conducted as a component of the filtration experiments described above, by varying the actinide concentration, and comparing growth curves measured by optical density and/or by direct cell counting. To increase the total concentration of actinides in solution, EDTA was added in some experiments in a one-to-one molar ratio with the actinide element. That approach was taken for some Pu experiments, and all of the Th, Np, and Am experiments.

Interpretation of Experimental Results

Proportionality constants (PROPMIC) describing the amount of actinide element bound to mobile microbes were determined from the data listed above. In addition, maximum concentrations of actinides that could be associated with microbes (CAPMIC) were determined from the experimental data. Those two parameters are suitable for use in PA calculations, when coupled with dissolved actinide solubility values.

The 0.4 µm filter rententate and 0.03 µm filtrate (acquired from the inoculated vessels, not the uninoculated control vessels) were selected to represent the microbial actinide and dissolved actinide concentrations, respectively. The ratio between the microbial actinide and dissolved actinide, both expressed in molarity, represents the proportionality constant value used for the PROPMIC parameter. The 0.4 µm filter rententate was selected to represent the microbial fraction because nearly all of the bacteria biomass was associated with that filter. A small concentration of actinides was associated with suspected biomass trapped on the 10 µm filter, as clumped microbes, and on the 0.03 µm filter, as lysed microbes. The contribution of actinides associated biomass consisting of clumped and lysed microbes was typically at least one order-of-magnitude less than the actinide concentration associated with the dispersed microbes collected on the 0.4 µm filter. The concentration of dissolved actinides measured from the 0.03 filter filtrate was used in the ratio because it provides the best indication of final dissolved actinide concentration. The individual proportionality constants for the filtration experiments are summarized in Table 1. Representative values for PROPMIC were developed from the individual proportionality constants on an element-by-element basis. Results of experiments using the BAB culture were disregarded, because of their lower uptake of actinides (especially plutonium), and because of the limited number of experiments conducted with that culture. For the WIPP-1A culture, the first sampling period (2 to 4 days, but generally 3 days) was disregarded in determining proportionality constants because steady state population had not yet been reached. The remaining values were averaged arithmetically (refer to comment column in Table 1).

The filtration experiments discussed above (see Table 1) also provided the basis for determining CAPMIC values. Final cell population numbers in the test vessels were estimated using measurements of optical density at a wavelength of 600 nm or by direct counting with epifluorescent microscopy. The magnitude of the toxicity effects were estimated by comparing final cell numbers obtained from a series of test vessels with varying actinide concentration. The direct counting technique provided the most dependable measure of cell number and was used where available. The CAPMIC value is defined as the actinide concentration in molarity at which no growth was observed. For cases where growth clearly diminished as actinide concentration increased, but the actinide concentration was not great enough to stop growth, CAPMIC values were determined by linear extrapolation of population numbers, and then adding an order-of-magnitude to account for uncertainty. It appears that the toxicity effects are due to chemical toxicity rather than radiotoxicity. Because of the high radiation levels of americium and safety considerations in the laboratory facility used, the molar concentration could not be increased to the point at which toxicity effects could be observed. Consequently no CAPMIC value is currently available for americium. The experimental basis for determination of CAPMIC values and comments on the determination of parameter values are summarized in Table 2.

The experiments conducted do not provide sufficient information to enable us to formulate a distribution of values for PROPMIC and CAPMIC. Therefore, single values for PROPMIC and CAPMIC are provided to the PA Department. Uncertainties due to analytical precision are small compared to uncertainties in knowledge of the microbe culture which might predominate in the WIPP repository or in the Culebra in an intrusion scenario. 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 microbes.

Summary

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

References

Brush, L. H., 1990. Test Plan for Laboratory and Modeling Studies of Repository and Radionuclide Chemistry for the Waste Isolation Pilot Plant. SAND90-0266. Albuquerque, NM: Sandia National Laboratories.

Francis, A. J., and J. B. Gillow, 1994. Effects of Microbial Processes on Gas Generation Under Expected Waste Isolation Pilot Plant Repository Conditions. Progress Report Through 1992. SAND93-7036. Albuquerque, NM: Sandia National Laboratories.

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

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

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.

Table 1.—Microbe filtration results.

