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Scientific Notebook #123 for
Sorption Modeling for HLW
Performance Assessment-Task

Project: Sorption Modeling for HLW Performance Assessment - Task 2

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Contents

Page

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9/9/94 PM

PM this notebook will contain data continuing from scientific notebook #057.

below is a copy of the objectives sheet written by Dr. David Turner from scientific notebook #057.

PM

Sorption Modeling for HLW Performance Assessment - Task 2

Objectives:

This scientific notebook contains the results of sorption modeling of radionuclide sorption using surface complexation modeling techniques. The objectives are to determine the model parameters necessary to reproduce the observed sorption behavior. The results are computer-based; the data used to determine the necessary model parameters are from the peer-reviewed with data sources as noted. Experimental conditions for the different data sources are noted as necessary. A basic understanding of chemical principles and DOS-based computer operation are the minimum requirements for these modeling efforts.

The computer equipment (hardware) includes:

Digitizing tablet for converting graphical data to numerical values
IBM Personal computers.

General DOS/Windows computer codes include:

Spreadsheets (Quattro, Quattro Pro, Lotus)
Graphics programs (Sigma Plot, Surfer)
Geochemical codes (EQ3/6, MINTEQA2, EQMOD)
Geochemical Parameter Estimation Code (FITEQL)

Potential sources of uncertainty and error include:

Digitization error
Experimental error/uncertainty
Conceptual model uncertainty/error
Thermodynamic data uncertainty/error

Sorption Binding Constant (K) Tables - Continued

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Tripathi 94 Concentration: [U(VI)] = 1e-6.7 M (50 ppb)	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.08 Abs Error (radionuclide): 1.7e-08	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2

	DLM Log K_+ = 7.24 Log K_- = -9.06			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ =5.89 Log K_- = -9.89 Log K_{Ca} = -7.64 Log K_{As} = 8.56		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	1.176	3.635	.07405	0.6519	3.416	.07412	-3.031	12.28	.1093
XOH-UO_2^{2+}	8.567	6.289	.07703	7.656	5.136	.07570	4.846	12.30	.1155
XO-UO_2OH^o	-6.259	1.755	.07568	-6.370	2.070	.07496	-8.396	7.345	.07925
XOH-UO_2OH^+	1.176	3.635	.07405	0.6519	3.416	.07412	-0.5580	7.735	.08213
XO-$UO_2(OH)_2^-$	-13.72	.8030	.08115	-13.40	1.175	.07800	-14.05	1.940	.07734
XOH-$UO_2(OH)_2^o$	-6.259	1.755	.07568	-6.370	2.070	.07496	-6.235	2.158	.07482
XOH_2-$UO_2(OH)_2^+$	1.176	3.635	.07405	0.6519	3.416	.07412	1.620	2.483	.07646
XOH-$UO_2(OH)_3^-$	-13.72	.8030	.08115	-13.40	1.175	.07800	-12.06	.5707	.09089
XOH_2-$UO_2(OH)_3^o$	-6.259	1.755	.07568	-6.370	2.070	.07496	-4.232	.5684	.08791
XOH-$UO_2(OH)_4^{2-}$	-21.21	.5975	.08959	-20.44	.7013	.08294	-17.93	1.281	.1191
XOH_2-$UO_2(OH)_4^-$	-13.72	.8030	.08115	-13.40	1.175	.07800	-10.16	1.383	.1136
XOH-$UO_2CO_3^o$	-2.647	2.215	.04662	-2.753	2.625	.04654	-2.616	2.777	.04660
XOH_2-$UO_2(CO_3)_2^-$	-6.968	2.203	.03880	-6.642	2.266	.03785	-5.794	9.157	.09508
XOH_2-$UO_2(CO_3)_3^{3-}$	-18.31	1.029	.07026	-17.22	2.404	.06947	-17.48	9.036	.1409
XOH_2-$(UO_2)_3CO_3(OH)_3^o$	-6.397	.9093	.09096	-6.499	1.037	.09060	-4.800	2.238	.1130

