

# **LABORATORY NOTEBOOK**

**GEOSCIENCES & ENGINEERING DIVISION**

SCIENTIFIC  
NOTEBOOK

# 1001

NOTEBOOK NO. \_\_\_\_\_  
ISSUED TO D.R. Turner  
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Surface Complexation modeling Approaches to Simulate Actinide Sorption

Project No. 14002.01.354 – Radionuclide Release Rates and Solubility Limits  
08/05/2009

8/5/2009  
DRT

David R. Turner (DRT)

The information in this scientific notebook is intended to support the staff review of the DOE approach to simulating transport through the engineered barrier system as presented in the 2008 safety analysis report (SAR) and the underlying references. Specifically, the information contained in this notebook is focused on surface complexation modeling (SCM) approaches used to simulate actinide sorption.

DRT

Anticipated software to be used includes:

PHREEQCi, Version 2.15.: This software and the necessary SCM modules were validated in accordance with TOP-018 on 12/11/2008. Additional modules will be validated on an "as needed" basis. Thermodynamic data are anticipated to be based on the Nuclear Energy Agency (NEA) thermodynamic database projects as referenced in the DOE SAR.

*[A large diagonal line is drawn across the page, with the handwritten signature 'DRT' and date '8/12/2009' written across it.]*

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**DIGITIZING NEPTUNIUM AND PLUTONIUM SORPTION DATA**

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As a check for the reported ranges in neptunium and plutonium sorption on iron (hydr)oxides, available experimental data for sorption as a function of geochemistry were identified and digitized (see references listed below). These results, usually reported as percent sorbed, were then converted to sorption coefficients ( $K_d$  in mL/g) for more ready comparison with the values reported by DOE in the SAR. As can be seen from the references, there is generally much more information available on neptunium sorption on Fe-(hydr)oxides. Only two studies, both from 1985, present sorption results for plutonium on Fe-(hydr)oxides.

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Zuyi, T. C. Taiwei, L. Weijuan, D. Jinzhou, D. Xiongxin, and G. Yingjie. 2004. "Cation Adsorption of  $\text{NpO}_2^+$ ,  $\text{UO}_2^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Yb}^{3+}$ , and  $\text{Am}^{3+}$  Onto Oxides of Al, Si, and Fe From Aqueous Solution: Ionic Strength Effect." *Colloids and Surfaces A: Physicochemical Engineering Aspects*. Vol. 242. pp. 39-45.

## PROCEDURE FOR CAPTURING DATA POINTS FROM GRAPH IMAGES

By: Deborah J. Waiting, Research Technologist

### Software used:

Seiko Epson Expression 10000 XL scanner & software  
 Adobe Illustrator, v. 10.0.3  
 ESRI ArcInfo Desktop v. 9.0.0 (Limited validation 2/22/2008)  
 ESRI ArcGIS Desktop v. 9.0 (Limited validation 5/24/2005)  
 ESRI ArcView v. 3.3 (Limited validation 7/23/20008)  
 Microsoft Excel 2003 SP3

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Each graph image was scanned from a copy of the original material using Epson Expression 10000 XL scanner to create individual tiff format image of the graph. The scanned tiff graph images were opened in Adobe Illustrator to straighten the image if tilted during copying of original material, and to add crossing lines aligned to the axes to create interior points to aid in registration of the graph. ArcInfo was used to create a grid with assigned coordinate points that correspond to points taken from the x and y axes of the grid image. The graph image was registered to the grid using ArcGIS, creating a world file that assigns the coordinates from the grid to the graph image. The registration of the image to the grid was checked in ArcView and random points on the image were verified with the grid. A point shapefile containing the x and y coordinates for each point was created in ArcView for each data series on the graph. Point coordinates for the graph data series were transferred to a Microsoft Excel worksheet for analysis.

Date \_\_\_\_\_



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<b>Herberling Figure 4 - Open Diamonds = pH 6.0</b>			
("X_COORD" & "Y_COORD" numbers are for digitizing grid)			
X_COORD	c [mol/L]	Y_COORD	q [mol/g]
-6.67851	-6.68	-8.00901	-8.01
-6.20867	-6.21	-7.69166	-7.69
-5.85010	-5.85	-7.49383	-7.49
-5.51214	-5.51	-7.28775	-7.29
-5.07114	-5.07	-7.03222	-7.03
-4.55184	-4.55	-6.74784	-6.75
<b>Herberling Figure 4 - Open Triangles = pH 7.2</b>			
("X_COORD" & "Y_COORD" numbers are for digitizing grid)			
X_COORD	c [mol/L]	Y_COORD	q [mol/g]
-6.78155	-6.78	-7.91421	-7.91
-6.27049	-6.27	-7.61335	-7.61
-5.92429	-5.92	-7.35782	-7.36
-5.53275	-5.53	-7.23005	-7.23
-5.07527	-5.08	-6.99925	-7.00
-4.56008	-4.56	-6.71487	-6.71
<b>Herberling Figure 4 - Open Circles = pH 8.3</b>			
("X_COORD" & "Y_COORD" numbers are for digitizing grid)			
X_COORD	c [mol/L]	Y_COORD	q [mol/g]
-6.92580	-6.93	-7.84003	-7.84
-6.33231	-6.33	-7.54740	-7.55
-6.10975	-6.11	-7.41552	-7.42
-5.93253	-5.93	-7.35782	-7.36
-5.71409	-5.71	-7.23830	-7.24
-5.55335	-5.55	-7.18059	-7.18
-5.26073	-5.26	-7.06519	-7.07
-5.08351	-5.08	-6.97452	-6.97
-4.87744	-4.88	-6.90858	-6.91
-4.74555	-4.75	-6.85088	-6.85
-4.56008	-4.56	-6.71487	-6.71
-4.41995	-4.42	-6.67778	-6.68
<b>Herberling Figure 4 - Open Squares = pH 9.4</b>			
("X_COORD" & "Y_COORD" numbers are for digitizing grid)			
X_COORD	c [mol/L]	Y_COORD	q [mol/g]
-6.76094	-6.76	-7.92658	-7.93
-6.32819	-6.33	-7.55153	-7.55
-5.88307	-5.88	-7.42788	-7.43
-5.53687	-5.54	-7.21357	-7.21
-5.08351	-5.08	-6.99101	-6.99
-4.56008	-4.56	-6.69838	-6.70

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Neptunium data pts - HEBERLING (2008)

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Jerdan Figure 1a - Open Squares = Np-U 4 hrs (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Closed Squares = Np 4 hrs (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Open Circles = Np-U 6 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Closed Circles = Np 6 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Open Triangles = Np-U 24 days (Y COORD' numbers are for digitizing grid)			
X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))	
3.51	1.03935	10.95		5.01	2.62714	423.78		5.00	2.17349	149.10		3.50	1.04692	11.14		3.50	1.00911	10.21	
5.00	2.28660	193.60		6.60	3.68567	4849.20		6.60	3.50420	3193.01		5.01	2.60446	402.22		5.00	2.25666	180.58	
6.60	3.30762	2030.58		8.91	4.94833	88783.04		8.81	4.75175	56461.19		6.61	3.78396	6080.79		6.61	3.77640	5875.86	
8.91	4.72907	53588.30										8.81	5.09955	125762.16		8.80	4.37371	23643.40	

Jerdan Figure 1b - Open Squares = Np-U 4 hrs (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Closed Squares = Np 4 hrs (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Open Circles = Np-U 6 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Closed Circles = Np 6 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Open Triangles = Np-U 24 days (Y COORD' numbers are for digitizing grid)			
X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)	
3.51	-6.20079	6.30E-07		6.60	-6.89594	1.27E-07		3.51	-6.16191	6.89E-07		3.50	-6.22142	6.01E-07		3.50	-6.13215	7.38E-07	
5.00	-6.20793	6.20E-07		8.92	-7.01497	9.66E-08		5.00	-6.18175	6.58E-07		4.99	-6.22142	6.01E-07		5.01	-6.19167	6.43E-07	
6.60	-6.59836	2.52E-07						6.61	-6.74715	1.79E-07		6.60	-6.98521	1.03E-07		6.61	-7.02489	9.44E-08	
8.92	-7.00505	9.88E-08										8.81	-7.01049	9.76E-08					

Neptunium data pts - JERDEN (2007)

Jerdan Figure 1a - Closed Triangles = Np 24 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Open Diamonds = Np-U 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - Closed Diamonds = Np 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - "X" = GW Np-U 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1a - "X" = GW Np 103 days (Y COORD' numbers are for digitizing grid)			
X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))		X COORD	Y COORD	Kd (mL/g - (mol/kg)/(mol/kg))	
3.71	1.00155	10.04		5.15	2.16593	146.53		5.94	3.33787	2177.06		8.09	5.07687	13363.06		8.03	5.21297	163293.91	
5.10	2.60446	402.22		6.30	3.54201	3483.45		6.46	3.80664	6406.78		8.11	5.00126	106290.55		8.06	5.16004	144567.29	
6.82	3.86981	7759.08		7.03	4.11864	13080.97		7.03	4.21493	16403.25									
8.80	4.71395	51754.72		8.00	4.13932	13782.25		8.21	4.16956	14776.11									

Jerdan Figure 1b - Closed Triangles = Np 24 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Open Diamonds = Np-U 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - Closed Diamonds = Np 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - "X" = GW Np-U 103 days (Y COORD' numbers are for digitizing grid)				Jerdan Figure 1b - "X" = GW Np 103 days (Y COORD' numbers are for digitizing grid)			
X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)		X COORD	Y COORD	Np In sol(moles/kg)(1.0E+)	
3.70	-6.20159	6.29E-07		3.51	-5.03111	9.31E-06		3.50	-5.08071	8.30E-06		8.09	-6.69756	2.01E-07		3.50	-5.08071	8.30E-06	
5.11	-6.25118	5.61E-07		5.16	-5.19874	6.31E-06		5.93	-5.57667	2.65E-06		8.10	-6.64795	2.25E-07		8.07	-6.64795	2.25E-07	
6.80	-7.02489	9.44E-08		6.31	-5.75522	1.76E-06		6.47	-6.01312	9.70E-07		8.03	-6.70747	1.96E-07		8.03	-6.70747	1.96E-07	
8.82	-7.02489	9.44E-08		7.03	-6.27102	5.36E-07		7.03	-6.30078	5.00E-07									
				8.00	-6.28086	5.12E-07		8.21	-6.28094	5.24E-07									

Neptunium data pts - JERDEN (2007)

JERDEN

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Khasanov Figure 1 - Closed Squares = c( $\beta$ -Fe <sub>2</sub> O <sub>3</sub> )=1.12 g/l										Khasanov Figure 1 - Open Circles = c( $\beta$ -Fe <sub>2</sub> O <sub>3</sub> )=0.71 g/l										Khasanov Figure 1 - Closed Triangles = c( $\beta$ -Fe <sub>2</sub> O <sub>3</sub> )=0.44 g/l										Khasanov Figure 1 - Open Diamonds = c( $\beta$ -FeOOH)=0.22 g/l									
alpha-Hematite, Cs=12 g/L, Np(tot)=6E-7 M										alpha-Hematite, Cs=0.71 g/L, Np(tot)=6E-7 M										alpha-Hematite, Cs=0.44 g/L, Np(tot)=6E-7 M										alpha-Goethite, Cs=0.22 g/L, Np(tot)=6E-7 M									
Asp (m2/g) = 6.4										Asp (m2/g) = 8.4										Asp (m2/g) = 8.4										Asp (m2/g) = 41.7									
X COORD	pH	Y COORD	Np(V) sorption, %	Kd	log Kd	log Ka (mL/m2)	X COORD	pH	Y COORD	Np(V) sorption, %	Kd	log Kd	log Ka (mL/m2)	X COORD	pH	Y COORD	Np(V) sorption, %	Kd	log Kd	log Ka (mL/m2)	X COORD	pH	Y COORD	Np(V) sorption, %	Kd	log Kd	log Ka (mL/m2)												
3.85	0.19085	1.91	17.4	1.240	0.434	4.51	0.38375	3.84	56.2	1.750	0.944	4.18	-0.10728	-1.07	-24.1	2.76	-0.01958	-0.20	-8.9	2.76	-0.01958	-0.20	-8.9	2.76	-0.01958	-0.20	-8.9												
6.27	1.36575	13.66	341.2	2.150	1.344	5.91	0.48896	4.89	72.4	1.800	1.054	2.65	0.19085	1.91	44.2	1.646	0.839	2.32	0.29607	2.96	138.7	2.142	0.522	3.44	0.19085	1.91	88.4	1.947	0.327										
6.27	1.94444	19.44	215.5	2.333	1.527	6.41	1.99704	19.97	351.5	2.546	1.740	3.95	0.03303	0.33	7.5	0.877	0.071	3.44	0.19085	1.91	88.4	1.947	0.327	4.09	0.82214	8.22	407.2	2.610	0.990										
6.58	1.57618	15.78	197.1	2.223	1.417	6.77	2.48005	24.88	466.5	2.889	1.863	5.16	0.26100	2.61	60.9	1.785	0.978	5.09	0.82214	8.22	407.2	2.610	0.990	5.11	1.54111	15.41	828.1	2.918	1.298										
6.67	1.06765	10.68	106.7	2.029	1.222	7.41	2.92844	29.26	582.7	2.765	1.959	5.20	0.03303	0.33	7.5	0.877	0.071	4.09	1.88140	18.81	918.8	2.963	1.343	6.28	0.86432	8.64	161.7	2.209	1.403										
6.81	3.03166	30.32	308.4	2.589	1.783	7.83	3.84541	38.45	808.0	2.907	2.101	6.70	0.40128	4.01	95.0	1.978	1.172	5.72	3.78570	37.86	2769.1	3.442	1.822	6.42	6.73172	67.32	8362.3	3.971	2.351										
7.42	3.17194	31.72	414.8	2.618	1.812	8.12	5.15349	51.53	1497.7	3.175	2.369	7.60	1.47097	14.71	392.0	2.583	1.787	6.42	6.73172	67.32	8362.3	3.971	2.351	6.55	7.71373	77.14	15330.1	4.186	2.566										
7.49	5.53928	55.39	3106.7	3.045	2.239	8.83	6.50375	65.04	2620.0	3.418	2.612	8.51	2.40037	24.00	717.8	2.856	2.050	6.55	7.71373	77.14	15330.1	4.186	2.566	8.05	2.76862	27.69	870.1	2.940	2.133										
7.83	8.73080	87.31	6141.9	3.788	2.982														10.04	9.51992	95.20	80135.7	4.955	3.335															
8.53	9.50238	95.02	17049.7	4.232	3.426																																		
9.66	9.32702	93.27	12374.4	4.093	3.286																																		
9.88	8.73080	87.31	6141.9	3.788	2.982																																		
6.32	0.69939	6.99	368.4	1.827	1.021																																		
6.42	0.64679	6.47	61.7	1.791	0.984																																		

Khasanov Figure 2 - Closed Squares = Np(V) in absence of HA											
alpha-Goethite, Cs=0.22 g/L, Np(tot)=5.8E-7 M											
Asp (m2/g) = 41.7											
X COORD	pH	Y COORD	Np sorption, %	Kd	log Kd	log Ka (mL/m2)					
2.30	0.31360	3.14	147.2	2.168	0.548	2.26	0.22593	2.26	105.1	2.021	0.401
4.07	0.83968	8.40	416.7	2.620	1.000	5.02	1.68894	16.99	830.3	2.969	1.348
5.11	1.54111	15.41	828.1	2.918	1.298	5.70	3.80323	38.03	2789.7	3.446	1.825
6.42	6.99665	69.97	9214.7	3.964	2.344	6.51	7.97678	79.77	17920.8	4.253	3.533
8.33	9.78341	97.83	32818.8	4.516	2.886	10.05	9.84884	98.85	83688.4	4.923	3.303

