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To: Chris Camphouse, MS 1395 (Org. 08881)

From: Paul S. Domski, MS 0779 (Org. 08882) Shelley R. Nielsen for

Subject: Th(IV), Np(V), and Am(III) Baseline Solubilities and Th(IV) and Am(III) Solubility Uncertainties for the CRA-2019 PA

Table 1 of this memorandum provides the parameter data entry information for the baseline solubilities of Th(IV), Np(V), and Am(III) for the WIPP PA Parameter Database for the CRA-2019 PA. These baseline solubilities are based on: (1) the concentrations of the organic ligands acetate, citrate, ethylenediaminetetraacetate (EDTA), and oxalate in two Waste Isolation Pilot Plant (WIPP) standard brines as a function of the volumes of these brines in the repository (Sisk-Scott, 2019); and (2) the Th(IV), Np(V), and Am(III) baseline solubilities predicted by EQ3/6 for these organic ligand concentrations (Domski and Sisk-Scott, 2019, Tables 6 and 7). Table 1 provides the solubilities of An(III), An(IV), and An(V) in Salado (GWB), and Castile (ERDA-6) brines.

Table 1. Parameter Data Entry for the Baseline Actinide Solubilities for the CRA-2019 PA (Domski and Sisk-Scott, 2019, Tables 6 and 7).

Parameter Description	Material	Property	Value	Units
Oxidation state III model, solubility in the minimum volume of Salado brine	SOLMOD3	SOLSOH	1.63×10^{-7}	M (mol/L)
Oxidation state III model, solubility in 2 × the minimum volume of Salado brine	SOLMOD3	SOLSOH2	1.58×10^{-7}	M

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Table 1. Parameter Data Entry for the Baseline Actinide Solubilities for the CRA-2019 PA (Domski and Sisk-Scott, 2019, Tables 6 and 7) (continued).

Parameter Description	Material	Property	Value	Units
Oxidation state III model, solubility in 3 × the minimum volume of Salado brine	SOLMOD3	SOLSOH3	1.56×10^{-7}	M (mol/L)
Oxidation state III model, solubility in 4 × the minimum volume of Salado brine	SOLMOD3	SOLSOH4	1.55×10^{-7}	M
Oxidation state III model, solubility in 5 × the minimum volume of Salado brine	SOLMOD3	SOLSOH5	1.54×10^{-7}	M
Oxidation state III model, solubility in the minimum volume of Castile brine	SOLMOD3	SOLCOH	1.78×10^{-7}	M
Oxidation state III model, solubility in 2 × the minimum volume of Castile brine	SOLMOD3	SOLCOH2	1.63×10^{-7}	M
Oxidation state III model, solubility in 3 × the minimum volume of Castile brine	SOLMOD3	SOLCOH3	1.58×10^{-7}	M
Oxidation state III model, solubility in 4 × the minimum volume of Castile brine	SOLMOD3	SOLCOH4	1.54×10^{-7}	M
Oxidation state III model, solubility in 5 × the minimum volume of Castile brine	SOLMOD3	SOLCOH5	1.52×10^{-7}	M
Oxidation state IV model, solubility in the minimum volume of Salado brine	SOLMOD4	SOLSOH	5.45×10^{-8}	M

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Table 1. Parameter Data Entry for the Baseline Actinide Solubilities for the CRA-2019 PA (Domski and Sisk-Scott, 2019, Tables 6 and 7) (continued).

Parameter Description	Material	Property	Value	Units
Oxidation state IV model, solubility in 2 × the minimum volume of Salado brine	SOLMOD4	SOLSOH2	5.45×10^{-8}	M (mol/L)
Oxidation state IV model, solubility in 3 × the minimum volume of Salado brine	SOLMOD4	SOLSOH3	5.45×10^{-8}	M
Oxidation state IV model, solubility in 4 × the minimum volume of Salado brine	SOLMOD4	SOLSOH4	5.45×10^{-8}	M
Oxidation state IV model, solubility in 5 × the minimum volume of Salado brine	SOLMOD4	SOLSOH5	5.45×10^{-8}	M
Oxidation state IV model, solubility in the minimum volume of Castile brine	SOLMOD4	SOLCOH	5.44×10^{-8}	M
Oxidation state IV model, solubility in 2 × the minimum volume of Castile brine	SOLMOD4	SOLCOH2	5.44×10^{-8}	M
Oxidation state IV model, solubility in 3 × the minimum volume of Castile brine	SOLMOD4	SOLCOH3	5.44×10^{-8}	M
Oxidation state IV model, solubility in 4 × the minimum volume of Castile brine	SOLMOD4	SOLCOH4	5.44×10^{-8}	M
Oxidation state IV model, solubility in 5 × the minimum volume of Castile brine	SOLMOD4	SOLCOH5	5.44×10^{-8}	M