1 2 3 4

.U33pg1

XOH-$UO_2(OH)_4^{-2}$	-21.46	7.652	.09217	-20.53	8.888	.08520	-17.92	10.47	.1188

.U33pg2

errors for input files numbered 1, 2, 3, and 4

	abs error (radion)		abs error (radion)		abs error (radion)		abs error (radion)	
UO_{2ads}	1	1.7E-08	2	1.7E-08	3	1.7E-08	4	1.7E-08
CO_{3ads}		1.7E-08		3.4E-08		5.1E-08		5.1E-08
H^+		0.0E-00		0.0E-00		0.0E-00		0.0E-00

* ;

this species was run in the presence of CO_2 - compare with the results obtained without CO_2 present (refer to the enteries following the tenth species in the table).

9/12/94 PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/g Data Source: Tripathi 84 Concentration: [U(VI)] = 1e-7.1 M (20 ppb)	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.08 Abs Error (radionuclide): 6.7e-09	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2

no CO_2	DLM Log K_+ = 7.24 Log K_- = -9.06			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 5.89 Log K_- = -9.89 Log K_{Ca} = -7.64 Log K_{As} = 8.56		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	1.246	3.605	.1026	0.7203	3.349	.1028	-2.947	16.00	.1496
XOH-UO_2^{2+}	8.660	6.853	.1048	7.737	5.363	.1034	4.882	16.22	.1558
XO-UO_2OH^o	-6.204	1.527	.1061	-6.312	1.861	.1049	-8.290	8.208	.1071
XOH-UO_2OH^+	1.246	3.605	.1026	0.7203	3.349	.1028	-.4580	8.803	.1095
XO-$UO_2(OH)_2^-$	-13.69	.5724	.1139	-13.36	0.9105	.1093	-14.01	1.694	.1066
XOH-$UO_2(OH)_2^o$	-6.204	1.527	.1061	-6.312	1.861	.1049	-6.176	1.956	.1046
XOH_2-$UO_2(OH)_2^+$	1.246	3.605	.1026	0.7203	3.349	.1028	1.671	2.288	.1051
XOH-$UO_2(OH)_3^-$	-13.69	.5724	.1139	-13.36	0.9105	.1093	-12.05	.2937	.1244
XOH_2-$UO_2(OH)_3^o$	-6.204	1.527	.1061	-6.312	1.861	.1049	-4.208	.2935	.1218
XOH-$UO_2(OH)_4^{2-}$	-21.20	.3730	.1235	-20.41	0.4180	.1155	-18.00	.8450	.1500
XOH_2-$UO_2(OH)_4^-$	-13.69	.5724	.1139	-13.36	0.9105	.1093	-10.18	.8330	.1456
XOH-$UO_2CO_3^o$									
XOH_2-$UO_2(CO_3)_2^-$									
XOH_2-$UO_2(CO_3)_3^{3-}$									
XOH_2-$(UO_2)_3CO_3(OH)_3^o$									

.U34

9/14/94 PM Plutonium K Tables

Plutonium (IV) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: goethite A_{SP}: 50 m^2/L Data Source: Sanchez Concentration: 1e-10 M	Rel Error (pH): * Abs Error (pH): Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-13	Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2 0.55 g/L

