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subject: Actinide Solubilities and Colloidal Source Terms in the CRA-2026 Interim State Repository PA

This memo is to provide a summary of the dissolved and colloidal actinide source terms in the CRA-2026 Interim State (IS) Repository Performance Assessment (PA) calculation. An example source term is calculated using median distribution values for PA sampled parameters.

Construction of Source Terms

Because PA does not differentiate dissolved from colloidal species for transport in the Salado, the total source term in the Salado is the sum of both components. To model transport within the Culebra, however, this simplification was replaced by separating the mobilized actinides delivered to the Culebra by Salado transport codes into five components (dissolved, humic, microbial, mineral-fragment, and intrinsic colloids) to account for differences in their transport behavior. This is important because transport within the repository occurs through, at most, hundreds of meters of poorly defined waste undergoing decomposition, whereas transport through the Culebra occurs over kilometers in a relatively homogeneous (compared to waste) fractured dolomite.

The parameters required to construct the source term were as follows:

1. Baseline solubilities for four oxidation states in Salado and Castile brines, the two brine end members. (SOLMODx:SOLyOHn for oxidation state x (x=3, 4, 5, and 6), brine y (y=S for Salado and C for Castile), and minimum brine volume multiplier n (when 1x minimum brine volume (n=1) is used, “1” is omitted)).

2. Uncertainty distributions to be applied to the baseline solubilities for oxidation states III and IV (SOLMODx:SOLVAR for oxidation state x).

3. A scheme for assigning sampled oxidation states ("low" or "high") (GLOBAL:OXSTAT and z:OXCUTOFF for actinide z in PU, NP, and U).

4. Colloidal concentrations for each actinide (AM, NP, PU, TH, and U) for intrinsic and mineral fragment colloids (z:CONCINT, z:CONCMIN for actinide z).

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5. Proportionality constants for each oxidation state and brine type and maximum actinide concentrations for each actinide associated with humic colloids (PHUMOXx:PHUMyIM for oxidation state x and brine y; and z:CAPHUM for actinide z).

6. Proportionality constants and maximum actinide concentrations for each actinide oxidation state for actinides associated with microbial colloids (z+x:PROPMIC and z+x:CAPMIC for actinide z and oxidation state x).

The parameters used in the CRA-2026 Interim State calculation (CRA26_IS) are presented in Table 1, along with the parameters used in the CRA-2019 Deferred Performance Assessment (DPA) (CRA19), the Replacement Panel Planned Change Request PA (RPPCR), and the CRA-2026 Final State calculation (CRA26_FS). Median solubility uncertainty values are given in Table 2.

These parameters are used to calculate a mobile concentration limit for each actinide in the PA calculations. The term "mobile concentration limit" is used for the combined mobile concentration limits of dissolved and colloidal species. The mobile concentration limits are not necessarily the actual concentrations, because the concentration could be limited by inventory availability. Both NUTS and PANEL assume that the mobile concentration limit for each element is constant throughout the course of a simulation for a given model realization. The calculation of the mobile concentration limit is performed by PANEL for each of 100 sampled vectors per replicate for all 3 replicates. A similar methodology to generate the mobile concentration limit was used for the CCA PA, the CCA PAVT, the CRA-2004 PA, the CRA-2004 PABC, the CRA-2009 PA, the CRA-2009 PABC, the CRA-2014 PA, and the CRA-2019 DPA.

For each actinide, the baseline solubility is determined by the oxidation state (dependent on oxidation state index (OXSTAT)) and source brine (dependent on the future scenario realization). The mineral and intrinsic concentrations are constants pulled from the parameter database for each actinide. The dissolved concentration (mol/L), the humic concentration (mol/L), the microbial concentration (mol/L), the sum of colloidal concentrations (mol/L) and the mobile concentration limit (mol/L) need to be calculated. To calculate the solubility a solubility uncertainty parameter is sampled from a given distribution; the distribution parameters are dependent on the given oxidation state. For the results displayed here the median value for the solubility uncertainty will be used. The solubility can then be calculated using the formula:

$$Dissolved = Baseline\ Solubility \times 10^{Sampled\ Solubility\ Uncertainty}$$

The humic concentration can then be calculated with the formula:

$$Humic = \min(Dissolved * PHUM, CAPHUM)$$

Where *PHUM* is the proportionality constant of humic colloids (PHUMSIM or PHUMCIM), and *CAPHUM* is the maximum concentration of actinide ions combined with mobile humic colloids. The microbial concentration is calculated using the formula:

$$Microbial = \min(Dissolved * PROPMIC, CAPMIC)$$

Where *PROPMIC* is the proportionality constant of microbial colloids and *CAPMIC* is the maximum concentration of actinide ions attached on microbes.