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Table 1. Parameter Data Entry for the Baseline Actinide Solubilities for the CRA-2019 PA (Domski and Sisk-Scott, 2019, Tables 6 and 7) (continued).

Parameter Description	Material	Property	Value	Units
Oxidation state V model, solubility in the minimum volume of Salado brine	SOLMOD5	SOLSOH	4.02×10^{-7}	M (mol/L)
Oxidation state V model, solubility in 2 × the minimum volume of Salado brine	SOLMOD5	SOLSOH2	2.83×10^{-7}	M
Oxidation state V model, solubility in 3 × the minimum volume of Salado brine	SOLMOD5	SOLSOH3	2.42×10^{-7}	M
Oxidation state V model, solubility in 4 × the minimum volume of Salado brine	SOLMOD5	SOLSOH4	2.21×10^{-7}	M
Oxidation state V model, solubility in 5 × the minimum volume of Salado brine	SOLMOD5	SOLSOH5	2.09×10^{-7}	M
Oxidation state V model, solubility in the minimum volume of Castile brine	SOLMOD5	SOLCOH	1.20×10^{-6}	M
Oxidation state V model, solubility in 2 × the minimum volume of Castile brine	SOLMOD5	SOLCOH2	7.27×10^{-7}	M
Oxidation state V model, solubility in 3 × the minimum volume of Castile brine	SOLMOD5	SOLCOH3	5.52×10^{-7}	M
Oxidation state V model, solubility in 4 × the minimum volume of Castile brine	SOLMOD5	SOLCOH4	4.61×10^{-7}	M

Table 1 continued on next page

Table 1. Parameter Data Entry for the Baseline Actinide Solubilities for the CRA-2019 PA (Domski and Sisk-Scott, 2019, Tables 6 and 7) (continued).

Parameter Description	Material	Property	Value	Units
Oxidation state V model, solubility in 5 × the minimum volume of Castile brine	SOLMOD5	SOLCOH5	4.05×10^{-7}	M (mol/L)

Tables 2 and 3 of this memorandum provide the parameter data entry information for the uncertainties in the solubilities of Am(III) and Th(IV) predicted for the WIPP PA Parameter Database for the CRA-2019 PA. These uncertainties are based on the differences between the logs of the measured and predicted solubilities of Th(IV) and Am(III) (Domski, 2019).

Table 2 of this memorandum provides the cumulative distribution function (CDF) Table 9 of Domski (2019). This CDF defines the solubility multiplier SOLVAR for the oxidation state III model material SOLMOD3 in the WIPP PA Parameter Database for the CRA-2019 PA.

Table 3 of this memorandum provides the CDF Table 6 of Domski (2019). It defines the solubility multiplier SOLVAR for the oxidation state IV model material SOLMOD4 in the WIPP PA Parameter Database for the CRA-2019 PA.

Table 2. CDF of the Differences between the Measured and Predicted Nd(III) and Am(III) Solubilities for CRA 2019 PA (Domski 2019). This CDF Defines the Solubility Multiplier SOLVAR for the Oxidation-State III Model Material SOLMOD3 in the WIPP PA Parameter Database.

D	*P(D<X)* for CRA 2019 PA
-1.142510	0.01220
-0.932358	0.02439
-0.875954	0.03659
-0.805676	0.04878
-0.694681	0.06098
-0.677855	0.07317
-0.665805	0.08537
-0.566530	0.09756
-0.562972	0.1098
-0.487951	0.1220
-0.486971	0.1341
-0.442671	0.1463
-0.417617	0.1585
-0.376826	0.1707
-0.291642	0.1829
-0.232110	0.1951
-0.228885	0.2073
-0.202533	0.2195
-0.166077	0.2317
-0.160532	0.2439
-0.122178	0.2561
-0.114771	0.2683
-0.112331	0.2805
-0.108348	0.2927
-0.100004	0.3049
-0.079188	0.3171
-0.069364	0.3293
-0.025201	0.3415
0.007030	0.3537
0.048993	0.3659
0.049039	0.3780

Table 2 continued on next page

Table 9. CDF of the Differences between the Measured and Predicted Nd(III) and Am(III) Solubilities for CRA 2019 PA. (Cont.)

