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date: November 18, 2009

to: Records Center

from: Daniel J. Clayton

Technical Review: James Garner

QA Review: Mario Chavez

subject: Update to the K_d values for the PABC-2009

As noted in the third set of the EPA's completeness comments (Kelly, 2009), comment 3-C-25, the matrix partition coefficient (K_d) values used in the 2009 Compliance Recertification Application (CRA-2009) Performance Assessment (PA) were derived from experimental data with low to intermediate organic ligand concentrations (Brush and Storz 1996). The predicted organic ligand concentrations have increased significantly since 1996. The EPA recommended that the K_d ranges be revisited based on the higher organic ligand concentrations.

A phone conversation with an EPA contractor was conducted and the results of those discussions were documented in email (Appendix A). Based these discussions, the K_d ranges will be expanded to account for the increased organic ligand concentrations. During the phone conversation, it was noted that the uranium(VI) range will not be modified, as the lower bound is already effectively zero and hence the effect of the high organic ligand concentration is already incorporated. Furthermore, although neptunium is not currently included in the Culebra transport calculations, we will update its K_d range to maintain consistency. Table 1 shows the K_d parameters that will be updated for the 2009 Performance Assessment Baseline Calculation (PABC-2009).

Table 1. K_d parameters to be updated for the PABC-2009.

Material	Property	Description
AM+3	MKD_AM	Matrix Partition Coefficient for Americium
NP+4	MKD_NP	Matrix Partition Coefficient for Neptunium
NP+5	MKD_NP	Matrix Partition Coefficient for Neptunium
PU+3	MKD_PU	Matrix Partition Coefficient for Plutonium
PU+4	MKD_PU	Matrix Partition Coefficient for Plutonium
TH+4	MKD_TH	Matrix Partition Coefficient for Thorium
U+4	MKD_U	Matrix Partition Coefficient for Uranium

QA-L gd 11/19/09

Two clarifications for the appropriate parameter ranges were addressed during the phone conversation. First, the experimental data used to develop the K_d ranges (Brush and Storz 1996) were rounded to one digit and because it is given in cm^3/g, it is converted to m^3/kg by dividing by a factor of 1,000 for use in PA. Second, since the K_d ranges utilize a lognormal distribution, zero is not a valid lower bound. Therefore, the CRA-2009 lower bound of uranium(VI), 0.00003 m^3/kg, is used to approximate the recommended lower bound of zero for the K_d range of the neptunium(V). Tables 2 to 8 show the updated PABC-2009 K_d ranges.

Table 2. Americium(III) K_d (AM+3:MKD_AM) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	0.4
Minimum	0.005
Mean	0.090
Median	0.045
Standard Deviation	0.10
Units	m^3/kg

Table 3. Neptunium(IV) K_d (NP+4:MKD_NP) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	10.0
Minimum	0.0005
Mean	1.0
Median	0.071
Standard Deviation	2.0
Units	m^3/kg

Table 4. Neptunium(V) K_d (NP+5:MKD_NP) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	0.2
Minimum	0.00003
Mean	0.023
Median	0.0024
Standard Deviation	0.042
Units	m^3/kg

Table 5. Plutonium(III) K_d (PU+3:MKD_PU) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	0.4
Minimum	0.005
Mean	0.090
Median	0.045
Standard Deviation	0.10
Units	m^3/kg

Table 6. Plutonium(IV) K_d (PU+4:MKD_PU) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	10.0
Minimum	0.0005
Mean	1.0
Median	0.071
Standard Deviation	2.0
Units	m^3/kg

Table 7. Thorium(IV) K_d (TH+4:MKD_TH) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	10.0
Minimum	0.0005
Mean	1.0
Median	0.071
Standard Deviation	2.0
Units	m^3/kg

Table 8. Uranium(IV) K_d (U+4:MKD_U) distribution for the PABC-2009.

Statistic	Value
Distribution	Loguniform
Maximum	10.0
Minimum	0.0005
Mean	1.0
Median	0.071
Standard Deviation	2.0
Units	m^3/kg

REFERENCES

Brush, L.H. and L.J. Storz 1996. Revised Ranges and Probability Distributions of Kds for Dissolved Pu, Am, U, Th and Np in the Culebra for the PA Calculations to Support the WIPP CCA. Memorandum to M.S. Tierney, Sandia National Laboratories, Albuquerque, NM. ERMS 241561.

Kelly, T.E. 2009. EPA Third Letter Requesting Additional Information on the CRA-2009. U.S. EPA, Office of Radiation and Indoor Air, Washington, D.C. ERMS 552374.

From: Janet Schramke [mailto:ja_schramke@enchemica.com]
Sent: Friday, November 06, 2009 1:34 PM
To: Clayton, Daniel James
Cc: Charles Byrum
Subject: RE: PABC09 Kds

Dan-

These Kd ranges are supported by the available data. I believe they are appropriate to use in the PABC calculations.

Regards,
Janet Schramke

At 09:45 AM 11/6/2009, you wrote:

> Janet,
>
> Based on our phone conversation. We will be modifying the Kd ranges per the table below.
>
Oxidation State	CRA-2009		Updated	
	High	Low	High	Low
III	0.4	0.02	0.4	0.005
IV	10	0.7	10	0.0005
V	0.2	0.001	0.2	0.00003
VI	0.02	0.00003	0.02	0.00003
>
> Let me know if you have any questions or comments.
>
> Thanks,
> Dan