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The sum of the colloidal concentrations can be calculated with:

$$Sum\ Colloidal = Humic + Microbial + Mineral + Intrinsic$$

The mobile concentration limit can then be calculated as the sum of the concentrations:

$$Total\ Mobile = Dissolved + Sum\ Colloidal$$

For actinides with more than one oxidation state, the oxidation state is specified by the sampled oxidation-state parameter GLOBAL:OXSTAT and a cutoff values for that actinide z:OXCUTOFF representing the likelihood of the actinide solubility being dominated by the lower possible oxidation state. OXSTAT is sampled from a uniform distribution between 0 and 1. If the value of OXSTAT is less than or equal to z:OXCUTOFF then the lower oxidation state is used, otherwise the higher oxidation state is used.

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Table 1 Parameter Values from the WIPP PA Database for the calculation of concentrations[1, 2]

Material	Property	CRA19	RPPCR	CRA26_FS	CRA26_IS
AM	CONCMIN	2.60E-08	2.60E-08	2.60E-08	2.60E-08
NP	CONCMIN	2.60E-08	2.60E-08	2.60E-08	2.60E-08
PU	CONCMIN	2.60E-08	2.60E-08	2.60E-08	2.60E-08
TH	CONCMIN	2.60E-08	2.60E-08	2.60E-08	2.60E-08
U	CONCMIN	2.60E-08	2.60E-08	2.60E-08	2.60E-08
AM	CONCINT	9.50E-09	6.70E-07	6.70E-07	6.70E-07
NP	CONCINT	4.30E-08	4.30E-08	4.30E-08	4.30E-08
PU	CONCINT	4.30E-08	4.30E-08	4.30E-08	4.30E-08
TH	CONCINT	4.30E-08	4.80E-07	4.80E-07	4.80E-07
U	CONCINT	1.40E-06	1.40E-06	1.40E-06	1.40E-06
AM+3[2]	PROPMIC	3.00E-02	3.52E+00	2.92E+00	2.92E+00
NP+4[2]	PROPMIC	2.10E-01	1.20E+01	1.20E+01	1.20E+01
NP+5[2]	PROPMIC	2.10E-01	1.20E+01	1.20E+01	1.20E+01
PU+3[2]	PROPMIC	2.10E-01	3.00E-01	2.92E+00	2.92E+00
PU+4[2]	PROPMIC	2.10E-01	3.00E-01	3.00E-01	3.00E-01
TH+4[2]	PROPMIC	2.10E-01	3.10E+00	3.10E+00	3.10E+00
U+4[2]	PROPMIC	2.10E-01	2.10E-03	2.10E-03	2.10E-03
U+6[2]	PROPMIC	2.10E-01	2.10E-03	2.10E-03	2.10E-03
AM+3[2]	CAPMIC	2.30E-09	9.00E-07	4.97E-07	4.97E-07
NP+4[2]	CAPMIC	3.80E-08	2.33E-06	1.52E-07	1.52E-07
NP+5[2]	CAPMIC	3.80E-08	2.33E-06	1.52E-07	1.52E-07
PU+3[2]	CAPMIC	3.80E-08	1.22E-09	4.97E-07	4.97E-07
PU+4[2]	CAPMIC	3.80E-08	1.22E-09	4.07E-09	4.07E-09
TH+4[2]	CAPMIC	3.80E-08	6.95E-04	6.95E-04	6.95E-04
U+4[2]	CAPMIC	3.80E-08	2.22E-06	9.65E-06	9.65E-06
U+6[2]	CAPMIC	3.80E-08	2.22E-06	9.65E-06	9.65E-06
AM	CAPHUM	1.10E-05	1.10E-05	1.10E-05	1.10E-05
NP	CAPHUM	1.10E-05	1.10E-05	1.10E-05	1.10E-05
PU	CAPHUM	1.10E-05	1.10E-05	1.10E-05	1.10E-05
TH	CAPHUM	1.10E-05	1.10E-05	1.10E-05	1.10E-05
U	CAPHUM	1.10E-05	1.10E-05	1.10E-05	1.10E-05
PHUMOX3	PHUMSIM	2.00E-01	2.00E-01	3.00E-01	3.00E-01
PHUMOX4	PHUMSIM	1.00E-02	1.00E-02	1.00E-02	2.00E-02
PHUMOX5	PHUMSIM	9.10E-04	9.10E-04	9.10E-04	9.10E-04
PHUMOX6	PHUMSIM	1.20E-01	1.20E-01	1.20E-01	1.20E-01
PHUMOX3	PHUMCIM	2.00E-01	2.00E-01	4.00E-01	3.00E-01
PHUMOX4	PHUMCIM	1.00E-02	1.00E-02	1.00E-02	1.00E-02
PHUMOX5	PHUMCIM	7.40E-03	7.40E-03	7.40E-03	7.40E-03
PHUMOX6	PHUMCIM	5.10E-01	5.10E-01	5.10E-01	5.10E-01
SOLMOD3	SOLSOH	1.63E-07	3.40E-06	1.14E-05	1.45E-05
SOLMOD4	SOLSOH	5.45E-08	5.34E-08	5.34E-08	5.34E-08
SOLMOD5	SOLSOH	4.02E-07	4.95E-07	7.97E-07	9.75E-07
SOLMOD6	SOLSOH	1.00E-03	1.00E-03	3.00E-06	3.00E-06
SOLMOD3	SOLCOH	1.78E-07	3.51E-06	1.15E-05	1.44E-05
SOLMOD4	SOLCOH	5.44E-08	5.73E-08	5.67E-08	5.63E-08
SOLMOD5	SOLCOH	1.20E-06	1.80E-06	3.14E-06	4.01E-06
SOLMOD6	SOLCOH	1.00E-03	1.00E-03	3.00E-06	3.00E-06
NP	OXCUTOFF	0.5[1]	0.5	0.5	0.5
PU	OXCUTOFF	0.5[1]	0.25	0.25	0.25
U	OXCUTOFF	0.5[1]	0.5	0.5	0.5