Fig 1a		DLM Log K_+ = 7.35 Log K_- = -9.17			CCM Log K_+ = 6.47 Log K_- = -9.03			TLM Log K_+ = 6.00 Log K_- = -10.00 Log K_{Ca} = -7.64 Log K_{As} = 8.78		
		Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-Pu^{3+}	xopu	12.42	66.61	.02907	13.79	18.99	.03335	-1.715	94.49	.04917
XO-$PuOH^{3+}$	xopu1	7.197	20.44	.02808	7.241	17.50	.03634	-4.143	87.51	.03955
XO-$Pu(OH)_2^+$	xopu2	1.366	17.89	.04100	.8612	16.44	.04014	-6.593	55.45	.02711
XOH-$Pu(OH)_2^{2+}$	xohpu2	7.197	20.44	.02808	7.341	17.50	.03634	.9415	61.27	.02804
XO-$Pu(OH)_3^o$	xopu3	-4.211	30.16	.04980	-5.638	18.72	.04615	-9.657	20.26	.03054
XOH-$Pu(OH)_3^+$	xohpu3	1.366	17.89	.04100	.8612	15.50	.04014	-2.026	21.11	.02936
XO-$Pu(OH)_4^-$	xopu4	-11.48	38.03	.06597	-12.07	22.61	.05080	-13.20	20.02	.04794
XOH-$Pu(OH)_4^o$	xohpu4	-4.211	30.16	.04980	-5.638	18.72	.04615	-5.562	18.26	.04542
XOH_2-$Pu(OH)_4^+$	xoh2pu4	1.366	17.89	.04100	.8612	16.44	.04014	2.088	16.69	.04280
XOH-$Pu(OH)_5^-$	xohpu5	-11.48	38.03	.06597	-12.07	22.61	.05080	-9.753	34.07	.06482
XOH_2-$Pu(OH)_5^o$	xoh2pu5	-4.211	30.16	.04980	-5.638	18.72	.04615	-2.035	33.12	.06495
OTHER SPECIES:										

*. not used in input files to allow convergence

BINDING4.PI

9/16/94 PM

Plutonium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: goethite A_{sp}: 50 m^2/g Data Source: Sanchez 85 Concentration: 1e-10		Rel Error (pH): * Abs Error (pH): Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-13		Ionic Strength (electrolyte): 0.1 M $NaNO_3$ N_s = 2.31 sites/nm^2 0.55 g/L

Fig 1c		DLM			CCM			TLM		
		Log K_+ = 7.35 Log K_- = -9.17			Log K_+ = 6.47 Log K_- = -9.03			Log K_+ = 6.00 Log K_- = -10.00 Log K_{Ca} = -7.64 Log K_{As} = 8.78		
		Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-PuO_2^+	xopuo2	-.01758	52.68	.03017	-1.414	28.11	.02372	-3.944	80.08	.02004
XOH-PuO_2^+	xohpuo2	5.611	7.532	.02153	5.115	6.351	.02161	4.030	85.69	.02173
XO-PuO_2OH^-	xopuo21	-5.282	38.65	.03997	-7.830	45.05	.0258	-8.973	34.74	.02429
XOH-PuO_2OH^o	xohpuo21	-.01758	52.68	.03017	-1.414	28.11	.02372	-1.339	25.40	.02349
XOH_2-PuO_2OH^+	xoh2po21	5.611	7.532	.02153	5.115	6.351	.02161	6.313	15.93	.02275
OTHER SPECIES:										

*: not used in input files to allow convergence

BINDING5.P1

9/20/94 PM

Plutonium (V) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: gamma (γ) alumina A_{sp}: 120 m^2/g Data Source: Righetto et al 91 Concentration: [Pu(V)] = 2e-10 M		Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e-13		Ionic Strength (electrolyte): 0.1 M $NaClO_4$ N_s = 2.31 sites/nm^2

fig 1 C_s = .2 g/L		DLM			CCM			TLM		
		Log K_+ = 6.78 Log K_- = -9.12 (modelled using delta alumina parameters)			Log K_+ = 6.92 Log K_- = -9.00			Log K_+ = 6.29 Log K_- = -10.29 Log K_{Ca} = -7.81 Log K_{As} = 8.11		
		Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
XO-PuO_2^+	xopuo2	-3.154	.06438	.07878	-3.134	.06555	.07860	-2.766	4.988	.1483
XOH-PuO_2^+	xohpuo2	4.628	.09360	.07685	4.647	.04451	.07684	5.731	5.228	.2214
XO-PuO_2OH^-	xopuo21	-10.91	.2396	.08261	-10.90	.2408	.08259	-11.20	.1026	.08012
XOH-PuO_2OH^o	xohpuo21	-3.154	.06438	.07878	-3.134	.06555	.07860	-3.095	.06366	.07789
XOH_2-PuO_2OH^+	xoh2po21	4.628	.09360	.07685	4.647	.04448	.07698	5.013	.03330	.07855
OTHER SPECIES:										