Khasanov Figure 3 - Closed Squares = Np(V) without HA											
alpha-Goethite, Cs=0.22 g/L, Np(tot)=5.8E-7 M											
Asp (m2/g) = 41.7, Np(HA) sequestered from solution, %											
X COORD	pH	Y COORD	Np sorption, %	Kd	log Kd	log Ka (mL/m2)					
2.30	-0.03711	-0.37	-16.8	#NUM!	#NUM!	2.37	-0.03711	-0.37	-16.8	#NUM!	#NUM!
2.74	-0.01958	-0.20	-8.9	#NUM!	#NUM!	2.79	-0.01958	-0.20	-8.9	#NUM!	#NUM!
3.41	0.20839	2.08	96.7	1.986	0.365	4.04	0.68188	6.82	332.6	2.522	0.902
4.30	0.92738	9.27	464.6	2.667	1.047	5.00	1.66386	16.64	807.3	2.958	1.338
5.09	2.38283	23.83	1421.9	3.153	1.533	5.30	4.60988	46.10	3887.5	3.590	1.970
5.91	6.73172	67.32	9362.3	3.971	2.351	6.46	7.38054	73.81	12807.2	4.107	2.487
6.51	7.69619	76.96	15184.7	4.181	2.561	7.32	8.48530	84.85	25463.5	4.406	2.786
7.72	9.99384	99.94	40630.8	4.609	2.989	8.35	9.18673	91.87	51345.6	4.711	3.090
10.07	9.50238	95.02	86798.4	4.939	3.318						

Khasanov Figure 4 - Closed Squares = Np(V) without HA											
alpha-Hematite, Cs=0.44 g/L, Np(tot)=7.05E-7 M											
Asp (m2/g) = 6.4, Np sorption, % by $\beta$ -Fe <sub>2</sub> O <sub>3</sub>											
X COORD	pH	Y COORD	Np sorption, %	Kd	log Kd	log Ka (mL/m2)					
2.13	0.36058	3.61	85.0	1.929	1.123	2.64	0.28914	2.89	67.7	1.830	1.024
3.59	0.00340	0.03	0.8	-0.112	-0.918	4.13	0.04422	0.44	10.1	1.004	0.198
5.28	0.06463	0.65	14.8	1.170	0.364	5.68	0.25853	2.59	60.3	1.780	0.974
6.23	0.67694	6.77	165.0	2.218	1.411	6.68	0.80961	8.10	290.2	2.301	1.495
7.31	1.59540	15.95	431.4	2.635	1.829	7.80	2.70776	27.08	843.9	2.926	2.120
8.28	3.20782	32.08	1073.4	3.031	2.225						

Khasanov Figure 5 - Closed Squares = Np(V) without HA											
alpha-Goethite, Cs=0.22 g/L, Np(tot)=5.8E-7 M											
Asp (m2/g) = 41.7, Np sorption, % onto $\beta$ -FeOOH											
X COORD	pH	Y COORD	Np sorption, %	Kd	log Kd	log Ka (mL/m2)					
2.72	-0.01958	-0.20	-8.9	#NUM!	#NUM!	2.78	-0.01958	-0.20	-8.9	#NUM!	#NUM!
3.42	0.31360	3.14	147.2	2.168	0.548	4.06	0.83968	8.40	416.7	2.620	1.000
4.30	0.92738	9.27	464.6	2.667	1.047	5.02	1.68140	16.81	918.8	2.963	1.343
5.09	1.55865	15.59	839.3	2.924	1.304	5.39	4.01386	40.14	3047.6	3.484	1.864
5.88	6.76679	67.67	9513.2	3.978	2.358	6.42	7.32794	73.28	12465.6	4.096	2.476
6.48	7.73126	77.31	15489.7	4.190	2.570	7.26	8.15212	81.52	20525.6	4.302	2.682
7.67	8.71327	87.13	30780.2	4.488	2.868	8.30	9.01138	90.11	41432.3	4.817	2.997
10.00	9.53745	95.37	93724.0	4.972	3.354						

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Y COORD numbers are for digitizing grid									
KOHLER Figure 3 - Hematite - Closed Triangles = Experiment (average of digitizing 3(a) and 3(b))									
Carbonate adsorption: Cs=5.75 of CO2(bst)=59 uM									
Aspm2(z)= 14.4 % Suspension									
X COORD pH	Y COORD	CO2 adsorbed	Kd	log Kd	log Ka (mL/m2)				
4.01	3.95511	39.56	113.8	2.056	0.896				
4.31	4.83480	46.35	150.2	2.177	1.018				
4.74	5.7424	57.74	237.6	2.376	1.216				
5.22	7.01584	70.16	406.9	2.612	1.453				
5.65	7.69522	76.95	580.7	2.764	1.606				
5.80	7.82669	78.27	626.3	2.797	1.638				
6.18	8.06864	80.80	736.5	2.867	1.709				
6.47	8.03851	80.39	712.7	2.853	1.695				
6.81	8.01880	80.17	702.9	2.847	1.689				
7.04	7.57105	75.71	542.1	2.734	1.576				
7.47	6.54848	65.48	330.0	2.518	1.360				

KOHLER Figure 4 - Goethite - Closed Circles = Experiment (average of digitizing 4(a) and 4(b))									
Carbonate sorption: Cs=2 of CO2(bst)=55 uM									
Aspm2(z)= 45 % Suspension									
X COORD pH	Y COORD	CO2 adsorbed	Kd	log Kd	log Ka (mL/m2)				
3.99	2.2534	22.54	145.9	2.163	0.510				
4.57	3.26893	32.69	242.8	2.385	0.720				
5.10	4.37185	43.72	386.4	2.589	0.936				
5.57	5.27756	52.78	556.8	2.747	1.094				
6.05	5.57103	55.71	630.5	2.800	1.146				
6.49	5.00000	50.00	500.0	2.699	1.046				
6.72	4.39376	43.94	391.9	2.593	0.940				
6.93	2.90372	29.04	204.6	2.311	0.658				
7.20	1.10691	11.07	82.2	1.914	0.441				
7.62	1.42099	14.21	82.8	1.916	0.265				

KOHLER Figure 5 - Hematite - Open Circles = 0.005M									
Cs=1 of: No CO2: I=0.1 M NaClO4									
Aspm2(z)= 14.4									
X COORD pH	Y COORD	% Np(V) adsorbed	Kd	log Kd	log Ka (mL/m2)				
4.94	0.03884	-0.40	-4.0	#N/A	#N/A				
6.01	0.15863	1.59	18.1	1.208	0.050				
6.15	1.57291	15.73	186.6	2.271	1.113				
6.77	4.12058	41.21	700.8	2.846	1.697				
6.81	4.81009	48.10	928.9	2.967	1.809				
6.91	4.05046	40.50	690.8	2.833	1.875				
7.53	8.59655	85.97	6125.3	3.787	2.829				
10.00	9.94050	99.41	16707.2	5.223	4.065				

KOHLER Figure 5 - Hematite - Closed Triangles = 0.01M									
Cs=1 of: No CO2: I=0.01 M NaClO4									
Aspm2(z)= 14.4									
X COORD pH	Y COORD	% Np(V) adsorbed	Kd	log Kd	log Ka (mL/m2)				
5.35	-0.01847	-0.18	-1.8	#N/A	#N/A				
5.87	0.02524	0.85	8.5	0.818	-0.340				
6.02	0.39258	3.93	40.8	1.611	0.453				
6.52	3.50120	35.01	538.7	2.731	1.573				
6.77	4.30757	43.08	756.7	2.879	1.721				
7.24	6.24754	62.48	1864.9	3.271	2.083				
7.23	6.92537	69.25	2252.4	3.353	2.184				
7.98	9.34448	93.44	14255.3	4.154	2.996				
9.21	9.82887	98.29	109468.9	5.145					
9.57	9.88378	98.94	93126.5	4.989					

KOHLER Figure 6 - Hematite - Closed Diamonds = 0.01M									
Cs=1 of: No CO2: I=0.1 M NaClO4									
Aspm2(z)= 14.4									
X COORD pH	Y COORD	% Np(V) adsorbed	Kd	log Kd	log Ka (mL/m2)				
4.05	-0.03984	-0.40	-4.0	#N/A	#N/A				
4.58	-0.02815	-0.28	-2.8	#N/A	#N/A				
4.81	-0.01847	-0.18	-1.8	#N/A	#N/A				
5.05	-0.00478	-0.05	-0.5	#N/A	#N/A				
5.78	-0.01847	-0.18	-1.8	#N/A	#N/A				
6.89	3.32950	33.26	498.3	2.698	1.539				
6.82	3.87849	38.76	581.4	2.764	1.606				
6.95	4.83885	48.39	975.8	2.989	1.821				
7.24	7.15810	71.59	3220.0	3.401	2.243				
9.44	9.81713	99.17	119670.9	5.078	3.920				

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Y_COORD numbers are for digitizing grid							NAGASAKI Figure 2 - Open Squares = 0.01 M NaClO <sub>2</sub>							NAGASAKI Figure 2 - Closed Circles = 0.01 M NaClO <sub>2</sub>							NAGASAKI Figure 2 - Cross Squares = 1 M NaClO <sub>2</sub>											
0.889g/L, No CO <sub>2</sub> , 0.01 M NaClO <sub>4</sub> , 1E-8 M							0.889g/L, No CO <sub>2</sub> , 0.01 M NaClO <sub>4</sub> , 1E-8 M							0.889g/L, No CO <sub>2</sub> , 0.01 M NaClO <sub>4</sub> , 1E-8 M							0.889g/L, No CO <sub>2</sub> , 1 M NaClO <sub>4</sub> , 1E-8 M											
Asp(m2/g)= 35.5							Asp(m2/g)= 35.5							Asp(m2/g)= 35.5							Asp(m2/g)= 35.5											
X_COORD	pH	Y_COORD	% Adsorbed	Kd	log Kd	log Ka (mL/m2)	X_COORD	pH	Y_COORD	% Adsorbed	Kd	log Kd	log Ka (mL/m2)	X_COORD	pH	Y_COORD	% Adsorbed	Kd	log Kd	log Ka (mL/m2)	X_COORD	pH	Y_COORD	% Adsorbed	Kd	log Kd	log Ka (mL/m2)					
4.00	0.20839	2.08	23.9	1.379	-0.171	0.400	4.49	0.59418	5.94	71.1	1.852	0.301	4.02	0.22593	2.28	26.0	1.415	-0.135	0.473	4.00	0.24348	2.43	28.1	1.448	-0.102	0.446						
4.51	0.73446	7.34	89.2	1.950	0.400	0.400	5.04	1.41836	14.18	185.9	2.269	0.719	4.53	0.85722	8.57	105.5	2.023	0.473	0.473	5.00	1.22547	12.25	157.1	2.196	0.646	5.00	1.22547	12.25	157.1	2.196	0.646	
5.06	1.13779	11.38	144.4	2.160	0.809	0.809	5.49	4.22409	42.24	822.8	2.915	1.385	4.97	1.31315	13.13	170.0	2.231	0.680	0.680	5.98	7.38301	73.83	3140.8	3.497	1.947	5.98	7.38301	73.83	3140.8	3.497	1.947	
5.55	3.82077	38.21	895.5	2.842	1.292	1.292	6.04	7.48340	74.83	3309.7	3.520	1.970	5.48	4.03120	40.31	759.7	2.881	1.330	1.330	6.55	9.29195	92.92	14761.9	4.169	2.619	6.55	9.29195	92.92	14761.9	4.169	2.619	
6.00	7.48576	74.86	3349.1	3.525	1.975	1.975	6.51	9.31936	93.19	15401.6	4.188	2.637	6.00	7.48576	74.86	3349.1	3.525	1.975	1.975	7.07	8.80759	88.08	27540.6	4.440	2.890	7.07	8.80759	88.08	27540.6	4.440	2.890	
6.51	9.06398	90.64	10892.6	4.037	2.487	2.487	7.50	9.68848	96.88	34753.5	4.541	2.991	6.55	9.29195	92.92	14761.9	4.169	2.619	2.619	8.04	9.81802	98.18	80687.4	4.783	3.233	8.04	9.81802	98.18	80687.4	4.783	3.233	
7.00	9.48484	94.85	20710.3	4.316	2.766	2.766							7.04	9.43224	94.32	18687.4	4.272	2.721	2.721													
7.56	9.80049	98.00	55256.2	4.742	3.182	3.182							7.49	9.88817	98.88	99461.7	4.988	3.447	3.447													
														8.04	9.88817	98.88	99461.7	4.988	3.447	3.447												

Neptunium data pts - NAGASAKI

("Y\_COORD" numbers are for digitizing grid)

NAKATA Figure 2 - Open Circles = Anaerobic							NAKATA Figure 2 - Closed Squares = Aerobic								
Magnetite; Cs=25 g/L; 6E-6M; No CO <sub>2</sub> ; 0.1 M NaNO <sub>3</sub>							Magnetite; Cs=25 g/L; 6E-6M; No CO <sub>2</sub> ; 0.1 M NaNO <sub>3</sub>								
Asp(m2/g)= 1							Asp(m2/g)= 1								
X_COORD	pH	Y_COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)	X_COORD	pH	Y_COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)		
5.06		6.43361		64.34	72.2	1.858	1.858	4.21		0.10317		1.03	0.4	-0.380	-0.380
5.25		9.34456		93.45	570.3	2.756	2.756	5.37		0.47143		4.71	2.0	0.296	0.296
5.23		8.87109		88.71	314.3	2.497	2.497	6.05		1.76908		17.69	8.6	0.934	0.934
5.28		8.43269		84.33	215.2	2.333	2.333	7.11		2.75108		27.51	15.2	1.181	1.181
5.76		8.25734		82.57	189.5	2.278	2.278	7.84		4.18902		41.89	28.8	1.460	1.460
6.02		8.06444		80.64	166.7	2.222	2.222								
7.19		9.78295		97.83	1802.9	3.256	3.256								
7.70		9.95831		99.58	9554.6	3.980	3.980								

NAKATA Figure 3 - Open Circles = Anaerobic							NAKATA Figure 3 - Closed Squares = Aerobic								
Hematite; Cs=25 g/L; 6E-6M; No CO <sub>2</sub> ; 0.1 M NaNO <sub>3</sub>							Hematite; Cs=25 g/L; 6E-6M; No CO <sub>2</sub> ; 0.1 M NaNO <sub>3</sub>								
Asp(m2/g)= 5.8							Asp(m2/g)= 5.8								
X_COORD	pH	Y_COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)	X_COORD	pH	Y_COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)		
4.92		2.75108		27.51	15.2	1.181	0.418	4.30		0.68186		6.82	2.9	0.466	-0.297
5.04		3.62788		36.28	22.8	1.357	0.594	4.72		2.36530		23.65	12.4	1.093	0.330
5.51		8.04691		80.47	164.8	2.217	1.454	5.58		8.38009		83.80	206.9	2.316	1.552
								6.74		9.95831		99.58	9554.6	3.980	3.217
								7.44		9.99338		99.93	60383.0	4.781	4.017

Neptunium data pts - NAKATA

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**TY COORD numbers are for digitizing grid)**  
**NAKAYAMA Figure 3a - Closed Circles = Natl Goethite**  
 Natural Hematite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 15.7

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
4.15	-0.02979	-0.30	-3.0	#NUM!	#NUM!
4.68	0.25518	2.55	26.2	1.418	0.222
5.56	1.03886	10.39	115.9	2.064	0.898
5.85	1.15285	11.53	130.3	2.115	0.919
6.08	1.50907	15.09	177.7	2.250	1.054
6.33	2.05052	20.51	257.9	2.412	1.216
6.49	2.96244	29.62	420.9	2.624	1.428
6.97	4.07383	40.74	687.4	2.837	1.641
7.06	4.08808	40.88	691.5	2.840	1.644
6.97	4.47280	44.73	809.2	2.908	1.712
7.06	4.41580	44.16	790.8	2.898	1.702
7.19	5.01425	50.14	1005.7	3.002	1.807
8.08	5.88342	58.83	1429.2	3.155	1.959
8.63	6.52461	65.25	1877.4	3.274	2.078
8.87	6.83860	68.39	1975.0	3.296	2.100
9.61	7.08031	70.80	2425.0	3.385	2.189
9.95	7.96373	79.64	3910.9	3.592	2.396
10.16	7.99223	79.92	3980.7	3.600	2.404
10.62	8.14896	81.49	4402.4	3.644	2.448

**NAKAYAMA Figure 3a - Open Triangles = Natl Hematite**  
 Natural Hematite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 3.2