[1] Hardcoded value not in the WIPP PA Database for CRA19.
[2] For CRA19 and the RPPCR, PROPMIC and CAPMIC specified for actinide materials (AM, NP, PU, TH, and U) not actinide-oxidation state materials.

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Table 2 Median Solubility Uncertainty Factors [3, 4]

Material	Property	CRA19	RPPCR	CRA26_FS	CRA26_IS
SOLMOD3	SOLVAR[3]	3.46E-01	-2.45E-01	-2.76E-01	-2.76E-01
SOLMOD4	SOLVAR[3]	-9.96E-02	-9.47E-01	-9.47E-01	-9.47E-01
SOLMOD5	SOLVAR[4]	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SOLMOD6	SOLVAR[4]	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Prior to the RPPCR the oxidation state cutoff value was hardcoded to be 0.5 for all multi-valent actinides (NP, PU, and U). Lucchini and Swanson (2023) specified parameter values of OXCUTOFF for these actinides for RPPCR, which were added to the WIPP PA database as new parameters. Kaplan et al. (2025) recommended the same OXCUTOFF values for the CRA-2026 calculations. For CRA26_IS, microbial colloid parameters Kaplan et al. recommended using actinide-oxidation state specific parameter rather than actinide specific parameter as has been used in all previous WIPP PA calculations. Baseline solubility values for the +3, +4, and +5 actinides were updated by Domski (2025a) and baseline solubility values for the +6 actinides were updated by Kaplan et al. (2025). Humic colloid proportionality constants were updated by Mariner (2025). Solubility uncertainty distributions were updated by Domski (2025b).