BINDING5.P2

9/22/94 PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92		Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.1 Abs Error (radionuclide): 1e-09	Ionic Strength (electrolyte): 0.1 M N_s = 2.31 sites/nm^2

fig 7.1 25 mg/25 mL solid/liquid ratio kaolinite was modelled with 1:1 AlOH/SiOH ratio		TLM					CCM				
		Log K_+ = 6.69 Log K_- = -10.69 Log K_{Ca} = -7.73 Log K_{As} = 9.90 alpha-alumina Log K_- = -4.79 Log K_{Si} = -6.22 silica					Log K_+ = 9.08 Log K_- = -8.32 alpha-alumina Log K_- = -7.05 silica				
		Log K_{AlOH}	σK_{AlOH}	Log K_{SiOH}	σK_{SiOH}	V_Y	Log K_{AlOH}	σK_{AlOH}	Log K_{SiOH}	σK_{SiOH}	V_Y
XO-UO_2^+	xouo2	.2103	div 0*	-26.00			3.465	.07220	1.270	.1372	13.33
XOH-UO_2^{2+}	xohuo2	6.737	div 0*	-18.80			?NC	*			
XO-UO_2OH^+	xouo21	-4.043	div 0*	-29.00			-4.050	.1305	-5.416	.08351	13.10
XOH-UO_2OH^+	xohuo21	1.052	div 0*	-24.27			3.465	.07220	1.270	.1872	13.33
XO-$UO_2(OH)_2^-$	xouo22	-9.694	.4690	-10.04	.05612	14.13	-12.66	1.552	-12.34	.06639	5.351
XOH-$UO_2(OH)_2^o$	xohuo22	-3.876	.1300	-5.270	.08358	13.00	-4.050	.1305	-5.416	.08351	13.10
XOH_2-$UO_2(OH)_2^+$	xoh2uo22	1.462	.07731	-.6511	.1757	13.34	3.465	.07220	1.270	.1872	13.33
XOH-$UO_2(OH)_3^-$	xohuo23	-25.27 nc	*	-8.706			err # 1	*			
XOH_2-$UO_2(OH)_3^o$	xoh2uo23	-21.90 nc	*	-3.7245			-4.050	.1305	-5.416	.08351	13.10
XOH-$UO_2(OH)_4^{2-}$	xohuo24	22.57	err # 1*	19.64			err #1	*			
XOH_2-$UO_2(OH)_4^-$	xoh2uo24	-23.44	err # 1*	-25.20			-12.66	1.552	-12.34	.05091	5.351
XOH-$UO_2CO_3^o$											

*: Abs err = $1e^{-07}$
?: no convergence, ? output

U.AS1

err#1: # iterations allowed was exceeded

9/26/94 PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92		Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.1 Abs Error (radionuclide): 1e-09	Ionic Strength (electrolyte): 0.1 M N_s = 2.31 sites/nm^2

fig 7.1 25 mg/25 mL solid/liquid ratio		DLM				
		K_+ = 8.22 K_- = -9.62 (Al) K_- = -7.10				
		Log K_{AlOH}	σK_{AlOH}	Log K_{SiOH}	σK_{SiOH}	V_Y
XO-UO_2^+	xouo2	2.603	.05992	1.173	.08929	10.48
XOH-UO_2^{2+}	xohuo2					nc?
XO-UO_2OH^+	xouo21	-4.807	.1279	-5.469	.07910	13.17
XOH-UO_2OH^+	xohuo21	2.603	.05992	1.173	.08927	10.48
XO-$UO_2(OH)_2^-$	xouo22	-13.68	4.854	-12.32	.07579	6.159 e = 1e-8
XOH-$UO_2(OH)_2^o$	xohuo22	-4.807	.1279	-5.469	.07910	13.17
XOH_2-$UO_2(OH)_2^+$	xoh2uo22	2.603	.05992	1.173	.08929	10.48
XOH-$UO_2(OH)_3^-$	xohuo23	-31.66	4.848	-12.29	.07579	16.73
XOH_2-$UO_2(OH)_3^o$	xoh2uo23	-4.807	.1279	-5.469	.07910	13.17
XOH-$UO_2(OH)_4^{2-}$	xohuo24					err # 1
XOH_2-$UO_2(OH)_4^-$	xoh2uo24	-13.68	4.854	-12.32	.07579	6.159 e = 1e-08
XOH-$UO_2CO_3^o$						