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
3.48	0.25518	2.55	26.2	1.418	0.913
4.17	0.38342	3.83	39.9	1.601	1.096
4.45	0.41192	4.12	43.0	1.633	1.128
5.18	1.01036	10.10	112.4	2.051	1.546
5.38	1.19560	11.96	135.8	2.133	1.628
5.95	0.38342	3.83	39.9	1.601	1.096
6.20	0.41192	4.12	43.0	1.633	1.128
6.76	0.58290	5.83	61.9	1.792	1.287
6.96	0.92487	9.25	101.9	2.008	1.503
7.04	0.63990	6.40	68.4	1.835	1.330
7.20	1.29534	12.95	148.8	2.173	1.667
8.38	0.86788	8.68	95.0	1.978	1.473
8.80	1.85104	18.51	227.2	2.356	1.851
8.94	1.25259	12.53	143.2	2.156	1.651
9.17	1.87853	18.80	231.5	2.364	1.859
9.52	1.32383	13.24	152.6	2.184	1.678
9.94	1.95078	19.51	242.4	2.384	1.879
10.36	2.57772	25.78	347.3	2.541	2.036
10.72	2.80570	28.06	390.0	2.591	2.086

**NAKAYAMA Figure 3a - Closed Squares = Natl Magnetite**  
 Natural Magnetite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 5.8

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
3.74	0.82513	8.25	89.9	1.954	1.190
4.31	0.78328	7.82	84.9	1.929	1.165
4.88	0.78328	7.82	84.9	1.929	1.165
5.33	0.96337	9.53	105.4	2.023	1.259
5.82	0.51166	5.12	53.9	1.732	0.968
5.98	0.87238	7.82	84.9	1.929	1.165
6.08	1.08161	10.82	121.3	2.084	1.320
6.43	0.58290	5.83	61.9	1.792	1.028
6.89	0.54016	5.40	57.1	1.757	0.993
7.43	0.95337	9.53	105.4	2.023	1.259
8.20	1.83679	18.37	225.0	2.352	1.589
8.43	1.87953	18.80	231.5	2.364	1.601
8.61	1.52332	15.23	179.7	2.255	1.491
9.10	2.54922	25.49	342.1	2.534	1.771
9.14	2.46373	24.64	326.9	2.514	1.751
9.44	2.52073	25.21	337.0	2.528	1.764
9.59	2.49223	24.92	332.0	2.521	1.758
9.94	3.70337	37.03	588.2	2.769	2.006
10.16	3.16192	31.62	462.4	2.665	1.902
10.66	4.82902	48.29	933.9	2.970	

**NAKAYAMA Figure 3a - Open Circles = Natl Biotite**  
 Natural Biotite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 7.5

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
4.52	0.24093	2.41	24.7	1.392	0.517
4.76	0.11268	1.13	11.4	1.087	0.382
4.94	0.14118	1.41	14.3	1.156	0.281
5.56	0.41192	4.12	43.0	1.633	0.758
6.03	0.51166	5.12	53.9	1.732	0.857
6.50	0.46891	4.69	49.2	1.662	0.817
6.67	0.51166	5.12	53.9	1.732	0.857
7.17	0.54016	5.40	57.1	1.757	0.882
7.88	0.55446	5.54	58.7	1.769	0.894
8.18	1.45202	14.53	169.9	2.230	1.355
8.44	0.92487	9.25	101.9	2.008	1.139
9.07	1.43782	14.38	167.9	2.225	1.350
7.29	1.18135	11.81	134.0	2.127	1.252
9.07	2.10751	21.08	267.0	2.427	1.581
9.54	2.15025	21.50	273.9	2.438	1.563
9.81	2.64895	26.49	369.4	2.567	1.682
9.89	2.77720	27.77	384.5	2.585	1.710
9.88	2.96244	29.62	420.9	2.624	1.749
10.32	2.89119	28.91	406.7	2.609	1.734
10.14	4.20207	42.02	724.8	2.850	1.885
10.61	4.58629	45.58	837.7	2.923	2.046
10.88	6.92358	69.24	2380.5	3.382	2.477
11.13	7.30822	73.08	2715.1	3.434	2.559

**NAKAYAMA Figure 3b - Closed Triangles = Synth Hematite**  
 Synthetic Hematite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 5.9

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
4.34	0.54016	5.40	57.1	1.757	0.985
4.82	0.32642	3.26	33.7	1.528	0.757
5.59	0.82513	8.25	89.9	1.954	1.183
6.46	0.79813	7.98	83.2	1.920	1.149
6.57	1.49482	14.95	175.8	2.245	1.474
6.66	1.16710	11.67	132.1	2.121	1.350
6.96	1.03886	10.39	115.9	2.064	1.293
7.24	1.13860	11.39	128.5	2.109	1.338
8.08	2.86269	28.63	401.1	2.603	1.832
8.71	3.17617	31.76	465.5	2.668	1.897
8.70	3.95894	39.60	655.6	2.817	2.046
8.87	3.81736	38.17	617.4	2.791	2.020
9.24	4.80052	48.01	923.3	2.965	2.194
9.45	6.05440	60.54	1534.5	3.186	2.415
10.19	4.43005	44.30	795.3	2.901	2.130
10.41	6.46187	64.62	1842.4	3.265	2.495
10.58	7.16005	71.80	2546.2	3.406	2.635
10.61	7.25130	72.51	2638.1	3.421	2.650
10.66	5.61289	56.13	1279.3	3.107	2.336
10.91	8.63342	86.33	6317.5	3.801	3.030

**NAKAYAMA Figure 3b - Open Squares = Synth Magnetite**  
 Synthetic Magnetite, Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 5.5

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
3.82	0.19819	1.98	20.2	1.306	0.565
4.75	0.41192	4.12	43.0	1.633	0.893
5.32	0.56865	5.69	60.3	1.780	1.040
6.03	0.83938	8.39	91.6	1.962	1.222
6.70	0.78238	7.82	84.9	1.929	1.188
6.82	1.15285	11.53	130.3	2.115	1.375
7.04	0.62513	6.25	69.9	1.954	1.214
7.04	1.29534	12.95	148.8	2.173	1.432
7.60	1.48057	14.81	173.8	2.240	1.500
7.87	1.93653	19.37	240.2	2.381	1.640
7.94	1.79404	17.94	218.6	2.340	1.599
8.28	1.73705	17.37	210.2	2.323	1.582
8.47	1.55181	15.52	183.7	2.264	1.524
8.71	2.34974	23.50	307.1	2.487	1.747
9.28	2.36399	23.64	309.6	2.491	1.750
9.24	3.04793	30.48	436.4	2.642	1.902
9.69	3.11917	31.19	453.3	2.656	1.916
9.99	3.36140	33.61	506.3	2.704	1.984
10.41	4.48705	44.87	813.9	2.911	2.170

**NAKAYAMA Figure 4 - Open Squares =  $\delta$ -Al<sub>2</sub>O<sub>3</sub>**  
 Synthetic alumina(alpha Al2O3), Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 2.5

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
5.73	0.81088	8.11	88.2	1.946	1.548
7.09	1.15285	11.53	130.3	2.115	1.717
7.09	0.96798	8.68	95.0	1.978	1.580
7.78	0.89637	8.96	98.5	1.993	1.595
8.07	0.98187	9.82	108.9	2.037	1.639
8.87	1.01036	10.10	112.4	2.051	1.653
9.34	1.42358	14.24	166.0	2.220	1.822
9.97	1.43782	14.38	167.9	2.225	1.827
10.55	1.95078	19.51	242.4	2.384	1.987
10.95	2.53497	25.35	339.6	2.531	2.133

**NAKAYAMA Figure 4 - Open Circles = Y-AIOOH**  
 Synthetic Boehmite(gamma AlOOH), Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 175

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
4.96	2.23575	22.36	288.0	2.459	0.216
5.51	1.02461	10.25	114.2	2.058	-0.186
6.40	3.57513	35.75	556.5	2.745	0.502
7.27	5.98420	59.84	1284.6	3.102	0.859
7.43	6.55311	65.53	1901.2	3.279	1.036
7.68	7.65026	76.50	3255.8	3.513	1.270
8.06	7.16580	71.66	2528.3	3.403	1.180
8.83	9.20337	92.03	11552.9	4.063	1.820
10.15	9.48834	94.88	18544.2	4.268	2.025
10.32	9.68782	96.88	31032.8	4.492	2.249

**NAKAYAMA Figure 4 - Open Triangles = Y-FeOOH**  
 Synthetic Lepidocrocite(gamma FeOOH), Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 36

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
3.70	1.35233	13.52	156.4	2.194	0.638
4.19	1.29534	12.95	148.8	2.173	0.616
5.52	1.39508	13.95	162.1	2.210	0.654
6.40	1.39508	13.95	162.1	2.210	0.654
6.80	1.52132	15.23	179.7	2.255	0.698
7.20	3.04793	30.48	438.4	2.642	1.086
8.71	7.22280	72.23	2600.7	3.415	1.859
9.37	7.84874	78.50	3650.6	3.562	2.006
10.01	8.84715	88.47	7674.2	3.885	2.329
10.66	9.60389	90.04	9039.1	3.956	2.406

**NAKAYAMA Figure 4 - Open Squares =  $\delta$ -Al<sub>2</sub>O<sub>3</sub>**  
 Synthetic alumina(alpha Al2O3), Cs=1 g/L, 6E-6M, No CO2, 0.1 M NaNO3  
 Asp(m2/g)= 2.5

X COORD	Y COORD	Np % sorbed	Kd	log Kd	log Ka (mL/m2)
5.73	0.81088	8.11	88.2	1.946	1.548
7.09	1.15285	11.53	130.3	2.115	1.717
7.09	0.96798	8.68	95.0	1.978	1.580
7.78	0.89637	8.96	98.5	1.993	1.595
8.07	0.98187	9.82	108.9	2.037	1.639
8.87	1.01036	10.10	112.4	2.051	1.653
9.34	1.42358	14.24	166.0	2.220	1.822
9.97	1.43782	14.38	167.9	2.225	1.827
10.55	1.95078	19			

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TY COORD numbers are for (Mn, Pb, Cu, Zn)											
NERO Figure 8a - Small Diamonds = [Pb] <sub>tot</sub> 0.001 µM					NERO Figure 8a - Large Diamonds = [Pb] <sub>tot</sub> 1 µM						
(A)Sulfide washed, Ca=20 µM, 1E-5M, Atm CO2, 0.1 M NaHCO4					(A)Sulfide washed, Ca=20 µM, 1E-5M, Atm CO2, 0.1 M NaHCO4						
Asim(20)	430				Asim(20)	430					
X COORD pH Y COORD	NH <sub>4</sub> % sorbed	Kd	log Kd	log Ka (mM/m2)	X COORD pH Y COORD	NH <sub>4</sub> % sorbed	Kd	log Kd	log Ka (mM/m2)		
4.33	0.29718	2.97	1.5	0.185	-2.448	3.01	0.29718	2.97	1.5	0.185	-2.448
4.61	0.30982	3.09	1.6	0.209	-2.431	3.98	0.83266	6.33	2.4	0.857	-1.916
4.76	0.59984	6.00	3.2	0.504	-2.130	4.21	1.35650	13.57	7.8	0.895	-1.739
5.29	0.64641	6.46	3.5	0.538	-2.095	4.59	1.25173	12.52	7.2	0.855	-1.778
5.27	0.55228	5.52	2.9	0.467	-2.167	5.50	0.80251	6.03	5.0	0.696	-1.938
5.61	0.66969	6.70	3.6	0.555	-2.079	6.38	2.52059	25.21	16.9	1.407	-1.467
6.02	1.03056	10.31	5.7	0.759	-1.874	6.44	2.45075	24.51	16.2	1.210	-1.423
6.24	1.0040	11.00	6.2	0.791	-1.842	6.56	3.96140	36.61	28.9	1.461	-1.173
6.45	1.39142	13.91	8.1	0.907	-1.726	6.80	5.53335	55.33	41.9	1.997	-1.011
6.77	1.71737	17.17	10.4	1.016	-1.618	7.58	4.90698	49.07	48.2	1.683	-0.951
6.81	1.90044	19.04	11.8	1.075	-1.563	7.48	8.73349	87.33	67.2	1.827	-0.866
6.92	2.14808	21.48	13.7	1.136	-1.497	8.82	6.71331	67.11	50.6	2.009	-0.825
7.01	2.45075	24.51	16.2	1.210	-1.423						
7.24	3.1296	31.29	20.4	1.357	-1.277						
7.58	3.71960	37.20	24.8	1.471	-1.162						
7.78	4.49854	45.00	30.9	1.612	-1.022						
7.87	5.24446	52.45	35.1	1.743	-0.892						
7.92	6.02450	60.25	39.8	1.879	-0.754						
8.31	7.27008	72.70	46.2	2.024	-0.509						
8.68	8.71820	87.18	54.9	2.253	-0.360						
8.91	8.51565	85.16	52.8	2.208	-0.376						

Recorded by: Date

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Project No.  
Book No.

NERO Flora 14a - Open Triangles + Sulf 2.3										NERO Flora 14a - Open Circles + Sulf 5										NERO Flora 14a - Open Squares + Sulf 10									
[ANALYSIS INHIBIT: SVAH(2.3) Ca-20 g/L, 1E-5M, ATM CO2 0.1 M NaCO3]										[ANALYSIS INHIBIT: SVAH(5) Ca-20 g/L, 1E-5M, ATM CO2 0.1 M NaCO3]										[ANALYSIS INHIBIT: SVAH(10) Ca-20 g/L, 1E-5M, ATM CO2 0.1 M NaCO3]									
Aspm2(n) 430										Aspm2(n) 430										Aspm2(n) 430									
X COORD	pH	COORD	No % sorbed	Kd	log Kd	log Ka (mM/L)	Kd	log Kd	log Ka (mM/L)	X COORD	pH	COORD	No % sorbed	Kd	log Kd	log Ka (mM/L)	Kd	log Kd	log Ka (mM/L)	X COORD	pH	COORD	No % sorbed	Kd	log Kd	log Ka (mM/L)	Kd	log Kd	log Ka (mM/L)
3.16	0.72211	7.02	3.9	0.500	-2.043	3.55	0.53714	5.32	2.8	0.453	-2.180	4.24	0.75056	7.51	4.1	0.608	-2.025												
3.89	1.00588	10.07	5.8	0.748	-1.856	4.80	0.90708	9.07	5.0	0.698	-1.936	4.84	0.87892	8.29	4.8	0.683	-1.961												
4.93	1.3233	12.03	7.5	1.020	-1.740	5.56	1.00348	18.03	11.0	1.041	-1.592	5.11	0.89295	8.93	4.9	0.690	-1.943												
5.27	2.27302	22.73	14.7	1.188	-1.468	5.96	2.27303	28.28	19.7	1.265	-1.339	5.40	1.14896	11.49	6.5	0.812	-1.821												
5.79	3.95199	39.52	32.7	1.514	-1.119	6.28	3.31170	33.12	24.8	1.384	-1.240	5.91	1.43354	14.34	8.4	0.923	-1.711												
5.86	3.69617	34.91	28.9	1.204	-1.204	6.28	4.98227	45.92	42.1	1.629	-1.056	6.05	1.80348	18.03	11.0	1.041	-1.592												
5.96	3.92353	39.24	32.3	1.509	-1.124	7.43	5.23256	52.32	54.9	1.739	-0.804	7.17	4.19387	41.84	36.1	1.558	-1.076												
6.59	4.67884	46.77	47.6	1.678	-0.956	7.56	5.67364	56.74	55.6	1.817	-0.817	7.50	4.36492	43.65	38.7	1.588	-1.045												
7.24	5.47444	54.74	60.2	1.852	-0.744	7.87	6.15431	61.57	60.1	1.904	-0.730	8.17	4.87844	48.78	42.1	1.629	-1.056												
7.63	5.81553	58.18	72.4	1.860	-0.774	8.67	7.89320	78.93	78.3	2.273	-0.361	7.66	5.36061	53.61	57.8	1.762	-0.872												
7.46	6.74078	67.41	102.4	2.015	-0.619	8.87	8.16364	81.64	222.3	2.347	-0.287	8.04	5.90130	59.01	72.0	1.867	-0.776												
7.94	7.46644	74.66	147.4	2.188	-0.465	8.87	8.16364	81.64	222.3	2.347	-0.287	8.47	6.54518	65.42	84.8	1.976	-0.658												
8.17	8.43398	84.34	269.3	2.430	-0.203							8.62	7.03958	70.40	118.9	2.075	-0.558												
8.71	8.47667	84.77	278.2	2.444	-0.189																								
8.95	8.57627	85.76	301.2	2.478	-0.158																								



("Y\_COORD" numbers are for digitizing grid)