Example Calculation

As an example, the Pu concentration in the Salado brine will be calculated assuming the high oxidation state Pu(IV) was sampled by GLOBAL:OXSTAT being greater than PU:OXCUTOFF. The sampled value for solubility uncertainty will use the median value of -0.947. The median brine solubility uses the SOLMOD*x* material where *x* is the oxidation state (in this case SOLMOD4) and the Salado brine corresponds to the property SOLSOH, giving the value 5.34×10^{-8} mol/L. The humic proportionality constant, PHUMOX4:PHUMSIM, is 0.02, the microbial proportionality constant, PU+4:PROPMIC, is 0.3, the humic cap, PU:CAPHUM, is 1.10×10^{-5} mol/L, the microbe cap, PU+4:CAPMIC, is 4.07×10^{-9} mol/L, the concentration of the actinide in mineral fragment forms, PU:CONCMIN, is 2.6×10^{-8} mol/L, and the intrinsic colloid concentration, PU:CONCINT, is 4.3×10^{-8} mol/L.

In this case, the dissolved concentration limit of Pu(IV) used in the PA would be:

$$Dissolved = Baseline\ Solubility \times 10^{Sampled\ Solubility\ Uncertainty}$$
$$= (5.34 \times 10^{-8}) \times (10^{-0.947}) = 6.03 \times 10^{-9} \frac{mol}{L}$$

The humic-complexed Pu limit would be:

$$Humic = \min(Dissolved * PHUM, CAPHUM)$$
$$= \min\left((6.03 \times 10^{-9}) \times (0.02), 1.10 \times 10^{-5}\right) = 1.21 \times 10^{-10} \frac{mol}{L}$$

The microbial-mobilized Pu limit would be:

[3] Median value used for Sampled Parameters
[4] Oxidation states +5 and +6 are assumed to have no uncertainty and therefore the uncertainty exponential takes on a value of 0.0. These values are not included in the WIPP PA Database.

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$$Microbial = \min(Dissolved * PROPMIC, CAPMIC)$$
$$= \min\left((6.03 \times 10^{-9}) \times (0.3), 4.07 \times 10^{-9}\right) = 1.81 \times 10^{-9} \frac{mol}{L}$$

The mobile concentration limit of Pu(IV) would then be the sum of the dissolved and colloidal contributions:

$$Total\ Mobile = Dissolved + (Humic + Microbial + Mineral + Intrinsic)$$
$$= 6.03 \times 10^{-9} + 1.21 \times 10^{-10} + 1.81 \times 10^{-9} + 2.60 \times 10^{-8} + 4.30 \times 10^{-8}$$
$$= 7.70 \times 10^{-8} \frac{mol}{L}$$

Calculated Solubilities

Table 3 shows the dissolved and colloidal components of the source term and the mobile concentration limits for each element obtained when median parameter values are used for the sampled uncertainty for the CRA26_IS. The 1× minimum brine volume baseline solubilities are used in Table 3.

Table 4 shows the dissolved, colloidal, and mobile concentration limits for the CRA26_IS when calculated using the minimum, median, mean, and maximum values for the uncertain parameters. Again the 1× minimum brine volume baseline solubilities are used.

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Table 3 Median Actinide Solubility and Colloidal Contributions for CRA-2026 IS [5]