date of experiment	actinide	form	initial target actinide concentration (M)	microbe culture	sampling time (days)	0.4 μm filter, filter retentate, inoculated vessel	uncertainty	0.03 μm filter, filtrate, inoculated vessel	uncertainty	proportionality constant (microbial An/dissolved An in M/M)	comments related to selection of PROPMIC values
PLUTONIUM											
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	3	3.59E-07	not available	1.30E-06	not available	0.2762	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	8	3.67E-08	not available	5.80E-07	not available	0.0633	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	15	7.85E-09	not available	1.66E-07	not available	0.0473	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	3	1.81E-07	not available	6.85E-08	not available	2.6423	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	8	7.55E-09	not available	3.05E-08	not available	0.2475	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	15	2.69E-09	not available	1.07E-08	not available	0.2514	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-07	WIPP-1A	3	7.28E-09	not available	1.94E-08	not available	0.3753	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-07	WIPP-1A	15	1.11E-10	not available	5.82E-08	not available	0.0019	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	2	3.16E-08	4.59E-10	1.38E-08	1.34E-09	2.2899	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	8	1.44E-09	9.50E-11	6.02E-09	1.11E-10	0.2392	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	11	9.24E-10	1.70E-10	6.33E-09	3.22E-10	0.1460	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	3	2.54E-07	not available	1.63E-06	not available	0.1558	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	8	5.18E-07	not available	1.16E-06	not available	0.4466	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	15	2.87E-08	not available	1.83E-06	not available	0.0157	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	3	2.43E-07	not available	9.94E-08	not available	2.4447	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	8	1.17E-08	not available	4.08E-08	not available	0.2868	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	15	1.00E-09	not available	2.01E-08	not available	0.0498	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	3	1.15E-08	not available	2.29E-08	not available	0.5022	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	8	2.93E-09	not available	1.43E-09	not available	2.0490	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	15	7.65E-11	not available	1.07E-07	not available	0.0007	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	3	2.52E-10	4.28E-11	5.68E-08	3.19E-10	0.0044	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	9	1.45E-09	1.14E-10	3.89E-08	5.96E-10	0.0373	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	21	1.22E-09	2.00E-10	5.46E-08	5.45E-10	0.0223	disregard
PROPMIC(Pu):	mean										3.0e-01
	standard deviation										5.44e-01
	number of samples										1.3e+01

Table 1.—Microbe filtration results.

date of experiment	actinide	form	initial target actinide concentration (M)	microbe culture	sampling time (days)	0.4 μm filter, filter retentate, inoculated vessel	uncertainty	0.03 μm filter, filtrate, inoculated vessel	uncertainty	proportionality constant (microbial An/dissolved An in M/M)	comments related to selection of PROPMIC values
AMERICIUM											
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	3	1.82E-08	1.15E-10	1.84E-09	2.12E-10	9.8913	disregard
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	7	6.32E-09	2.52E-10	3.35E-09	6.65E-10	1.8866	include in mean for Am
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	11	1.22E-08	5.33E-10	2.28E-09	1.05E-10	5.3509	include in mean for Am
PROPMIC(Am):	mean										3.6e+00
	standard deviation										2.45e+00
	number of samples										2.0e+00
NEPTUNIUM											
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	3	6.24E-06	1.58E-07	8.04E-06	4.11E-06	0.7761	disregard
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	7	2.33E-06	1.24E-06	1.98E-07	8.89E-09	11.7677	include in mean for Np
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	11	not available	not available	not available	not available	not available	disregard
PROPMIC(Np):	mean										1.2e+01
	standard deviation										not applicable
	number of samples										1.0e+00
THORIUM											
11-Mar-96	Th-232	Th EDTA	1.00E-03	WIPP-1A	7	4.90E-04	1.41E-04	2.72E-04	9.14E-05	1.8015	include in mean for Th
11-Mar-96	Th-232	Th EDTA	1.00E-03	WIPP-1A	13	6.95E-04	7.55E-05	1.55E-04	6.10E-06	4.4839	include in mean for Th
PROPMIC(Th):	mean										3.1e+00
	standard deviation										1.90e+00
	number of samples										2.0e+00
URANIUM											
9-Feb-96	U-238	U(VI) nitrate	1.00E-03	WIPP-1A	4	5.30E-07	3.18E-08	2.93E-04	1.06E-06	0.0018	disregard
9-Feb-96	U-238	U(VI) nitrate	1.00E-03	WIPP-1A	13	2.11E-06	2.61E-07	9.83E-04	1.68E-05	0.0021	include in mean for U
22-Feb-96	U-238	U(VI) nitrate	1.00E-03	BAB	5	2.17E-06	1.64E-07	1.24E-03	4.20E-06	0.0018	disregard
22-Feb-96	U-238	U(VI) nitrate	1.00E-03	BAB	13	2.22E-06	1.89E-07	1.16E-03	4.20E-06	0.0019	disregard
PROPMIC(U):	mean										2.1e-03
	standard deviation										not applicale
	number of samples										1

Table 2.—Microbe toxicity results.