**WILK Figure 1, [Np] = 10<sup>-4</sup>M - Open Squares = Manganite**  
 Manganite (MnOOH); Cs=2.5 mg/mL; 1E-4M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
4.11	1.75163	17.52	84.9	1.929
4.95	2.33843	23.38	122.1	2.087
5.66	3.07192	30.72	177.4	2.249
6.60	5.46102	54.61	481.3	2.682
7.73	6.86514	68.65	876.0	2.942
7.84	6.48792	64.88	738.9	2.869
9.66	5.02093	50.21	403.4	2.606
10.17	4.72753	47.28	358.7	2.555

**WILK Figure 1, [Np] = 10<sup>-4</sup>M - Open Circles = Hausmanite**  
 Hausmannite (Mn<sub>3</sub>O<sub>4</sub>); Cs=3.35 mg/mL; 1E-4M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
4.05	1.81450	18.15	67.2	1.827
5.03	2.48513	24.85	100.2	2.001
6.04	3.17671	31.77	141.1	2.149
7.02	3.26054	32.61	146.6	2.166
8.03	2.17077	21.71	84.0	1.924
9.08	8.56266	85.63	1805.2	3.257
10.06	6.57174	65.72	580.9	2.764

**WILK Figure 1, [Np] = 10<sup>-5</sup>M - Open Squares = Manganite**  
 Manganite (MnOOH); Cs=2.5 mg/mL; 1E-5M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
4.05	-0.59555	-5.96	-22.5	#NUM!
4.88	2.14982	21.50	109.5	2.040
5.60	4.64370	46.44	346.8	2.540
6.56	6.04782	60.48	612.1	2.787
7.65	5.02093	50.21	403.4	2.606
8.99	7.89204	78.92	1497.6	3.175
10.08	5.56581	55.66	502.1	2.701

**WILK Figure 1, [Np] = 10<sup>-5</sup>M - Open Circles = Hausmanite**  
 Hausmannite (Mn<sub>3</sub>O<sub>4</sub>); Cs=3.35 mg/mL; 1E-5M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
5.87	3.07192	30.72	134.4	2.128
6.27	2.12886	21.29	82.0	1.914
6.33	3.21862	32.19	143.8	2.158
6.46	2.10790	21.08	80.9	1.908
7.44	5.08380	50.84	313.4	2.496
7.96	7.22141	72.21	787.6	2.896
8.80	7.82917	78.29	1092.9	3.039
10.42	6.63462	66.35	597.4	2.776

**WILK Figure 1, [Np] = 10<sup>-6</sup>M - Open Squares = Manganite**  
 Manganite (MnOOH); Cs=2.5 mg/mL; 1E-6M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
4.42	-0.80512	-8.05	-29.8	#NUM!
5.43	3.76351	37.64	241.4	2.383
5.87	2.75757	27.58	152.3	2.183
6.02	1.77259	17.73	86.2	1.935
6.04	2.65278	26.53	144.4	2.160
7.99	5.67059	56.71	523.9	2.719
8.93	7.82917	78.29	1442.6	3.159
10.35	6.02686	60.27	606.8	2.783

**WILK Figure 1, [Np] = 10<sup>-6</sup>M - Open Circles = Hausmanite**  
 Hausmannite (Mn<sub>3</sub>O<sub>4</sub>); Cs=3.35 mg/mL; 1E-6M; Atm CO<sub>2</sub>; 0.1 M NaClO<sub>4</sub>

X_COORD pH	Y_COORD	Np % sorbed	Kd	log Kd
5.85	2.29651	22.97	90.3	1.956
6.37	2.88331	28.83	122.8	2.089
6.67	4.22456	42.25	221.7	2.346
6.73	3.80542	38.05	186.2	2.270
6.85	1.60493	16.05	57.9	1.763
8.22	5.92208	59.22	440.1	2.644
8.84	7.47290	74.73	896.1	2.952
10.27	8.16448	81.64	1347.9	3.130

Neptunium data pts - WILK (2005)

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*Handwritten date: 9/12/2004*

12/2009

ZUYI Figure 1 - Circles = $C_s = 0.1 \text{ mol l}^{-1}$				ZUYI Figure 1 - Squares = $C_s = 0.01 \text{ mol l}^{-1}$				ZUYI Figure 1 - Triangles = $C_s = 0.001 \text{ mol l}^{-1}$			
AI2O3: Ca=1 g/100 mL; Np(tot)=1E-5M; CO2: 0.1 M NaNO3				AI2O3: Ca=1 g/100 mL; Np(tot)=1E-5M; CO2: 0.01 M NaNO3				AI2O3: Ca=1 g/100 mL; Np(tot)=1E-5M; CO2: 0.001 M NaNO3			
Adsorption %				Adsorption %				Adsorption %			
X_COORD	pH	Y_COORD	log Kd	X_COORD	pH	Y_COORD	log Kd	X_COORD	pH	Y_COORD	log Kd
3.54	2.1244	2.12	2.2	2.85	0.18394	1.84	1.9	4.12	0.06995	0.70	0.7
4.45	1.79404	17.94	2.19	4.38	0.71114	7.11	7.7	6.37	1.13860	11.39	12.8
5.94	4.2057	42.31	73.3	5.83	2.70596	27.06	37.1	6.87	6.43912	64.39	180.8
6.84	8.04922	80.49	412.6	6.80	6.05440	60.54	153.4	7.01	7.92098	79.21	381.0
7.41	9.43135	94.31	1658.6	7.24	8.13472	81.35	436.1	7.07	8.06347	80.63	418.4
7.64	9.54534	95.45	2099.4	7.40	8.84715	88.47	767.4	7.26	9.01813	90.18	918.5
8.00	9.63083	96.31	2608.8	7.50	9.06088	90.61	964.8	7.34	9.34585	93.46	1428.7
				7.57	9.64508	96.45	2717.5	7.54	9.56959	95.60	2170.6
								10.35	9.94430	99.44	17853.3

Neptunium data pts - ZUYI

(“Y\_COORD” numbers are for digitizing grid)

**ZAVARIN Figure 10 - Open Circles = at 24 Hours**

Calcite; Cs=50 mg/40 mL; 1E-7M; .03% CO2; 0.1 M NaClO4

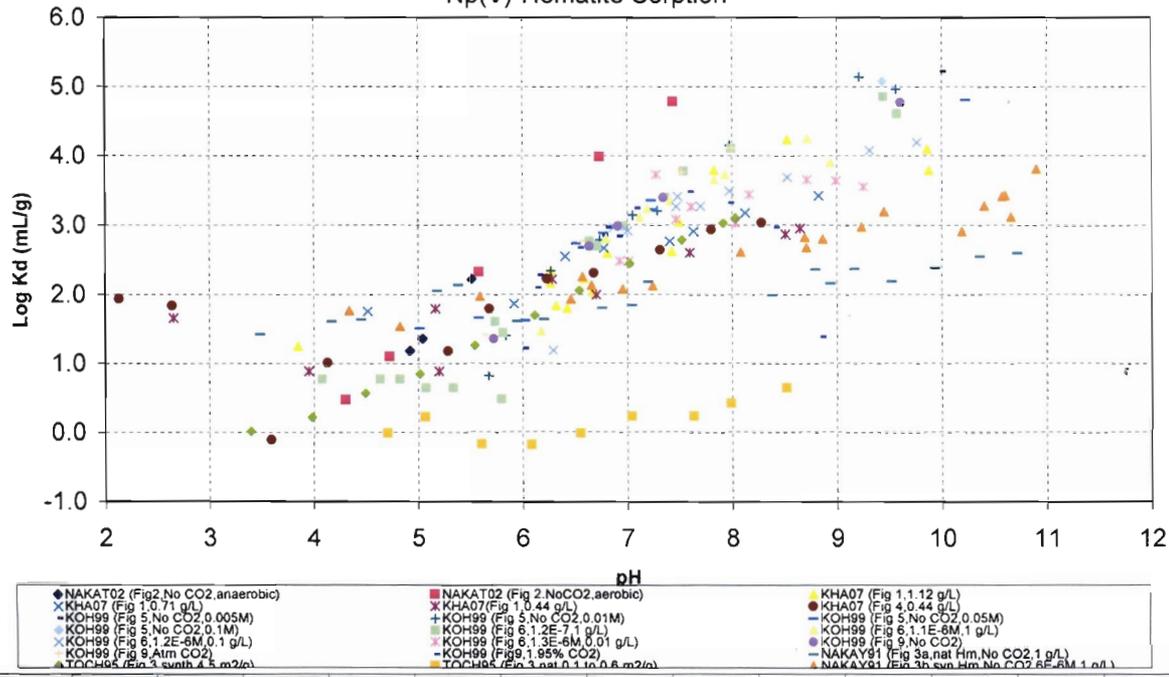
X_COORD	pH	Y_COORD	Np % sorbed	Kd	log Kd
7.11		1.54162	15.42	145.8	2.164
7.22		1.31824	13.18	121.5	2.084
7.61		1.54162	15.42	145.8	2.164
7.88		1.98839	19.88	198.6	2.298
8.16		2.11870	21.19	215.1	2.333
8.50		2.21177	22.12	227.2	2.356
8.82		1.39270	13.93	129.4	2.112
9.17		1.53231	15.32	144.8	2.161
9.33		1.02040	10.20	90.9	1.959
9.62		0.00586	0.06	0.5	-0.329

Neptunium data pts - ZAVARIN (2005)

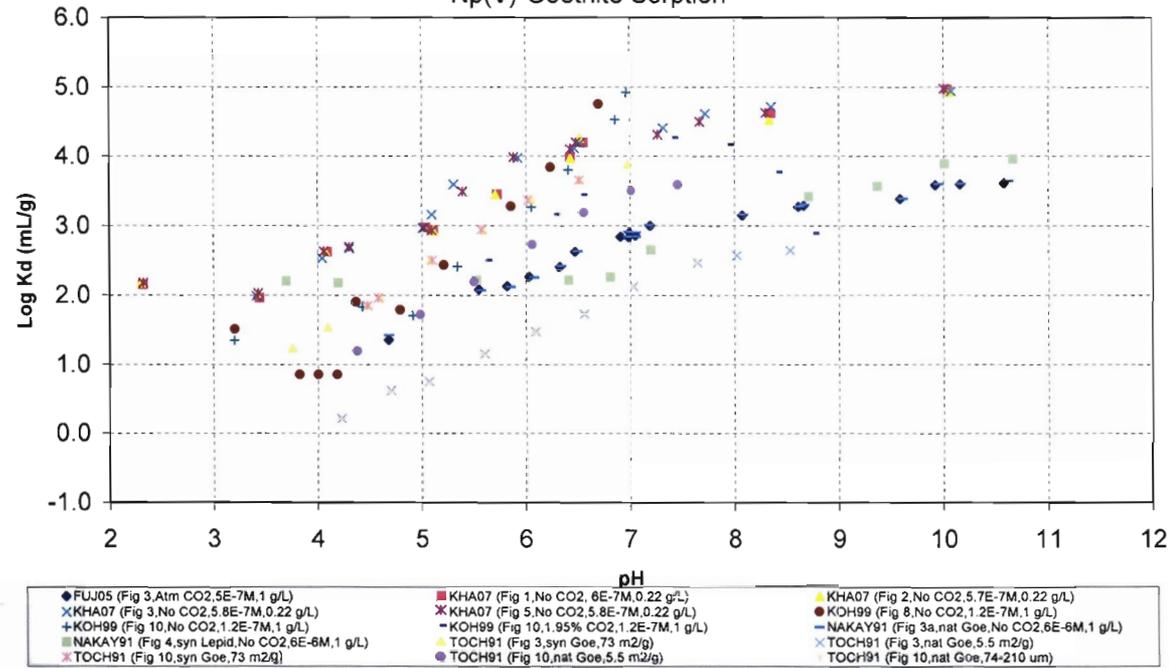
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### Np(V)-Hematite Sorption



### Np(V)-Goethite Sorption



	Hm	Goe	HFO	Mt	SiO2	Al-oxide	Al-Silicate	Cc
FUJ95		X		X				
GIR91			X					
HEB08								X
JER07		X						
KHA07	X	X						
KOH99	X	X			X			
NAG98			X					
NAKAT02	X			X				
NAKAY91	X	X		X		X	X(bt)	
DELNER04							X	
TOCH95	X	X	X	X				
WILK05								
ZAV05					X	X		X
ZUY104								

TITLE

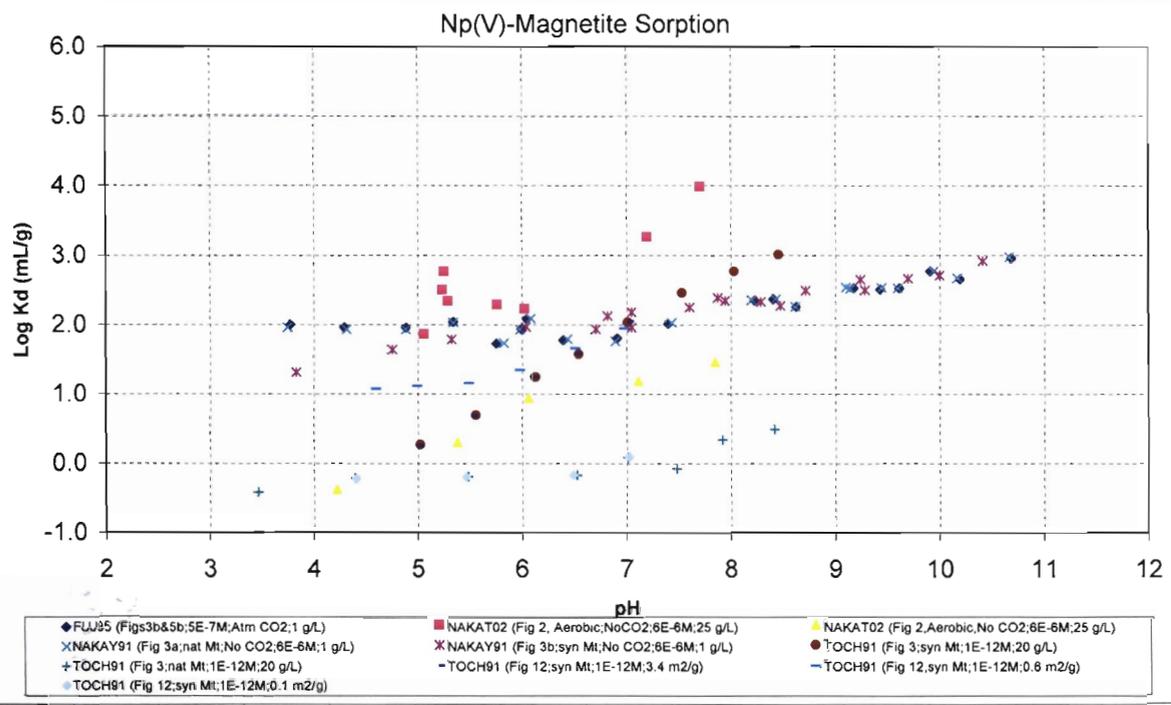
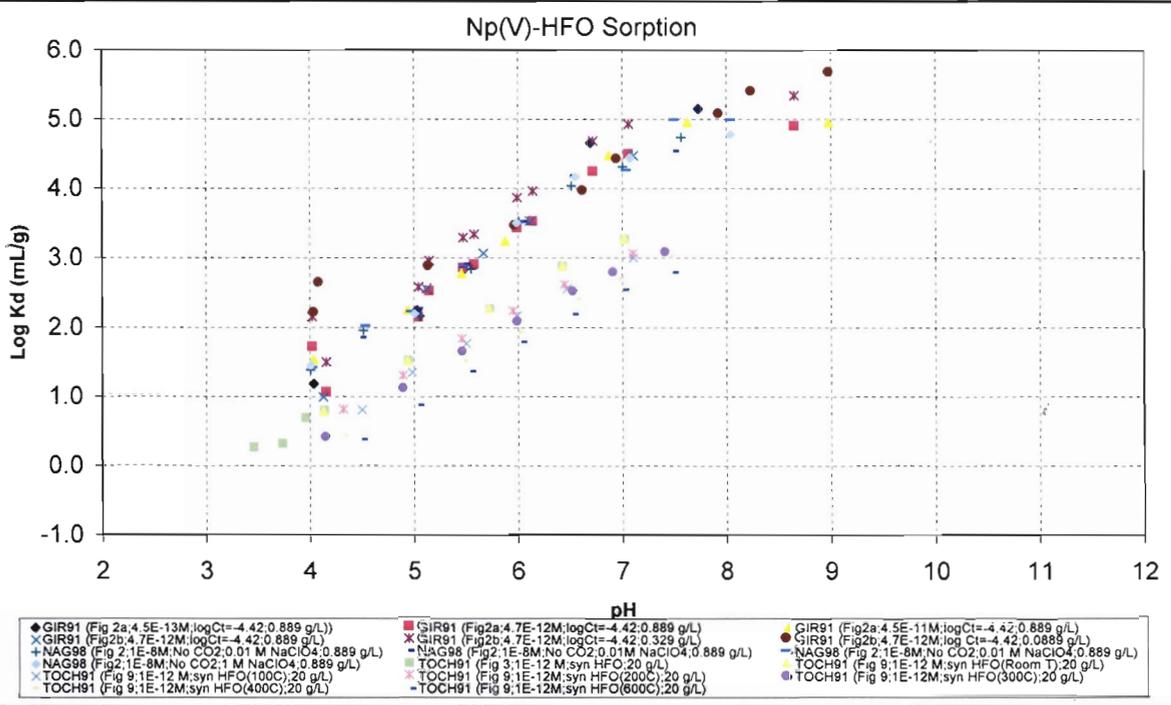
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Book No. \_\_\_\_\_