An	Brine	Baseline Solubility[6] (mol/L)	Uncertainty Exponent[7] (-)	Dissolved (mol/L)	Mineral (mol/L)	Intrinsic (mol/L)	Humic (mol/L)	Microbial (mol/L)	Sum Colloidal (mol/L)	Total Mobile[8] (mol/L)
Am(III)	Salado (GWB)	1.45E-05	-2.76E-01	7.68E-06	2.60E-08	6.70E-07	2.30E-06	4.97E-07	3.50E-06	1.12E-05
Am(III)	Castile (ERDA-6)	1.44E-05	-2.76E-01	7.63E-06	2.60E-08	6.70E-07	2.29E-06	4.97E-07	3.48E-06	1.11E-05
Np(IV)	Salado (GWB)	5.34E-08	-9.47E-01	6.03E-09	2.60E-08	4.30E-08	1.21E-10	7.24E-08	1.42E-07	1.48E-07
Np(IV)	Castile (ERDA-6)	5.63E-08	-9.47E-01	6.36E-09	2.60E-08	4.30E-08	6.36E-11	7.63E-08	1.45E-07	1.52E-07
Np(V)	Salado (GWB)	9.75E-07	0.00E+00	9.75E-07	2.60E-08	4.30E-08	8.87E-10	1.52E-07	2.22E-07	1.20E-06
Np(V)	Castile (ERDA-6)	4.01E-06	0.00E+00	4.01E-06	2.60E-08	4.30E-08	2.97E-08	1.52E-07	2.51E-07	4.26E-06
Pu(III)	Salado (GWB)	1.45E-05	-2.76E-01	7.68E-06	2.60E-08	4.30E-08	2.30E-06	4.97E-07	2.87E-06	1.06E-05
Pu(III)	Castile (ERDA-6)	1.44E-05	-2.76E-01	7.63E-06	2.60E-08	4.30E-08	2.29E-06	4.97E-07	2.85E-06	1.05E-05
Pu(IV)	Salado (GWB)	5.34E-08	-9.47E-01	6.03E-09	2.60E-08	4.30E-08	1.21E-10	1.81E-09	7.09E-08	7.70E-08
Pu(IV)	Castile (ERDA-6)	5.63E-08	-9.47E-01	6.36E-09	2.60E-08	4.30E-08	6.36E-11	1.91E-09	7.10E-08	7.73E-08
Th(IV)	Salado (GWB)	5.34E-08	-9.47E-01	6.03E-09	2.60E-08	4.80E-07	1.21E-10	1.87E-08	5.25E-07	5.31E-07
Th(IV)	Castile (ERDA-6)	5.63E-08	-9.47E-01	6.36E-09	2.60E-08	4.80E-07	6.36E-11	1.97E-08	5.26E-07	5.32E-07
U(IV)	Salado (GWB)	5.34E-08	-9.47E-01	6.03E-09	2.60E-08	1.40E-06	1.21E-10	1.27E-11	1.43E-06	1.43E-06
U(IV)	Castile (ERDA-6)	5.63E-08	-9.47E-01	6.36E-09	2.60E-08	1.40E-06	6.36E-11	1.34E-11	1.43E-06	1.43E-06
U(VI)	Salado (GWB)	3.00E-06	0.00E+00	3.00E-06	2.60E-08	1.40E-06	3.60E-07	6.30E-09	1.79E-06	4.79E-06
U(VI)	Castile (ERDA-6)	3.00E-06	0.00E+00	3.00E-06	2.60E-08	1.40E-06	1.53E-06	6.30E-09	2.96E-06	5.96E-06

[5] Spreadsheet used to obtain final results stored in the WIPP PA CVS archive at: /data/cvs/CVSLIB/WIPP_EXTERNAL/APPENDIXSOTERM/CRA26/
[6] The baseline solubility is calculated using the minimum brine volume.
[7] The median distribution value is used for sampled parameters
[8] = Dissolved + (Mineral + Intrinsic + Humic + Microbial)

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Table 4. Concentrations (mol/L) of Dissolved, Colloidal, and Total Mobile Actinides Obtained Using Minimum, Median, Mean, and Maximum Parameter Values for the CRA-2026 IS PA.

Actinide Oxidation State and Brine	Minimum	Mean	Median	Maximum
Am(III), dissolved, Salado brine	2.52E-08	4.88E-06	7.68E-06	5.75E-05
Am(III), colloidal, Salado brine	7.77E-07	2.66E-06	3.50E-06	1.22E-05
Am(III), total mobile, Salado brine	8.02E-07	7.54E-06	1.12E-05	6.97E-05
Am(III), dissolved, Castile brine	2.50E-08	4.85E-06	7.63E-06	5.71E-05
Am(III), colloidal, Castile brine	7.77E-07	2.65E-06	3.48E-06	1.22E-05
Am(III), total mobile, Castile brine	8.02E-07	7.49E-06	1.11E-05	6.93E-05
Np(IV), dissolved, Salado brine	5.22E-10	9.25E-09	6.03E-09	1.81E-07
Np(IV), colloidal, Salado brine	7.53E-08	1.80E-07	1.42E-07	2.25E-07
Np(IV), total mobile, Salado brine	7.58E-08	1.89E-07	1.48E-07	4.05E-07
Np(IV), dissolved, Castile brine	5.50E-10	9.76E-09	6.36E-09	1.90E-07
Np(IV), colloidal, Castile brine	7.56E-08	1.86E-07	1.45E-07	2.23E-07
Np(IV), total mobile, Castile brine	7.62E-08	1.96E-07	1.52E-07	4.13E-07
Np(V), dissolved, Salado brine	9.75E-07	9.75E-07	9.75E-07	9.75E-07
Np(V), colloidal, Salado brine	2.22E-07	2.22E-07	2.22E-07	2.22E-07
Np(V), total mobile, Salado brine	1.20E-06	1.20E-06	1.20E-06	1.20E-06
Np(V), dissolved, Castile brine	4.01E-06	4.01E-06	4.01E-06	4.01E-06
Np(V), colloidal, Castile brine	2.51E-07	2.51E-07	2.51E-07	2.51E-07
Np(V), total mobile, Castile brine	4.26E-06	4.26E-06	4.26E-06	4.26E-06
Pu(III), dissolved, Salado brine	2.52E-08	4.88E-06	7.68E-06	5.75E-05
Pu(III), colloidal, Salado brine	1.50E-07	2.03E-06	2.87E-06	1.16E-05
Pu(III), total mobile, Salado brine	1.75E-07	6.91E-06	1.06E-05	6.90E-05
Pu(III), dissolved, Castile brine	2.50E-08	4.85E-06	7.63E-06	5.71E-05