U.AS2

nc?: output gave ????? as results
e=1e-8: Abs error was relaxed to $1.0e^{-8}$
err#1: # iterations allowed was exceeded

9/27/94 PM

PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92 Concentration: 1.00e-6 M UO_2^{+2}	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e*	Ionic Strength (electrolyte): 0.1 M N_s = 2.31 sites/nm^2

fig 7.2 modelled with 1:1 AlOH/SiOH ratio 100 mg/25 mL solid/liquid ratio		TLM: Log K_+ = 6.69; Log K_- = -10.69; Log K_{Ca} = -7.73; Log K_{Al} = 9.90 alpha alumina; Log K_- = -4.79; Log K_{Ca} = -6.22 silica					CCM: Log K_+ = 9.08; Log K_- = -8.32 alpha alumina; Log K_- = -7.05 silica				
		Log K_{AlOH}	σ K_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y	Log K_{AlOH}	σK_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y
$XO\text{-}UO_2^+$	xouo2	div 0				*-7	3.176	.1560	1.046	.1984	3.874*-8
$XOH\text{-}UO_2^{2+}$	xohuo2	ao				*-7	10.18	.06545	7.865	.05418	12.75-10
$XO\text{-}UO_2OH^o$	xouo21	-5.086	.09868	-7.333	.1059	14.51*-9	-3.945	.6387	-5.837	.6466	.2487*-7
$XOH\text{-}UO_2OH^+$	xohuo21	-.2561	.07026	-2.719	.08746	24.42*-10	3.176	.1560	1.046	.1984	3.874*-8
$XO\text{-}UO_2(OH)_2^-$	xouo22	-9.047	1.376	-10.32	.3838	.2565*-7	-11.60	2.050	-12.53	.3256	.2919*-7
$XOH\text{-}UO_2(OH)_2^o$	xohuo22	-3.760	.6350	-5.711	.6797	.2456*-7	-3.945	.6387	-5.837	.6466	.2487*-7
$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo22	1.183	.1835	-.8153	.1794	4.116*-8	3.176	.1560	1.046	.1984	3.874*-8
$XOH\text{-}UO_2(OH)_2^-$	xohuo23	err # 1					-11.60	2.050	-12.53	.3256	.2919*-7
$XOH_2\text{-}UO_2(OH)_2^o$	xoh2uo23	nc-25.44		-3.806		*-7	-3.945	.6387	-5.837	.6466	.2487*-7

U.AS3 pg1

$XOH\text{-}UO_2(OH)_3^{2-}$	xohuo24	err # 1				*-7	NC-40.30		NC-19.38		*-6
$XOH_2\text{-}UO_2(OH)_2^-$	xoh2uo24	err # 1				*-7	-11.60	2.049	-12.53	.3256	.2919*-7
$XOH\text{-}UO_2CO_3^o$											
$XOH_2\text{-}UO_2(CO_3)_2^-$											
$XOH_2\text{-}(UO_2)_3CO_3(OH)_3^+$											

U.AS3 pg2

*: Abserror ranged from 1.0e-10 to 1.0e-6, as listed under V_y.
div 0: error due to division by 0
ao: error due to arithmetic overflow
err #1: # iterations allowed was exceeded
nC: no convergence

9/28/94 PM

PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92 Concentration: 1.00e-6 M UO_2^{2+}	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.1 Abs Error (radionuclide): 1e*	Ionic Strength (electrolyte): N_s = 2.31 sites/nm^2

fig 7.2 100 mg/25 mL solid/liquid ratio		DLM: K_+ = 8.22; K_- = -9.62 (Al); K_- = -7.10				
		Log K_{AlOH}	σ K_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y
$XO\text{-}UO_2^+$	xouo2	2.178	.1014	.9603	.03507	7.722*-10
$XOH\text{-}UO_2^{2+}$	xohuo2	9.196	.03086	5.728	.1573	12.98*-10
$XO\text{-}UO_2OH^o$	xouo21	-4.738	.5905	-5.836	.4451	.2543*-7
$XOH\text{-}UO_2OH^+$	xohuo21	2.178	.1014	.9603	.03507	7.722*-10
$XO\text{-}UO_2(OH)_2^-$	xouo22	-12.56	3.360	-12.43	.2804	.3674*-7
$XOH\text{-}UO_2(OH)_2^o$	xohuo22	-4.738	.5905	-5.836	.4451	.2543*-7