date of experiment	actinide	form	initial target actinide concentration (M)	0.2 μm filter, filtrate (actinide solubility; M)	final cell number (cells/mL)	final optical density at 600 nm (units)	final pH	magnitude of toxicity (relative to no actinide control)	toxic concentration - observed (M)	toxic concentration - extrapolated (M)	comments related to selection of CAPMIC values
THORIUM											
13-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.567	8.08	not applicable			
13-Mar-96	Th-232	Th(IV) nitrate	4.30e-04	0 (ppt.)	not analyzed	0.645	8.22	none			
13-Mar-96	Th-232	Th(IV) nitrate	1.10e-03	0 (ppt.)	not analyzed	0.58	8.28	none			
13-Mar-96	Th-232	Th(IV) nitrate	2.20e-03	0 (ppt.)	not analyzed	0.352 (ppt.)	6.05	extreme	1.90e-03		use for Th
13-Mar-96	Th-232	Th(IV) nitrate	4.30e-03	0 (ppt.)	not analyzed	0.427 (ppt.)	5.76	extreme	3.46e-03		disregard, toxicity observed at lower value
13-Mar-96	Th-232	Th(IV) EDTA	4.30e-04	3.41e-04	not analyzed	0.063	6.45	inconclusive			
13-Mar-96	Th-232	Th(IV) EDTA	1.10e-03	1.01e-03	4.24e+06	0.071	6.13	moderate			
13-Mar-96	Th-232	Th(IV) EDTA	2.20e-03	1.90e-03	not analyzed	0.004	6.08	extreme	2.20e-03		disregard, toxicity observed at lower value
13-Mar-96	Th-232	Th(IV) EDTA	4.30e-03	3.46e-03	not analyzed	0	6.32	extreme	4.30e-03		disregard, toxicity observed at lower value
URANIUM											
17-Oct-95	control (none)	not applicable	not applicable	not applicable	2.62e+08	0.541	8.1	not applicable	not applicable	not applicable	
17-Oct-95	U-238	U(VI) nitrate	4.20e-04	4.20e-04	2.57e+08	0.543	8.04	none			
17-Oct-95	U-238	U(VI) nitrate	1.10e-03	1.00e-03	3.08e+08	0.539	7.94	none			
17-Oct-95	U-238	U(VI) nitrate	2.10e-03	0 (ppt.)	2.24e+05	0.272	6.26	extreme	2.10e-03		use for U
17-Oct-95	U-238	U(VI) nitrate	4.20e-03	0 (ppt.)	2.02e+05	0.533	5.9	extreme	4.20e-03		disregard, toxicity observed at lower value
17-Oct-95	U-238	U(VI) citrate	4.20e-04	4.20e-04	2.77e+08	0.514	8.01	none			
17-Oct-95	U-238	U(VI) citrate	1.10e-03	1.10e-03	2.39e+08	0.508	7.96	none			
17-Oct-95	U-238	U(VI) citrate	2.10e-03	0 (ppt.)	2.58e+05	0.318	6.11	extreme	2.10e-03		use for U
17-Oct-95	U-238	U(VI) citrate	4.20e-03	0 (ppt.)	1.93e+05	0.344	5.91	extreme	4.20e-03		disregard, toxicity observed at lower value
NEPTUNIUM											
19-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.8	8.04	none			
19-Mar-96	Np-237	Np(V) EDTA	5.00e-06	2.70e-06	not analyzed	0.788	8.02	none			
19-Mar-96	Np-237	Np(V) EDTA	5.00e-05	2.53e-05	not analyzed	0.802	7.95	none			
19-Mar-96	Np-237	Np(V) EDTA	5.00e-04	2.65e-04	not analyzed	0.141	6.57	, but some growth	2.65e-04		use for Np, but increase by one order of magnitude because of some growth
PLUTONIUM											
28-Nov-95	control (none)	not applicable	not applicable	not applicable	3.40e+08	0.672	8.157	not applicable	not applicable	not applicable	
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-07	5.01e-08	3.20e+08	0.683	8.197	none			
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-06	6.90e-07	1.40e+08	0.453	8.327	moderate			
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-05	8.80e-06	5.50e+07	0.237	7.94	extreme		7.71e-06	disregard, toxicity observed at lower value
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-07	5.50e-08	2.80e+08	0.691	8.223	none			
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-06	6.20e-07	1.20e+08	0.499	8.387	moderate			
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-05	8.00e-06	9.80e+07	0.532	8.363	extreme		6.83e-06	use for Pu, but increase by one order of magnitude
AMERICIUM											
5-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.89	7.93	not applicable			
5-Mar-96	Am-243	Am(III) EDTA	5.00e-08	2.62e-08	not analyzed	0.864	7.98	none			
5-Mar-96	Am-243	Am(III) EDTA	5.00e-07	3.36e-07	not analyzed	0.821	8.04	none			
5-Mar-96	Am-243	Am(III) EDTA	5.00e-06	2.65e-06	not analyzed	0.79	8.04	slight	>2.65E-06		inconclusive; Am concentrations not sufficiently high

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

copy to:

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

SWCF-A:WBS1.1.10.2.1

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

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.

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;

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:

MS 1328	Hong-Nian Jow, 6741
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MS 1328	Mary-Alena Martell, 6749
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MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt W. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

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.

copy to:

MS 1328	Hong-Nian Jow, 6741
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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).

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:

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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).

29 March 1996

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

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