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Actinide Oxidation State and Brine	Minimum	Mean	Median	Maximum
Pu(III), colloidal, Castile brine	1.50E-07	2.02E-06	2.85E-06	1.16E-05
Pu(III), total mobile, Castile brine	1.75E-07	6.87E-06	1.05E-05	6.86E-05
Pu(IV), dissolved, Salado brine	5.22E-10	9.25E-09	6.03E-09	1.81E-07
Pu(IV), colloidal, Salado brine	6.92E-08	7.20E-08	7.09E-08	7.67E-08
Pu(IV), total mobile, Salado brine	6.97E-08	8.12E-08	7.70E-08	2.57E-07
Pu(IV), dissolved, Castile brine	5.50E-10	9.76E-09	6.36E-09	1.90E-07
Pu(IV), colloidal, Castile brine	6.92E-08	7.20E-08	7.10E-08	7.50E-08
Pu(IV), total mobile, Castile brine	6.97E-08	8.18E-08	7.73E-08	2.65E-07
Th(IV), dissolved, Salado brine	5.22E-10	9.25E-09	6.03E-09	1.81E-07
Th(IV), colloidal, Salado brine	5.08E-07	5.35E-07	5.25E-07	1.07E-06
Th(IV), total mobile, Salado brine	5.08E-07	5.44E-07	5.31E-07	1.25E-06
Th(IV), dissolved, Castile brine	5.50E-10	9.76E-09	6.36E-09	1.90E-07
Th(IV), colloidal, Castile brine	5.08E-07	5.36E-07	5.26E-07	1.10E-06
Th(IV), total mobile, Castile brine	5.08E-07	5.46E-07	5.32E-07	1.29E-06
U(IV), dissolved, Salado brine	5.22E-10	9.25E-09	6.03E-09	1.81E-07
U(IV), colloidal, Salado brine	1.43E-06	1.43E-06	1.43E-06	1.43E-06
U(IV), total mobile, Salado brine	1.43E-06	1.44E-06	1.43E-06	1.61E-06
U(IV), dissolved, Castile brine	5.50E-10	9.76E-09	6.36E-09	1.90E-07
U(IV), colloidal, Castile brine	1.43E-06	1.43E-06	1.43E-06	1.43E-06
U(IV), total mobile, Castile brine	1.43E-06	1.44E-06	1.43E-06	1.62E-06
U(VI), dissolved, Salado brine	3.00E-06	3.00E-06	3.00E-06	3.00E-06
U(VI), colloidal, Salado brine	1.79E-06	1.79E-06	1.79E-06	1.79E-06
U(VI), total mobile, Salado brine	4.79E-06	4.79E-06	4.79E-06	4.79E-06

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Actinide Oxidation State and Brine	Minimum	Mean	Median	Maximum
U(VI), dissolved, Castile brine	3.00E-06	3.00E-06	3.00E-06	3.00E-06
U(VI), colloidal, Castile brine	2.96E-06	2.96E-06	2.96E-06	2.96E-06
U(VI), total mobile, Castile brine	5.96E-06	5.96E-06	5.96E-06	5.96E-06

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