BINDINGU.AS4, pt1

PM

$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo22	2.178	.1014	.9603	.03507	7.722*-10
$XOH\text{-}UO_2(OH)_3^-$	xohuo23	-12.56	3.360	-12.43	.2804	.3674*-7
$XOH_2\text{-}UO_2(OH)_2^o$	xoh2uo23	-4.738	.5905	-5.836	.4451	.2543*-7
$XOH\text{-}UO_2(OH)_4^{2-}$	xohuo24	NC	err # 1			*-7
$XOH_2\text{-}UO_2(OH)_2^-$	xoh2uo24	-12.56	3.360	-12.43	.2804	.3674*-7
$XOH\text{-}UO_2CO_3^o$						
$XOH_2\text{-}UO_2(CO_3)_2^-$						

U.AS4 (pt 2)

for error explanations, see listings under 9/27/94.

9/30/94 PM

PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92 Concentration: 1.00e-6 M UO_2^{2+}	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Ref Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e*	Ionic Strength (electrolyte): 0.1 M N_s = 2.31 sites/nm^2

fig 7.3 modelled with 1:1 AlOH/SiOH ratio 400 mg/25 mL solid/liquid ratio		TLM: Log K_+ = 6.69; Log K_- = -10.69; Log K_{Ca} = -7.73; Log K_{Al} = 9.90 alpha alumina; Log K_- = -4.79; Log K_{Ca} = -6.22 silica					CCM: Log K_+ = 9.08; Log K_- = -8.32 alpha alumina; Log K_- = -7.05 silica				
		Log K_{AlOH}	σ K_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y	Log K_{AlOH}	σK_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y
$XO\text{-}UO_2^+$	xouo2	ao				*-7	3.121	.1615	1.027	.05724	10.69*-10
$XOH\text{-}UO_2^{2+}$	xohuo2	ao				*-7	10.18	.1068	7.219	.3699	3.750*-8
$XO\text{-}UO_2OH^o$	xouo21	-5.066	.09018	-7.803	.1098	8.861*-10	nc-4.502		-5.648		*-6
$XOH\text{-}UO_2OH^+$	xohuo21	div 0				*-7	3.121	.1615	1.027	.05724	10.69*-10
$XO\text{-}UO_2(OH)_2^-$	xouo22	nc-10.52		-10.16		*-7	nc-12.84		-12.36		*-6
$XOH\text{-}UO_2(OH)_2^o$	xohuo22	nc-4.521		-5.449		*-7	nc-4.459		-5.605		*-7
$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo22	nc1.040		-0.8837		*-7	3.121	.1615	1.027	.05724	10.69*-10
$XOH\text{-}UO_2(OH)_3^-$	xohuo23	err # 1				*-7	nc-28.84		-12.29		*-7
$XOH_2\text{-}UO_2(OH)_2^o$	xoh2uo23	err # 1				*-8	err # 1				*-7
$XOH\text{-}UO_2(OH)_4^{2-}$	xohuo24	ao				*-7	err # 1				*-6
$XOH_2\text{-}UO_2(OH)_2^-$	xoh2uo24	ao				*-7	nc-28.84		-12.29		*-7
$XOH\text{-}UO_2CO_3^o$											