8/12/2009



Neptunium data pts - Graphs - Log Kd

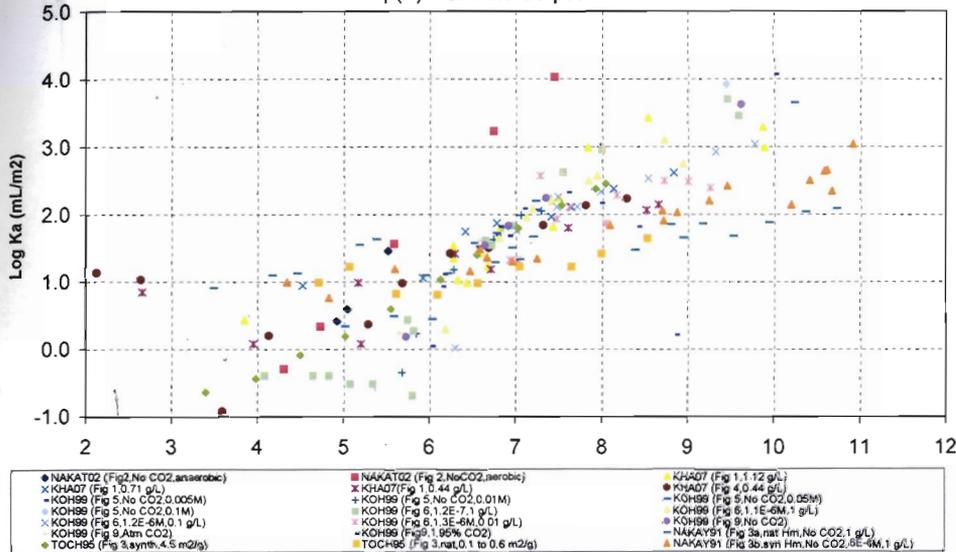
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TITLE \_\_\_\_\_

Book No. \_\_\_\_\_

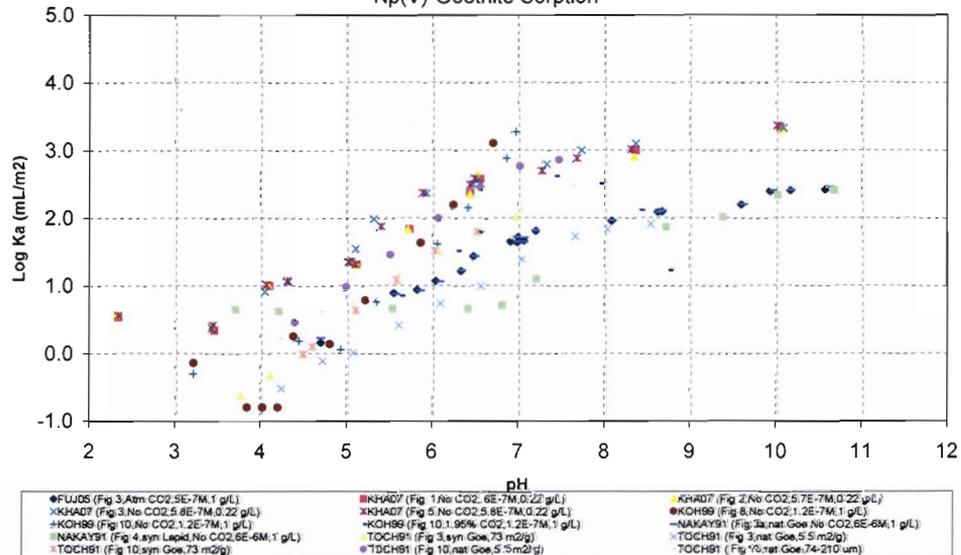
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Np(V)-Hematite Sorption



	Hm	Goe	HFO	Mt	SiO <sub>2</sub>	Al-oxide	Al-Silicate	Cc
FUJ95		X		X				
SIR91			X					
HEB08								X
JER07		X						
KHA07	X	X						
KOH99	X	X			X			
NAG98			X					
NAKAT02	X			X				
NAKAY91	X	X		X		X	X (b)	
DELNER04							X	
TOCH95	X	X	X	X				
WILK05								
ZAV05					X	X		
ZUY104								

Np(V)-Goethite Sorption



Neptunium data pts - Graphs - Log Ka

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Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)				Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)				Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)				Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)				Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)				Keeney Figure 4a ( <sup>137</sup> Pu 10 <sup>-10</sup> M)									
Closed Circles = Aragonite (deionized water)				Open Circles = Aragonite (S=35 seawater)				Closed Squares = Calcite (deionized water)				Open Squares = Calcite (S=35 seawater)				Closed Triangles = Goethite (deionized water)				Open Triangles = Goethite (S=35 seawater)									
1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L				1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L				1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L				1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L				1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L				1E-10 M. Atm CO <sub>2</sub> : pH=7.8 to 8.2, 5 m2/L									
X COORD	Y COORD	% Adsorption	Log Time (min)	Ka (mL/m)	log Ka (mL/m2)	X COORD	Y COORD	% Adsorption	Log Time (min)	Ka (mL/m)	log Ka (mL/m2)	X COORD	Y COORD	% Adsorption	Log Time (min)	Ka (mL/m)	log Ka (mL/m2)	X COORD	Y COORD	% Adsorption	Log Time (min)	Ka (mL/m)	log Ka (mL/m2)	X COORD	Y COORD	% Adsorption	Log Time (min)	Ka (mL/m)	log Ka (mL/m2)
0.71	0.60914	96.89	5444.0	3.77	0.74	5.81488	56.15	156.1	2.41	0.70	7.38782	73.88	505.9	2.75	0.75	3.18973	31.89	92.8	1.97	0.70	8.88200	88.82	1784.0	3.25	0.73	2.23421	22.34	57.5	1.75
1.52	0.71037	97.10	6705.4	3.83	1.48	6.88307	68.83	443.7	2.65	1.52	7.45853	74.57	586.3	2.77	1.81	4.87786	48.77	190.1	2.28	1.47	8.83498	88.34	11852.0	4.07	1.50	4.88908	48.89	197.6	2.30
2.10	0.77909	97.29	8853.5	3.95	2.12	8.29485	82.95	972.9	2.90	2.09	7.91006	79.10	757.0	2.88	2.10	8.35709	83.57	348.0	2.54	2.57	9.97148	99.71	99950.0	4.64	2.12	8.30568	83.06	382.4	2.86
2.58	0.86154	98.02	14244.6	4.15	2.58	8.11440	81.14	2222.5	3.35	2.81	8.19995	81.99	810.3	2.96	3.10	8.21238	82.12	818.8	2.98	2.84	9.98887	99.98	1041547.0	6.29	2.84	9.50423	95.04	3834.1	3.58
2.94	0.83408	98.34	11852.5	4.07	3.08	9.49049	94.90	3795.3	3.57	2.91	8.37231	83.72	1032.5	3.03	3.10	8.21238	82.12	818.8	2.98	3.27	9.99897	99.99	1041547.0	6.29	3.08	9.81417	98.14	4983.0	3.70
3.27	0.86154	98.02	14244.6	4.15	3.23	9.50423	95.04	3834.1	3.58	3.28	8.48725	84.87	1122.1	3.05	3.52	8.22813	82.28	827.6	2.97	3.52	9.98522	99.85	135209.0	5.13	3.52	9.87284	98.72	4483.2	3.95
3.53	0.84903	98.89	17822.9	4.25	3.42	8.51787	85.18	3949.1	3.60	3.52	8.54222	85.42	1171.9	3.07	3.58	8.28736	82.87	954.3	2.88	3.88	9.98522	99.85	135209.0	5.13	3.88	9.71037	97.10	6705.4	3.83
3.68	0.90277	99.03	20389.8	4.31	3.63	9.56669	95.67	4639.0	3.67	3.88	8.44802	84.48	1087.0	3.04	3.85	8.21238	82.12	818.8	2.98	4.20	9.98522	99.78	15837.2	4.20	4.20	9.71037	97.10	6705.4	3.83

Plutonium\_data\_pu - KEENEY

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Banchez Fluera 1a - Pu (IV) 10 <sup>11</sup> on Goethite										Banchez Fluera 1a - Pu (IV) 10 <sup>11</sup> on Goethite										Banchez Fluera 1a - Pu (IV) 10 <sup>11</sup> on Goethite										Banchez Fluera 1a - Pu (IV) 10 <sup>11</sup> on Goethite									
Open Circles = 1 Hr (10 <sup>11</sup> M Pu)										Open Circles = 24 Hrs (10 <sup>11</sup> M Pu)										Open Sources = 96 Hrs (10 <sup>11</sup> M Pu)										Closed Circles = 24 Hrs (10 <sup>11</sup> M Pu)									
soeithe 1E-11M Pu(VI) Alm CO2 28.5 m2/L										soeithe 1E-11M Pu(VI) Alm CO2 28.5 m2/L										soeithe 1E-11M Pu(VI) Alm CO2 28.5 m2/L										soeithe 1E-10M Pu(VI) Alm CO2 28.5 m2/L									
X COORD	Y COORD	% Pu (VI) Ads/Kd	Kd	log Kd (mL/mg)	log Ka (mL/mg)	X COORD	Y COORD	% Pu (VI) Ads/Kd	Kd	log Kd (mL/mg)	log Ka (mL/mg)	X COORD	Y COORD	% Pu (VI) Ads/Kd	Kd	log Kd (mL/mg)	log Ka (mL/mg)	X COORD	Y COORD	% Pu (VI) Ads/Kd	Kd	log Kd (mL/mg)	log Ka (mL/mg)																
2.20	2.63276	29.33	330.9	2.97	1.10	2.46	2.50907	25.09	872.5	2.94	1.07	2.29	2.98930	20.89	879.7	2.83	0.99	2.29	0.91489	9.15	762.3	2.42	0.95																
2.86	3.73219	37.10	1551.1	3.19	1.32	2.84	3.42985	34.30	1359.8	3.13	1.26	2.43	2.84885	28.49	1089.4	3.04	1.17	2.99	2.55030	25.50	891.7	2.95	1.08																
3.42	4.99005	49.89	2672.8	3.41	1.54	2.97	4.61554	45.18	2144.7	3.34	1.46	3.05	3.92459	39.25	1882.7	3.23	1.36	3.08	3.30616	33.06	1286.6	3.11	1.24																
3.90	5.34012	53.40	2985.1	3.47	1.60	3.21	4.44563	44.47	2085.9	3.32	1.45	3.23	7.25039	72.50	8889.7	3.84	1.97	3.75	5.20289	52.03	2625.0	3.61	1.58																
4.04	7.89630	78.96	9771.4	3.99	2.12	4.08	7.99502	79.95	10195.6	4.01	2.14	4.04	9.86154	98.62	18529.2	5.27	3.40	3.72	5.46380	54.64	3137.5	3.90	1.63																
4.84	9.35306	93.53	37859.5	4.58	2.71	6.22	9.49049	94.90	48620.0	4.69	2.82	6.93	9.87529	98.75	20628.7	5.31	3.44	4.15	6.10972	61.10	4091.0	3.85	1.74																
4.84	9.73789	97.38	96764.3	4.99	3.12	8.18	9.88903	98.89	232130.8	5.37	3.50	7.56	9.80657	98.07	132062.1	5.12	3.25	4.20	6.30212	63.02	4439.3	3.85	1.78																
5.01	9.71037	97.10	87332.7	4.94	3.07	8.95	9.89903	98.99	232130.8	5.37	3.50							5.11	9.09184	90.92	26081.2	4.42	2.55																
8.55	9.77909	97.79	115310.2	5.06	3.19													6.02	9.64166	96.42	20087.6	2.85	2.98																
8.55	9.77909	97.79	115310.2	5.06	3.19																																		
8.73	9.82032	98.20	142361.4	5.15	3.28																																		
9.50	9.80657	98.07	132062.1	5.12	3.25																																		

BET (m<sup>2</sup>/g) measurements for soeithe using methods of Altonson et al. (1967)

78. Wina and Schiffrin (1955) J. 20011

46. Labouard and Ehrhard (1964) after modification of Altonson et al. (1967) methodology by van Goin et al. (1964)

82. Labouard and Ehrhard (1964) after modification of Altonson et al. (1967) methodology by Goin et al. (1964)

79. J. Apest et al. (1964) J. 20011

47.5. Denis and Strain (1964)

87.87. (1964) J. 20011

84.5. Denis et al. (1964) after modification of Altonson et al. (1967) methodology by Wina et al. (1964)

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**Shaughnessy Figure 3a - Manganite**

Down Triangle = Pu(VI) =  $1 \cdot 10^{-7} M$  Asp=9.5 m2/g  
MnOOH;1E-7M Pu(VI);Atm CO2;10 g/L

X_COORD pH	Y_COORD	% Pu Sorbed in 24 Hours	Kd	log Kd (m)	log Ka (mL/m2)
3.15	4.16259	41.63	71.3	1.85	0.88
3.99	3.81976	38.20	61.8	1.79	0.81
5.19	5.58066	55.81	126.3	2.10	1.12
6.14	7.51297	75.13	302.1	2.48	1.50
6.95	9.61669	96.17	2508.9	3.40	2.42
8.01	9.94394	99.44	17738.0	4.25	3.27
8.95	9.97510	99.75	40060.6	4.60	3.62
10.43	9.64786	96.48	2739.8	3.44	2.46

**Shaughnessy Figure 3a - Manganite**

Closed Square = Pu(VI) =  $5 \cdot 10^{-6} M$   
MnOOH;5E-6M Pu(VI);Atm CO2;10 g/L

X_COORD pH	Y_COORD	% Pu Sorbed in 24 Hours	Kd	log Kd (m)	log Ka (mL/m2)
3.79	1.91862	19.19	23.7	1.38	0.40
5.04	3.07177	30.72	44.3	1.65	0.67
6.36	5.39366	53.94	117.1	2.07	1.09
7.06	6.26631	62.66	167.8	2.22	1.25
7.97	9.61669	96.17	2508.9	3.40	2.42
8.82	9.95952	99.80	24603.6	4.39	3.41
9.98	8.18304	81.83	450.4	2.65	1.68

**Shaughnessy Figure 3a - Manganite**

Closed Circle = Pu(VI) =  $8 \cdot 10^{-2} M$   
MnOOH;8E-5M Pu(VI);Atm CO2;10 g/L

X_COORD pH	Y_COORD	% Pu Sorbed in 24 Hours	Kd	log Kd (m)	log Ka (mL/m2)	#NUM!	#NUM!
3.00	-0.06044	-0.60	-0.6				
4.90	0.50055	5.01	5.3	0.72	-0.26		
5.01	0.74988	7.50	8.1	0.91	-0.07		
5.83	1.23296	12.33	14.1	1.15	0.17		
7.02	3.00944	30.09	43.1	1.63	0.66		
8.03	8.16746	81.67	445.7	2.65	1.67		
8.25	9.61669	96.17	2508.9	3.40	2.42		
8.82	9.86802	98.66	7363.8	3.87	2.89		
9.00	9.61669	96.17	2508.9	3.40	2.42		
9.70	6.59356	65.94	193.6	2.29	1.31		
10.01	4.44309	44.43	80.0	1.90	0.93		