D	*P(D<X)* for CRA 2019 PA
0.049806	0.3902
0.074136	0.4024
0.074136	0.4146
0.106091	0.4268
0.155677	0.4390
0.160394	0.4512
0.215051	0.4634
0.254326	0.4756
0.313025	0.4878
0.346357	0.5000
0.685282	0.5122
0.701582	0.5244
0.749390	0.5366
0.778205	0.5488
0.802090	0.5610
0.850272	0.5732
0.889953	0.5854
0.952970	0.5976
1.028720	0.6098
1.068567	0.6220
1.095435	0.6341
1.170804	0.6463
1.215464	0.6585
1.217682	0.6707
1.232646	0.6829
1.236077	0.6951
1.236170	0.7073
1.285946	0.7195
1.295231	0.7317
1.418860	0.7439
1.419674	0.7561
1.451948	0.7683
1.518970	0.7805

Table 2 continued on next page

Table 2. CDF of the Differences between the Measured and Predicted Nd(III) and Am(III) Solubilities for CRA 2019 PA. (Cont.)

D	*P(D<X)* for CRA 2019 PA
1.557256	0.7927
1.570299	0.8049
1.643798	0.8171
1.672233	0.8293
1.703691	0.8415
1.792566	0.8537
1.916789	0.8659
1.963935	0.8780
2.023033	0.8902
2.059652	0.9024
2.068615	0.9146
2.175439	0.9268
2.251789	0.9390
2.343682	0.9512
2.372998	0.9634
2.627935	0.9756
2.683488	0.9878
2.971474	1.0000

Table 3. CDF of the Differences between Measured and Predicted Th(IV) Solubilities for CRA 2019 PA (Domski 2019). This CDF Defines the Solubility Multiplier SOLVAR for the Oxidation-State IV Model Material SOLMOD4 in the WIPP PA Parameter Database.

D	*P(D<X)* for CRA 2019 PA
-2.0098	0.0227
-1.4885	0.0455
-1.3031	0.0682
-1.0158	0.0909
-0.9475	0.1136
-0.8003	0.1364
-0.7203	0.1591
-0.7103	0.1818
-0.6458	0.2045
-0.6103	0.2273
-0.6103	0.2500
-0.5612	0.2727
-0.5603	0.2955
-0.5552	0.3182
-0.5403	0.3409
-0.5203	0.3636
-0.4645	0.3864
-0.4252	0.4091
-0.4192	0.4318
-0.4041	0.4545
-0.3303	0.4773
-0.0996	0.5000
-0.0803	0.5227
0.0297	0.5455
0.1597	0.5682
0.2697	0.5909
0.2897	0.6136
0.3919	0.6364
0.4597	0.6591
0.6797	0.6818

Table 3 continued on next page

Table 3. CDF of the Differences between the Measured and Predicted Th(IV) Solubilities for CRA 2019 PA (Domski 2019) (Cont.).

D	*P(D<X)* for CRA 2019 PA
0.6897	0.7045
0.7340	0.7273
0.7497	0.7500
0.7740	0.7727
0.7873	0.7955
0.7890	0.8182
0.8085	0.8409
0.8228	0.8636
0.8640	0.8864
0.8897	0.9091
1.1567	0.9318
1.2526	0.9545
1.2953	0.9773
1.4266	1.0000

REFERENCES

Domski, P.S. 2019. "Uncertainty Analysis of Actinide Solubilities for CRA 2019". Carlsbad, NM: Sandia National Laboratories. ERMS pending.

Domski, P.S. and C. Sisk-Scott. 2019. "Prediction of Baseline Actinide Solubilities for CRA 2019 with an Updated EQ3/6 Pitzer Thermodynamic Database, DATA0.FM4". Carlsbad, NM: Sandia National Laboratories. ERMS pending.

Sisk-Scott, C. 2019. "Calculation of Organic-Ligand Concentrations for the WIPP CRA-2019 Deferred PA" Carlsbad, NM: Sandia National Laboratories. ERMS 571011.

Distribution:

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