U.AS5

10/4/94 PM

PM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: kaolinite A_{sp}: 11 m^2/g Data Source: Payne et al 92 Concentration: 1.00e-6 M UO_2^{2+}	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 1.0e*	Ionic Strength (electrolyte): 0.1 M N_s = 2.31 sites/nm^2

fig 7.3		DLM: K_+ = 8.22; K_- = -9.62 (Al); K_- = -7.10				
		Log K_{AlOH}	σ K_{AlOH}	Log K_{SiOH}	σ K_{SiOH}	V_y
$XO\text{-}UO_2^+$	xouo2	2.715	.06732	-.07609	.08080	12.62*-10
$XOH\text{-}UO_2^{2+}$	xohuo2	???????				*-6
$XO\text{-}UO_2OH^o$	xouo21	nc-5.074		-5.735		*-6
$XOH\text{-}UO_2OH^+$	xohuo21	2.715	.06732	-.07609	.08080	12.62*-10
$XO\text{-}UO_2(OH)_2^-$	xouo22	nc-32.23		-12.23		*-6
$XOH\text{-}UO_2(OH)_2^o$	xohuo22	nc-5.074		-5.735		*-6
$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo22	2.715	.06731	-.07611	.08080	12.62*-10
$XOH\text{-}UO_2(OH)_3^-$	xohuo23	nc-32.23		-12.23		*-6
$XOH_2\text{-}UO_2(OH)_2^o$	xoh2uo23	nc-5.074		-5.735		*-6
$XOH\text{-}UO_2(OH)_4^{2-}$	xohuo24	err # 1				*-6
$XOH_2\text{-}UO_2(OH)_2^-$	xoh2uo24	nc-32.23		-12.23		*-6

U.AS6

10/06/94 PM MINTEQA2 PLOTS

PM Np(V) sorption data on goethite for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Nakayama and Sakamoto '91. The log K values calculated in FITEQL can be found in scientific notebook # 057, table Binding.NP, page 128. Below is a copy of the MINTEQA2 input file for TLM, species XO-NpO_2. The file is saved on a floppy disk (a:\naknp\naknp31t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\NAKNP\.

PM

```
Np(V) Sorption on Goethite, XO-NpO2, TLM
   25.00 MOLAL  0.000  0.00000E-01
   0 0 1 0 3 0 0 0 1 2 1 1 1
   ACTIVITY   330 29
     0.25
   NAKNP31T.SST      552
   3   1   6
   1.000E+00    50.00 0.800 0.200 81
       330  0.000E-01   -4.00 y                /H+1
       500  1.000E-01   -1.00 y                /Na+1
       492  1.000E-01   -1.00 y                /NO3-1
       552  6.000E-06   -5.22 y                /NpO2+1   <- components
       813  0.000E-01    0.00 y                /ADS1PSIo
       814  0.000E-01    0.00 y                /ADS1PSIb
       815  0.000E-01    0.00 y                /ADS1PSId
       811  1.918E-04   -3.72 y                /ADS1TYP1

     3   1
       330      4.0000      0.0000             /H+1   <- Fixed activity species
     6   3
       813      0.0000      0.0000             /ADS1PSIo
       814      0.0000      0.0000             /ADS1PSIb   <- excluded
       815      0.0000      0.0000             /ADS1PSId

     2   5
   8113300 XOH2+          0.0000    6.0000   0.000   0.000 0.00 0.00 0.00   0.0000
    0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
   0   0.000   0   0.000   0   0.000   0
   8113301 XO-            0.0000  -10.0000   0.000   0.000 0.00 0.00 0.00   0.0000
    0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
   0   0.000   0   0.000   0   0.000   0
   8115000 XONa           0.0000   -7.6400   0.000   0.000 0.00 0.00 0.00   0.0000
    0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
   0   0.000   0   0.000   0   0.000   0
   8114920 XOH2NaN3       0.0000    8.7800   0.000   0.000 0.00 0.00 0.00   0.0000
    0.00 5   1.000 811   1.000 492   1.000 330   1.000 813  -1.000 814   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
   0   0.000   0   0.000   0   0.000   0
   8115520 XONPO2         0.0000   -5.3100   0.000   0.000 0.00 0.00 0.00   0.0000
    0.00 5   1.000 811   1.000 552  -1.000 330  -1.000 813   1.000 814   0.000   0
     0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
```

PM Next is a listing from the MINTEQA2 handbook explaining the input file.

PM Table 1. Line-by-Line description of a typical MINTEQA2 input file.