**Shaughnessy Figure 3b - Hausmannite**

Closed Square = Pu(VI) =  $8 \cdot 10^{-5} M$  Asp=20.4 m2/g  
Mn3O4;8E-5M Pu(VI);Atm CO2;4 g/L

X_COORD pH	Y_COORD	% Pu Sorbed in 24 Hours	Kd	log Kd (m)	log Ka (mL/m2)
3.23	8.21421	82.14	1149.9	3.06	1.75
4.04	7.12339	71.23	619.1	2.79	1.48
5.11	8.30771	83.08	1227.3	3.09	1.78
5.88	8.04279	80.43	1027.3	3.01	1.70
6.91	9.64786	96.48	6849.4	3.84	2.53
8.18	9.91277	99.13	28409.9	4.45	3.14
8.85	9.94394	99.44	44345.1	4.65	3.34
9.81	6.28190	62.82	422.4	2.63	1.32

**Shaughnessy Figure 3b - Hausmannite**

Closed Circle = Pu(VI) =  $1 \cdot 10^{-4} M$   
Mn3O4;8E-5M Pu(VI);Atm CO2;4 g/L

X_COORD pH	Y_COORD	% Pu Sorbed in 24 Hours	Kd	log Kd (m)	log Ka (mL/m2)
3.14	6.03257	60.33	380.1	2.58	1.27
4.01	5.93907	59.39	365.6	2.56	1.25
5.07	5.42483	54.25	296.4	2.47	1.16
6.03	5.90790	59.08	360.9	2.56	1.25
6.91	6.43773	64.38	451.8	2.65	1.35
8.06	9.72577	97.26	8866.4	3.95	2.64
8.87	8.27654	82.77	1200.6	3.08	1.77
9.82	6.26631	62.66	419.6	2.62	1.31

**Shaughnessy Figure 4 - Pu(VI) =  $8 \cdot 10^{-6} M$**

Closed Circle = 10 mg Mn2O4  
Mn3O4;8E-5M Pu(VI);Atm CO2;4 g/L

X_COORD pH	Y_COORD	% Pu(VI) Sorbed in 24 Hrs (mg/m <sup>2</sup> )
3.17	20.07289	0.20
4.01	17.42981	0.17
5.10	20.34017	0.20
5.88	19.62743	0.20
6.89	23.54752	0.24
8.16	24.17117	0.24
8.91	24.23056	0.24
9.86	15.38067	0.15

**Shaughnessy Figure 4 - Pu(VI) =  $8 \cdot 10^{-6} M$**

Closed Triangle = 25 mg MnOOH  
MnOOH;8E-5M Pu(VI);Atm CO2;10 g/L

X_COORD pH	Y_COORD	% Pu Adsorbed in 24 Hrs (mg/m <sup>2</sup> )
3.00	-0.03240	0.00
4.87	1.00702	0.01
4.99	1.60097	0.02
5.82	2.61069	0.03
7.00	6.38229	0.06
8.01	17.07343	0.17
8.22	20.10259	0.20
8.85	20.60745	0.21
9.02	20.10259	0.20
9.71	13.74730	0.14
10.00	9.26296	0.09

Plutonium\_data\_pts - SHAUGHNESSY

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Date

8/12/2009  
DPA





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**Comparing DOE SCM modeling results to experimental data from the open literature**

As described in the Safety Analysis Report and the supporting AMRs, DOE used a surface complexation model (SCM) within the USGS geochemistry code PHREEQCi to simulate sorption of Am, Np, Pu, U, and Th on stationary Fe corrosion products. Nickel was included in the SCM to represent competition for sorption sites, but the sorbed mass of nickel was not explicitly tracked for transport purposes.

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The SCM is not directly incorporated in the TSPA model abstraction, but the sorption coefficients (Kd) developed from the SCM are directly applicable to the transport of uranium, neptunium, and thorium, which are assumed to undergo rapid and reversible sorption. To represent parameter uncertainty in the SCM, the applicant conducted about 5,000 PHREEQC simulations, each with a unique combination of surface properties and aqueous chemistry parameters as inputs. The following graphs show comparison of the DOE SCM results to SCM sorption results to experimental data reported in the peer-reviewed scientific literature. The comparison was made for Np and Pu, the two principal drivers of dose to the RMEI.

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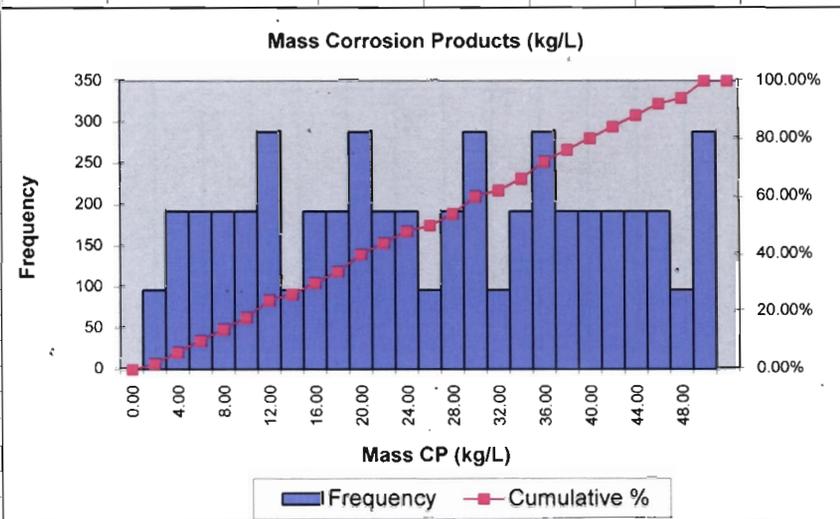
Recorded by:

Date

Verified by:

Date

soln	CP Mass (kg/L)				
1	17.511		<b>Mass Corrosion Products (kg/L)</b>		
2	17.511				
3	17.511		Mean	25.541	
4	17.511		Standard Error	0.204	
5	17.511		Median	25.785	
6	17.511		Mode	17.511	
7	17.511		Standard Deviation	14.113	
8	17.511		Sample Variance	199.165	
9	17.511		Kurtosis	-1.183	
10	17.511		Skewness	0.003	
11	17.511		Range	48.099	
12	17.511		Minimum	1.484	
13	17.511		Maximum	49.583	
14	17.511		Sum	122596.906	
15	17.511		Count	4800	
16	17.511		Confidence Level(95.0%)	0.39934063	
17	17.511				
18	17.511		<b>Bin</b>	<b>Frequency</b>	<b>Cumulative %</b>
19	17.511	0.00	0.00	0	0.00%
20	17.511	2.00	2.00	96	2.00%
21	17.511	4.00	4.00	192	6.00%
22	17.511	6.00	6.00	192	10.00%
23	17.511	8.00	8.00	192	14.00%
24	17.511	10.00	10.00	192	18.00%
25	17.511	12.00	12.00	288	24.00%
26	17.511	14.00	14.00	96	26.00%
27	17.511	16.00	16.00	192	30.00%
28	17.511	18.00	18.00	192	34.00%
29	17.511	20.00	20.00	288	40.00%
30	17.511	22.00	22.00	192	44.00%
31	17.511	24.00	24.00	192	48.00%
32	17.511	26.00	26.00	96	50.00%
33	17.511	28.00	28.00	192	54.00%
35	17.511	30.00	30.00	288	60.00%
36	17.511	32.00	32.00	96	62.00%
37	17.511	34.00	34.00	192	66.00%
38	17.511	36.00	36.00	288	72.00%
39	17.511	38.00	38.00	192	76.00%
40	17.511	40.00	40.00	192	80.00%
41	17.511	42.00	42.00	192	84.00%
42	17.511	44.00	44.00	192	88.00%
43	17.511	46.00	46.00	192	92.00%
44	17.511	48.00	48.00	96	94.00%
45	17.511	50.00	50.00	288	100.00%



DOE  
 Mass of Corrosion Products  
 (sampled distribution,  
 DOE reports using a  
 uniform distribution from  
 1 to 50 kg/L

*[Handwritten signature]*

Date

*[Handwritten initials]*

2/16/2010  
 [Signature]

pH values calculated by  
 DOE using PHREEQC

PO<sub>2</sub> sampled as PHREEQC  
 input parameters. DOE  
 reports sampling by PO<sub>2</sub>  
 from a uniform distribution.

$$-4.0 < \log P_{O_2} < -2.0$$

EBS Transport ARMIC  
 Section 6.5.2.4.1  
 ANL-WIS-PA-000001 Rev.03

[Signature]

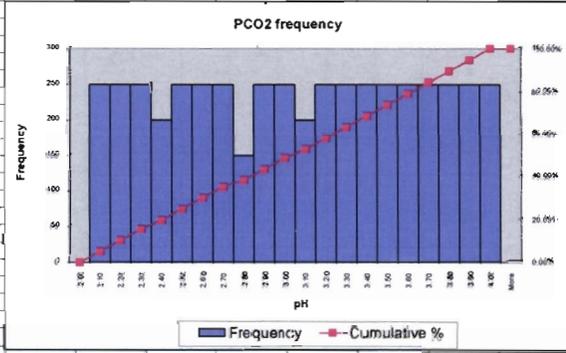
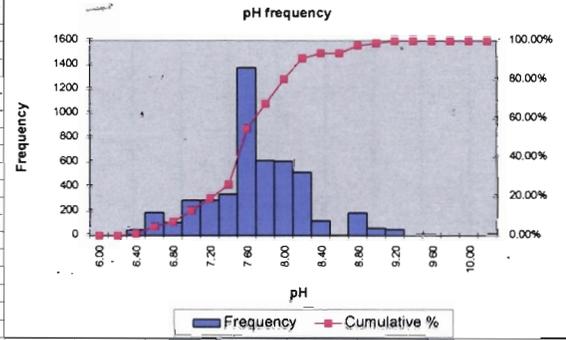
soln	pH	pCO2	pH stats		PCO2 stats	
1	7.29	2.80				
2	7.56	2.65				
3	7.14	3.31				
4	7.45	2.79				
5	6.51	2.43				
6	7.63	2.52				
7	7.42	2.46				
8	8.13	3.24				
9	7.58	2.38				
10	8.00	3.24				
11	7.60	2.92				
12	6.97	2.42				
13	8.00	3.67				
14	6.76	2.40				
15	7.44	2.95				
16	7.44	3.49				
17	7.43	3.87				
18	8.83	3.41				
19	7.06	2.10				
20	7.75	3.80				
21	8.06	3.66				
22	7.83	3.71				
23	8.00	2.86				
24	7.44	3.26				
25	8.77	3.50				
26	8.80	3.96				
27	7.52	2.49				
28	7.68	2.14				
29	6.97	3.26				
30	7.47	2.29				
31	7.06	2.83				
32	8.04	3.38				
33	7.97	3.96				
35	7.01	2.58				
36	7.72	3.07				
37	7.45	2.88				
38	7.29	3.12				
39	8.63	3.40				
40	8.06	3.43				
41	6.57	2.36				
42	8.14	3.97				
43	8.32	3.14				
44	7.88	2.01				
45	7.35	2.99				
46	7.49	2.19				
47	7.46	3.20				
48	7.55	3.65				
49	6.61	2.23				
50	7.50	3.52				
51	7.52	2.48				

pH stats			PCO2 stats		
Mean	7.601		Mean	3.013	
Standard Error	0.006		Standard Error	0.008	
Median	7.582		Median	3.041	
Mode	7.632		Mode	2.801	
Standard Deviation	0.529		Standard Deviation	0.584	
Sample Variance	0.279		Sample Variance	0.341	
Kurtosis	0.584		Kurtosis	-1.223	
Skewness	0.190		Skewness	-0.046	
Range	2.911		Range	1.970	
Minimum	6.249		Minimum	2.010	
Maximum	9.160		Maximum	3.981	
Sum	36482.587		Sum	14462.710	
Count	4800.000		Count	4800.000	
Confidence Level(95.0%)	0.015		Confidence Level(95.0%)	0.017	

pH frequency			PCO2 stats		
Bin	Frequency	Cumulative %	Bin	Frequency	Cumulative %
6.00	0	0.00%	2.00	0	0.00%
6.20	0	0.00%	2.10	250	5.21%
6.40	46	1.00%	2.20	250	10.42%
6.60	189	4.94%	2.30	250	15.63%
6.80	108	7.19%	2.40	200	19.79%
7.00	290	13.23%	2.50	250	25.00%
7.20	286	19.25%	2.60	250	30.21%
7.40	340	26.33%	2.70	250	35.42%
7.60	1378	55.04%	2.80	280	38.54%
7.80	612	67.79%	2.90	260	43.75%
8.00	608	80.46%	3.00	250	48.96%
8.20	517	91.23%	3.10	200	53.13%
8.40	121	83.75%	3.20	250	58.33%
8.60	2	93.79%	3.30	250	63.54%
8.80	187	97.69%	3.40	250	68.75%
9.00	61	98.96%	3.50	250	73.96%
9.20	50	100.00%	3.60	250	79.17%
9.40	0	100.00%	3.70	250	84.38%
9.60	0	100.00%	3.80	250	89.58%
9.80	0	100.00%	3.90	250	94.79%
10.00	0	100.00%	4.00	250	100.00%
More	0	100.00%	More	0	100.00%

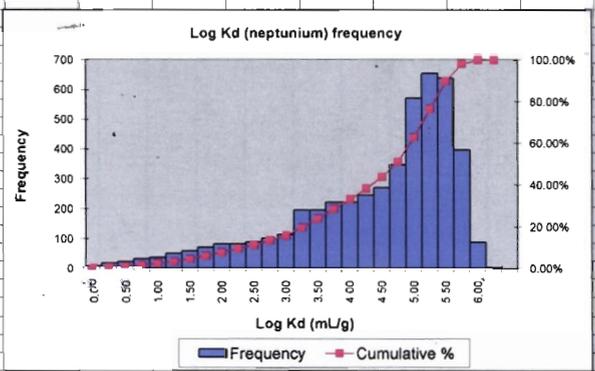


CNWRA\_pH\_PCO2\_stats

2/16/10  
BWS

Summary Statistics  
for Kd (log) values  
calculated by DDE  
using SCW in PHREEQC

4,800 calculations based  
on sampling input parameters



0.56 < Kd < 1,030,386  
10^-0.250 10^6.03

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soln	pH	pCO2	CP [Sp. Sur]	>Np_CP	Np	CP Mass (kg/ Kd (mL/g)	logKd	
1	7.290	2.801	46.370	4.631E-07	3.874E-13	17.511	68266.5	4.834
2	7.560	2.647	46.370	5.618E-02	3.040E-08	17.511	105542.1	5.023
3	7.137	3.315	46.370	2.058E-06	2.206E-08	17.511	5.3	0.727
4	7.451	2.791	46.370	9.632E-01	5.858E-07	17.511	93888.3	4.973
5	6.514	2.432	46.370	1.562E-04	6.659E-07	17.511	13.4	1.127
6	7.631	2.517	46.370	1.397E-02	8.306E-09	17.511	96066.4	4.983
7	7.420	2.456	46.370	2.209E-05	1.292E-11	17.511	97694.2	4.990
8	8.132	3.244	46.370	5.842E-02	4.472E-08	17.511	74597.9	4.873
9	7.578	2.376	46.370	2.236E-06	1.534E-12	17.511	83220.7	4.920
10	7.995	3.239	46.370	1.328E+00	7.289E-07	17.511	104050.2	5.017
11	7.600	2.922	46.370	7.834E-05	6.989E-11	17.511	64008.7	4.806
12	6.970	2.415	46.370	2.808E-04	6.560E-10	17.511	2444.7	4.388
13	8.004	3.675	46.370	6.641E-07	1.709E-13	17.511	221866.2	5.346
14	6.763	2.398	46.370	1.015E-05	4.494E-10	17.511	1289.5	3.110
15	7.442	2.950	46.370	6.889E-05	4.645E-11	17.511	84749.4	4.928
16	7.445	3.488	46.370	4.822E-06	8.551E-12	17.511	32206.3	4.508
17	7.428	3.871	46.370	7.400E-04	2.890E-09	17.511	14623.1	4.165
18	8.832	3.414	46.370	6.488E-02	5.881E-06	17.511	630.0	2.798
19	7.064	2.105	46.370	5.736E-02	9.550E-06	17.511	34300.9	4.535
20	7.745	3.803	46.370	6.647E-08	5.006E-13	17.511	7582.0	3.680
21	8.063	3.858	46.370	4.650E-01	1.885E-06	17.511	14083.6	4.149
22	7.825	3.706	46.370	2.045E-07	8.745E-14	17.511	133554.5	5.126
23	8.001	2.864	46.370	1.680E-01	2.066E-07	17.511	46422.4	4.667
24	7.437	3.289	46.370	1.161E-05	2.905E-11	17.511	26461.0	4.423
25	8.768	3.504	46.370	8.372E-08	2.379E-12	17.511	2010.0	3.303
26	8.803	3.981	46.370	9.600E-10	1.911E-14	17.511	2869.1	3.458
27	7.523	2.485	46.370	6.719E-02	6.051E-08	17.511	63415.2	4.802
28	7.675	2.141	46.370	1.662E+00	4.885E-06	17.511	19428.9	4.288
29	6.975	3.279	46.370	1.925E-10	3.954E-13	17.511	27.8	1.444
30	7.473	2.295	46.370	1.619E-03	1.360E-09	17.511	67964.9	4.832
31	7.056	2.828	46.370	2.622E-06	1.262E-10	17.511	1186.7	3.074
32	8.045	3.379	46.370	2.683E-05	1.084E-11	17.511	141371.1	5.150
33	7.971	3.956	46.370	3.329E-01	9.603E-08	17.511	197972.8	5.297
35	7.006	2.579	46.370	7.002E-03	4.451E-08	17.511	8982.9	3.953
36	7.718	3.988	46.370	4.297E-02	1.471E-06	17.511	166783.2	5.222
37	7.434	2.854	46.370	4.108E-01	2.198E-07	17.511	106734.2	5.028
38	7.292	3.115	46.370	9.355E-06	3.433E-09	17.511	155.6	2.192
39	8.625	3.399	46.370	4.394E-09	1.663E-13	17.511	1508.8	3.179
40	8.061	3.426	46.370	7.741E-01	3.028E-07	17.511	146078.4	5.165
41	6.566	2.358	46.370	1.530E-04	1.109E-07	17.511	78.8	1.896
42	9.144	3.973	46.370	5.919E-07	2.811E-11	17.511	1202.4	3.080
43	8.317	3.142	46.370	5.774E-01	2.672E-06	17.511	12340.5	4.091
44	7.660	2.010	46.370	1.972E+00	1.047E-05	17.511	10757.1	4.032
45	7.351	2.591	46.370	3.225E-04	5.571E-10	17.511	33062.7	4.519
46	7.494	2.192	46.370	8.894E-01	1.816E-06	17.511	27965.2	4.447
47	7.460	3.205	46.370	4.551E-02	6.046E-06	17.511	42965.8	4.633
48	7.547	3.853	46.370	8.679E-08	7.601E-14	17.511	65204.1	4.814
49	6.607	2.227	46.370	5.244E-07	5.128E-11	17.511	584.0	2.766
50	7.500	3.520	46.370	2.038E-01	3.773E-07	17.511	30861.2	4.488

CNwRA\_Kd\_Np\_plots

Date \_\_\_\_\_

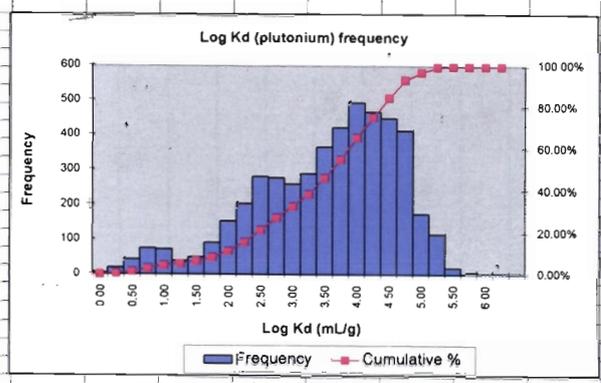
2/16/10  
C.R.

Summary statistics for  
K<sub>d</sub>, Pu  
calculated by

DOE SAM using  
PHREEQC.

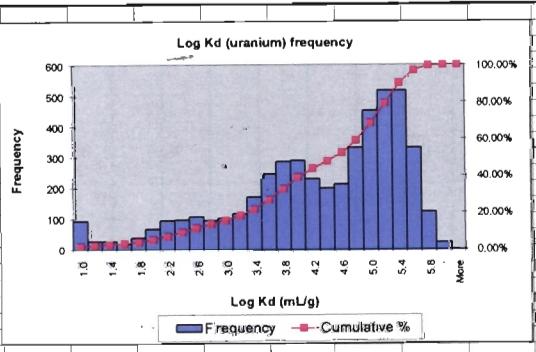
soln	pH	pCO2	CP	Sp. Surf	>Pu_CP	Pu	CP Mass (kg)	Kd (mL/g)	logKd
1	7.290	2.801	46.370	5.277E-08	3.671E-13	17.511	8209.3	3.914	
2	7.560	2.647	46.370	1.008E-03	1.006E-08	17.511	5717.5	3.757	
3	7.137	3.315	46.370	1.639E-09	3.015E-11	17.511	3.1	0.492	
4	7.451	2.791	46.370	4.207E-09	2.993E-14	17.511	8028.1	3.905	
5	6.514	2.432	46.370	3.119E-12	4.468E-14	17.511	4.0	0.601	
6	7.631	2.517	46.370	2.281E-07	3.281E-12	17.511	3969.9	3.599	
7	7.420	2.456	46.370	8.340E-03	1.044E-07	17.511	4561.8	3.659	
8	8.132	3.244	46.370	6.331E-06	5.636E-11	17.511	6195.3	3.792	
9	7.578	2.376	46.370	9.478E-09	1.827E-13	17.511	2962.6	3.472	
10	7.995	3.239	46.370	4.457E-07	2.767E-12	17.511	9199.7	3.964	
11	7.600	2.922	46.370	2.708E-05	2.831E-10	17.511	5462.4	3.737	
12	6.970	2.415	46.370	7.603E-04	1.749E-03	17.511	2483.3	3.395	
13	8.004	3.675	46.370	6.312E-09	8.563E-15	17.511	42096.4	4.624	
14	6.763	2.398	46.370	4.599E-09	1.319E-12	17.511	199.1	2.299	
15	7.442	2.950	46.370	2.301E-04	1.271E-09	17.511	10338.6	4.014	
16	7.445	3.488	46.370	3.833E-05	1.704E-10	17.511	12844.6	4.109	
17	7.428	3.871	46.370	6.932E-04	2.771E-09	17.511	14287.0	4.155	
18	8.832	3.414	46.370	2.002E-09	8.395E-13	17.511	121.7	2.085	
19	7.064	2.105	46.370	4.475E-06	1.741E-10	17.511	1467.6	3.167	
20	7.745	3.803	46.370	3.019E-06	5.491E-11	17.511	3138.7	3.497	
21	8.063	3.858	46.370	1.349E-07	2.230E-12	17.511	3455.0	3.538	
22	7.825	3.706	46.370	1.252E-05	1.878E-11	17.511	38066.2	4.581	
23	8.001	2.864	46.370	1.449E-08	3.061E-13	17.511	2703.9	3.432	
24	7.437	3.289	46.370	4.395E-07	3.652E-12	17.511	6873.0	3.837	
25	8.788	3.504	46.370	1.321E-03	2.220E-07	17.511	339.9	2.531	
26	8.803	3.981	46.370	1.503E-07	1.769E-11	17.511	486.0	2.687	
27	7.523	2.485	46.370	3.746E-09	7.819E-14	17.511	2736.1	3.437	
28	7.675	2.141	46.370	1.349E-07	1.177E-11	17.511	654.4	2.816	
29	8.975	3.279	46.370	1.817E-04	4.603E-07	17.511	20.1	1.303	
30	7.473	2.295	46.370	2.101E-08	5.200E-13	17.511	2307.1	3.363	
31	7.056	2.828	46.370	3.860E-09	8.736E-13	17.511	252.4	2.402	
32	8.045	3.379	46.370	1.179E-04	4.542E-10	17.511	14819.0	4.171	
33	7.971	3.956	46.370	1.298E-03	1.034E-06	17.511	71681.8	4.855	
35	7.006	2.579	46.370	1.690E-08	7.952E-13	17.511	1213.6	3.084	
36	7.718	3.068	46.370	1.353E-02	4.964E-08	17.511	15567.6	4.192	
37	7.434	2.854	46.370	2.621E-09	1.392E-14	17.511	10752.6	4.032	
38	7.282	3.115	46.370	2.580E-09	3.921E-12	17.511	37.6	1.575	
39	8.825	3.399	46.370	2.620E-04	6.957E-08	17.511	215.0	2.333	
40	8.061	3.426	46.370	1.299E-02	4.568E-08	17.511	16242.9	4.211	
41	6.566	2.358	46.370	1.007E-06	3.308E-09	17.511	17.4	1.240	
42	8.144	3.973	46.370	4.077E-07	1.131E-10	17.511	205.9	2.314	
43	8.317	3.142	46.370	1.255E-04	6.489E-09	17.511	1104.0	3.043	
44	7.660	2.010	46.370	3.174E-08	4.886E-12	17.511	371.0	2.569	
45	7.351	2.591	46.370	2.594E-02	6.559E-07	17.511	2258.3	3.354	
46	7.494	2.192	46.370	1.242E-07	8.515E-12	17.511	832.9	2.921	
47	7.460	3.205	46.370	2.061E-04	1.335E-09	17.511	8818.5	3.945	
48	7.547	3.653	46.370	7.400E-07	1.410E-12	17.511	29974.4	4.477	
49	6.607	2.227	46.370	1.643E-03	1.077E-06	17.511	87.1	1.940	
50	7.500	3.520	46.370	2.664E-02	1.299E-07	17.511	11706.2	4.068	

Bin	Frequency	Cumulative %	
0.00	0.00	5	0.10%
0.25	0.25	20	0.52%
0.50	0.50	44	1.44%
0.75	0.75	76	3.02%
1.00	1.00	73	4.54%
1.25	1.25	40	5.38%
1.50	1.50	50	6.42%
1.75	1.75	93	8.35%
2.00	2.00	154	11.56%
2.25	2.25	204	15.81%
2.50	2.50	282	21.69%
2.75	2.75	278	27.48%
3.00	3.00	261	32.92%
3.25	3.25	290	38.96%
3.50	3.50	367	46.50%
3.75	3.75	423	55.42%
4.00	4.00	495	65.73%
4.25	4.25	468	75.48%
4.50	4.50	450	84.85%
4.75	4.75	414	93.48%
5.00	5.00	176	97.15%
5.25	5.25	117	99.58%
5.50	5.50	19	99.98%
5.75	5.75	1	100.00%
6.00	6.00	0	100.00%
6.25	More	0	100.00%



0.65 < K<sub>d</sub> < 345,934  
 10<sup>-0.187</sup>                      10<sup>5.539</sup>

CNwRA\_Kd\_Pu\_plots



$0.09 < K_d < 125,314$   
 $10^{-1.634}$   $10^{+5.980}$

pH	pCO2	CP Sp. Sur	>U_CP	U	CP Mass (kg/Kd (mL/g)	logKd
7.290	2.801	46.370	5.365E+00	4.758E-06	17.511	64389.1
7.560	2.647	46.370	2.050E-01	1.196E-07	17.511	97894.9
7.137	3.315	46.370	1.160E+01	1.025E-01	17.511	6.5
7.451	2.791	46.370	1.632E+00	1.690E-06	17.511	55147.2
6.514	2.432	46.370	1.161E+01	6.419E-03	17.511	103.3
7.631	2.517	46.370	5.362E-02	1.741E-08	17.511	175893.6
7.420	2.456	46.370	4.442E-01	2.364E-07	17.511	107335.0
8.132	3.244	46.370	3.863E-03	3.269E-09	17.511	67486.1
7.578	2.376	46.370	1.146E-02	3.210E-09	17.511	203926.7
7.995	3.239	46.370	3.032E-01	3.030E-07	17.511	57135.2
7.600	2.922	46.370	8.952E-03	1.971E-06	17.511	25836.0
6.970	2.415	46.370	7.804E+00	8.825E-06	17.511	50505.5
8.004	3.675	46.370	1.522E-02	4.714E-08	17.511	18436.8
6.763	2.398	46.370	1.134E+01	1.098E-04	17.511	5894.2
7.442	2.950	46.370	1.775E+00	2.110E-06	17.511	48027.1
7.445	3.488	46.370	6.878E-07	1.171E-10	17.511	335.3
7.428	3.871	46.370	4.340E-01	3.965E-06	17.511	6204.6
8.832	3.414	46.370	9.430E-03	1.663E-07	17.511	3238.2
7.064	2.105	46.370	1.394E+00	1.845E-06	17.511	43144.3
7.746	3.803	46.370	1.123E+01	1.721E-04	17.511	3725.3
8.063	3.858	46.370	9.729E+00	1.506E-04	17.511	3689.9
7.825	3.706	46.370	4.325E-06	8.113E-11	17.511	3044.1
8.001	2.864	46.370	4.267E-03	2.483E-09	17.511	98124.3
7.437	3.289	46.370	3.092E-05	2.021E-09	17.511	874.0
8.768	3.504	46.370	5.477E-04	5.204E-09	17.511	6009.7
8.803	3.981	46.370	1.300E+00	5.492E-05	17.511	1352.0
7.523	2.485	46.370	1.877E-02	1.215E-08	17.511	86224.2
7.675	2.141	46.370	1.912E-02	6.188E-09	17.511	176503.2
6.975	3.279	46.370	1.162E+01	1.114E-02	17.511	59.6
7.473	2.295	46.370	9.386E-02	3.567E-08	17.511	150271.6
7.056	2.628	46.370	1.146E+01	2.253E-04	17.511	2903.1
8.045	3.379	46.370	1.567E-02	1.642E-08	17.511	58204.0
7.971	3.866	46.370	1.595E-05	4.048E-10	17.511	2249.8
7.006	2.579	46.370	1.031E+01	2.772E-05	17.511	21246.9
7.718	3.068	46.370	3.176E-01	2.848E-07	17.511	63982.6
7.434	2.854	46.370	2.136E+00	1.969E-06	17.511	62276.2
7.292	3.115	46.370	1.147E+01	2.653E-03	17.511	247.0
8.625	3.399	46.370	2.373E-03	3.215E-08	17.511	4214.9
8.061	3.426	46.370	2.869E-03	3.362E-09	17.511	50259.9
6.506	2.358	46.370	1.159E+01	1.107E-03	17.511	598.3
9.144	3.973	46.370	2.235E-02	1.007E-06	17.511	1267.3
8.317	3.142	46.370	2.726E-01	4.988E-07	17.511	31205.5
7.660	2.010	46.370	3.730E-02	1.307E-08	17.511	162943.1
7.351	2.591	46.370	6.183E-01	1.462E-06	17.511	23826.2
7.484	2.192	46.370	5.591E-02	3.369E-08	17.511	95064.9
7.460	3.205	46.370	2.567E-08	6.024E-11	17.511	2433.9
7.547	3.653	46.370	8.992E-08	1.188E-11	17.511	432.2
6.607	2.227	46.370	1.144E+01	1.685E-04	17.511	3876.0
7.500	3.520	46.370	2.299E-02	3.146E-07	17.511	4173.7
7.516	2.477	46.370	7.760E-02	3.902E-08	17.511	113565.6
8.075	3.838	46.370	1.110E+01	4.681E-03	17.511	136.1

Bin	Frequency	Cumulative %
1.0	93	1.94%
1.2	28	2.52%
1.4	28	3.10%
1.6	20	3.52%
1.8	39	4.33%
2.0	67	5.73%
2.2	94	7.69%
2.4	96	9.69%
2.6	107	11.92%
2.8	94	13.68%
3.0	102	16.00%
3.2	116	18.42%
3.4	170	21.96%
3.6	244	27.04%
3.8	285	32.98%
4.0	289	39.00%
4.2	229	43.77%
4.4	198	47.90%
4.6	211	52.29%
4.8	331	59.19%
5.0	451	68.56%
5.2	516	79.33%
5.4	516	90.08%
5.6	331	96.96%
5.8	122	99.52%
6.0	23	100.00%
More	0	100.00%

CNwRA\_Kd\_U\_plots

Summary Statistics  
 for K<sub>d</sub> calculated  
 by DDE SCM using  
 DIRECTAC software  
 parameter sampling  
 ASDD calculations

2/16/10  
 JES

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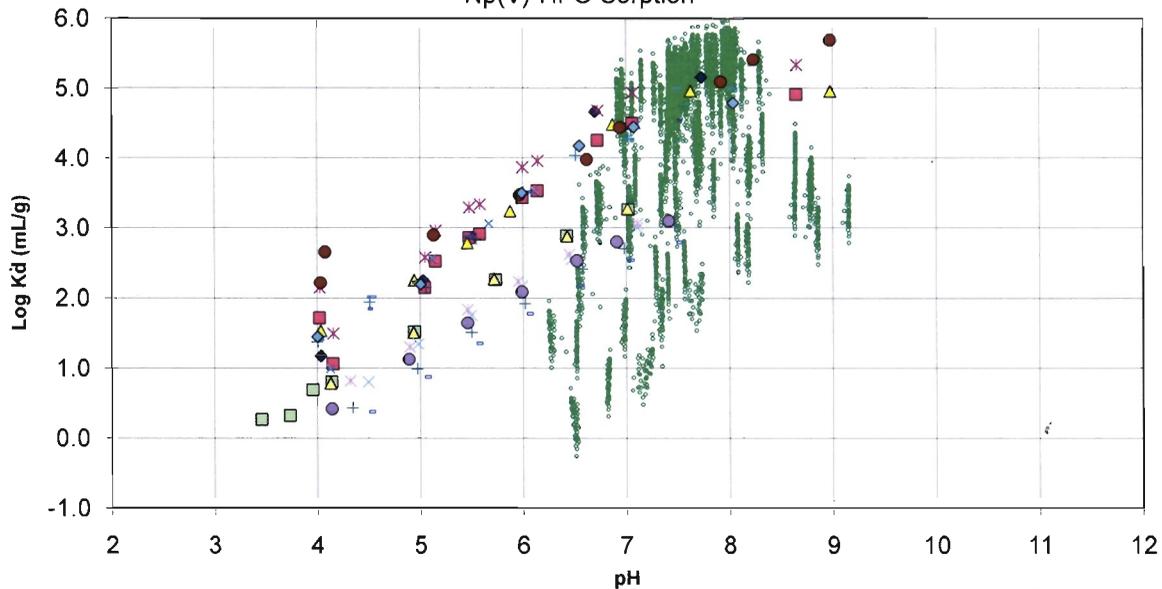
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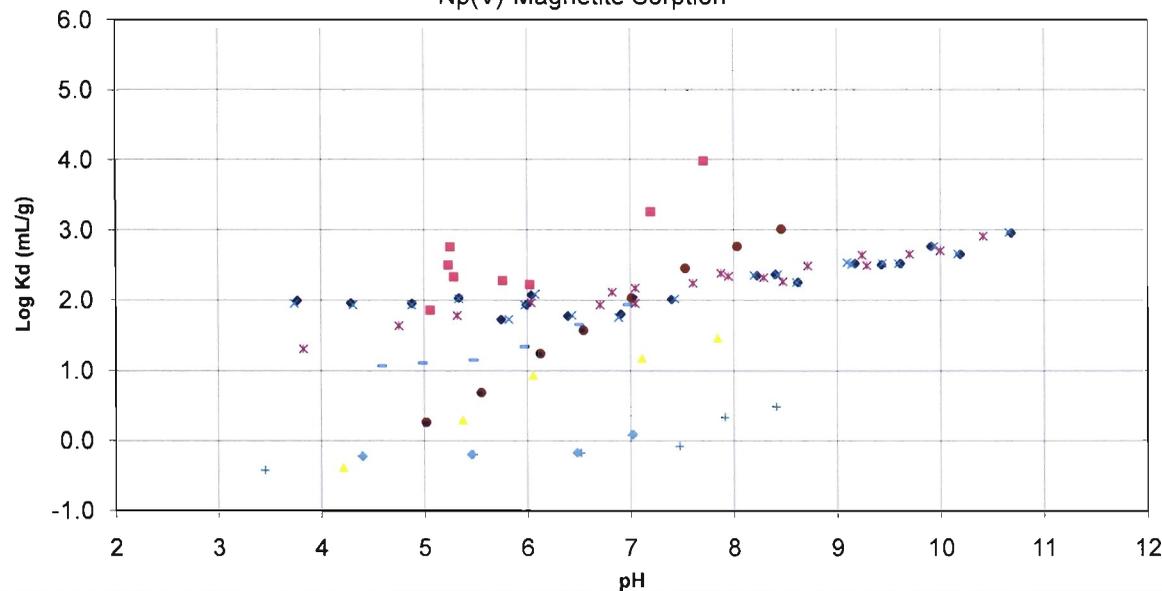


### Np(V)-HFO Sorption



- ◆ DOE PHREEQC data
- △ GIR91 (Fig 2a; 4.5E-11M; logCt=-4.42; 0.889 g/L)
- GIR91 (Fig 2b; 4.7E-12M; log Ct=-4.42; 0.889 g/L)
- NAG98 (Fig 2; 1E-8M; No CO2; 0.01 M NaClO4; 0.889 g/L)
- △ TOCH91 (Fig 9; 1E-12 M; syn HFO(Room T); 20 g/L)
- TOCH91 (Fig 9; 1E-12M; syn HFO(300C); 20 g/L)
- ◆ GIR91 (Fig 2a; 4.5E-13M; logCt=-4.42; 0.889 g/L)
- × GIR91 (Fig 2b; 4.7E-12M; logCt=-4.42; 0.889 g/L)
- × NAG98 (Fig 2; 1E-8M; No CO2; 0.01 M NaClO4; 0.889 g/L)
- NAG98 (Fig 2; 1E-8M; No CO2; 1 M NaClO4; 0.889 g/L)
- △ TOCH91 (Fig 9; 1E-12 M; syn HFO(100C); 20 g/L)
- TOCH91 (Fig 9; 1E-12M; syn HFO(400C); 20 g/L)
- ◆ GIR91 (Fig 2a; 4.7E-12M; logCt=-4.42; 0.889 g/L)
- × GIR91 (Fig 2b; 4.7E-12M; logCt=-4.42; 0.329 g/L)
- NAG98 (Fig 2; 1E-8M; No CO2; 0.01M NaClO4; 0.889 g/L)
- TOCH91 (Fig 3; 1E-12 M; syn HFO; 20 g/L)
- △ TOCH91 (Fig 9; 1E-12M; syn HFO(200C); 20 g/L)
- TOCH91 (Fig 9; 1E-12M; syn HFO(600C); 20 g/L)

### Np(V)-Magnetite Sorption



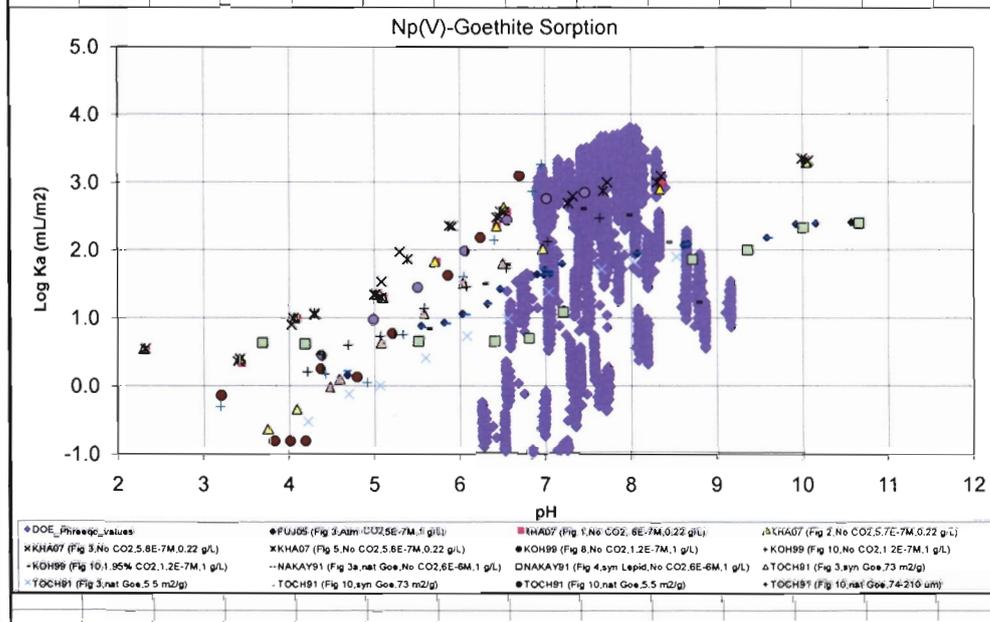
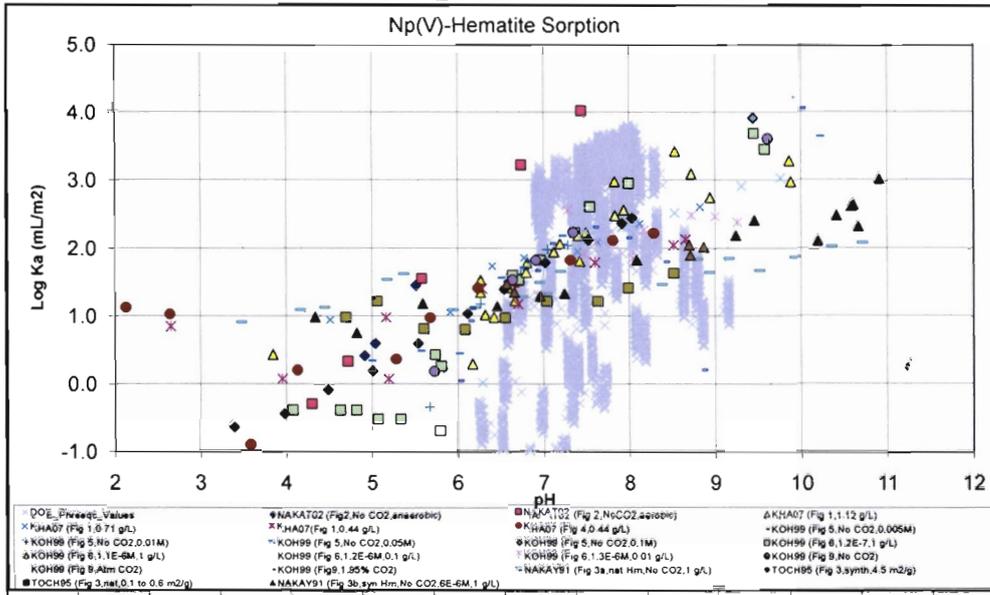
- ◆ FUJ95 (Figs 3b&5b; 5E-7M; Atm CO2; 1 g/L)
- × NAKAY91 (Fig 3b; syn Mt; No CO2; 6E-6M; 1 g/L)
- TOCH91 (Fig 12; syn Mt; 1E-12M; 0.6 m2/g)
- ◆ NAKAT02 (Fig 2, Aerobic; No CO2; 6E-6M; 25 g/L)
- TOCH91 (Fig 3; syn Mt; 1E-12M; 20 g/L)
- ◆ NAKAY91 (Fig 3a; nat Mt; No CO2; 6E-6M; 1 g/L)
- TOCH91 (Fig 3; nat Mt; 1E-12M; 20 g/L)
- TOCH91 (Fig 12; syn Mt; 1E-12M; 0.1 m2/g)
- TOCH91 (Fig 12; syn Mt; 1E-12M; 3.4 m2/g)

Neptunium data pts - Graphs - Log Kd

Same as pg. 32  
 Np(V)-HFO  
 Np(V)-Mt

*[Handwritten signature]*

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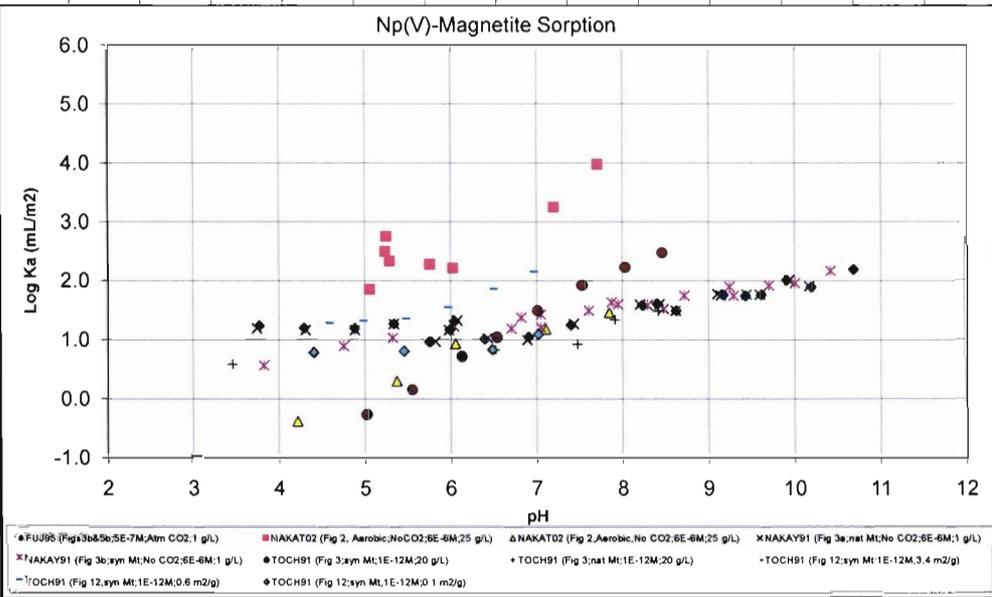
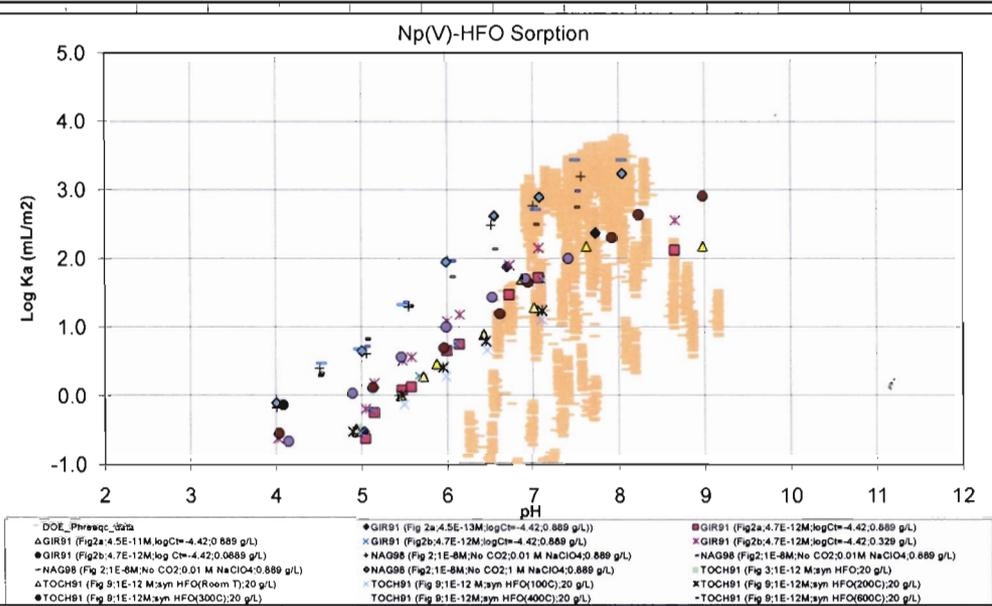


	Hm	Goe	HFO	Mt	SiO2	Al-oxide	Al-Silicate	Cc
FUJ85		X		X				
GIR51			X					
HEB08								X
JER07		X						
KHA07	X	X						
KOH99	X	X			X			
NAG98			X					
NAKAT02	X			X				
NAKAY91	X	X		X		X	X(bt)	
DELNER04							X	
TOCH95	X	X	X	X				
WILK05								
ZAV05					X	X		
ZUY104								

Comparison SEM to Experiment  
 Data, normalized to SA<sub>sp</sub>  
 DOE data normalized using sample  
 SA<sub>sp</sub> for individual PHREEQC simulations

Neptunium data pts - Graphs - Log Ka

2/16/10  
 [Signature]



Normalized for SAsp, including surface area sampled for individual DOE PHRECAL runs.

Neptunium data pts - Graphs - Log Ka

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2/16/2010  
 2010





No. *104* *Further entries.*  
*ECF* *7/22/2010*

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Date

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<b>Remarks:</b> (computer runs, etc.)	Notebook supplemental material