Line No.	Description
1	Problem Title
2	Problem Title
3	i) Temperature in °C
	ii) Concentration Units
	iii) Fixed ionic strength [see line 4, flag (vii) ISOPT)]

PM

4	i) Flag - Alkalinity (0=Total carbonate specified; 1=alkalinity)
	ii) Flag -
	iii) Flag - Terminate if Charge Imbalance exceeds 30% (0=Yes; 1=No)
	iv) Flag - Print options for solids (0=Ppt only allowed solids; 1=
	v) Flag - Maximum number of iterations (0=40; 1=10; 2=100; 3=200; 4=500)
	vi) Flag -
	vii) Flag - Ionic strength option (0=computed; 1=fixed)
	viii) Flag -
	ix) Flag - Activity coefficient option (0=Debye Huckel; 1=Davies Equation)
	x) Flag - Output options (0=Full; 1=Intermediate; 2=Abbreviated)
	xi) Flag - Sweep Options [0=No sweep; 1=Yes(-log c); 2=Yes(conc)]
	xii) Flag - Number components for spreadsheet (0 to 6)
	xiii) Flag - Type of output to spreadsheet [0=No file; 1=Equil mass %; 2=Equil mass conc (molal); 3=Equil conc(molal)]
5	No line entry if no sweep option (ISWEEP = 0)

PM

Line No.	Description
6	No line entry if no sweep option (ISWEEP = 0)
7	No line entry if no output to spreadsheet (N123 and NTYP123 = 0)
8	No line entry if no output to spreadsheet (N123 and NTYP123 = 0)
9	i) Flag - Model Sorption? (0=No sorption; 1-4 Check for model specific parameters)
	ii) Number of sorption surfaces (0=No sorption; 1-5 maximum)
	iii) Flag - Sorption model (0= No sorption; 1-7 for specific models)
10	No line entry if no sorption model
11	i) Water chemistry - Component ID# (must be in COMP.DBS)
	ii) Total dissolved concentration
	iii) log free activity guess
	iv) Flag - Adjust/Improve guess (N=No; Not N (e.g., blank, Y)=Yes)
	REPEAT (i-iv) FOR N COMPONENTS
	BLANK LINE
12	i) Types (3-6)
	ii) Number of Type (3-6)
13	i) Species/Component ID (Must be in THERMO.DBS/COMP.DBS)
	ii) Equilibrium constant (Log K from THERMO.DBS)
	iii) Enthalpy of reaction (From THERMO.DBS)
	iv) If Type 4, concentration of finite solid
	REPEAT LINES 12-13 for Types (3-6) Type 3 = Fixed activity Type 4 = Finite solids Type 5 = Possible solids Type 6 = Excluded species (e.g., non specified redox couples, infinite solids)
	BLANK LINE

PM After the blank line, the species involved in the surface reaction and the stoichiometry of their reactions are listed. Recorded (in order) is the species ID#, species name, 0.0000, log K value, seven 0.0s, # of components in the reaction, ID# of the components and their stoichiometry, and twelve 0.000 0s.

PM

Reactions considered for Np(V) sorption on Goethite - protonation/deprotonation, anion/cation

PM

$XOH + H^+ \rightleftharpoons XOH_2^+$

$XOH \rightleftharpoons XO^- + H^+$

$XOH + H^+ + ClO_4^- = XOH_2ClO_4$ } Used in TLM not DLM, CCM

$XOH + Na^+ = XONa + H^+$ }

PM

surface reactions

PM

$XOH + NpO_2^+ \rightleftharpoons XONpO_2^0 + H^+$ 0.0

$XOH + NpO_2^+ \rightleftharpoons XOHNpO_2^+$ +0.11

$2XOH + NpO_2^+ \rightleftharpoons (XO)_2NpO_2^- + 2H^+$ -0.11

$XOH + NpO_2^+ + H_2O \rightleftharpoons XONpO_2OH^- + 2H^+$ -0.11

$XOH + NpO_2^+ + H_2O \rightleftharpoons XOHNpO_2OH^0 + H^+$ 0

$XOH + NpO_2^+ + H_2O \rightleftharpoons XOH_2NpO_2OH^+$ +0.11

PM

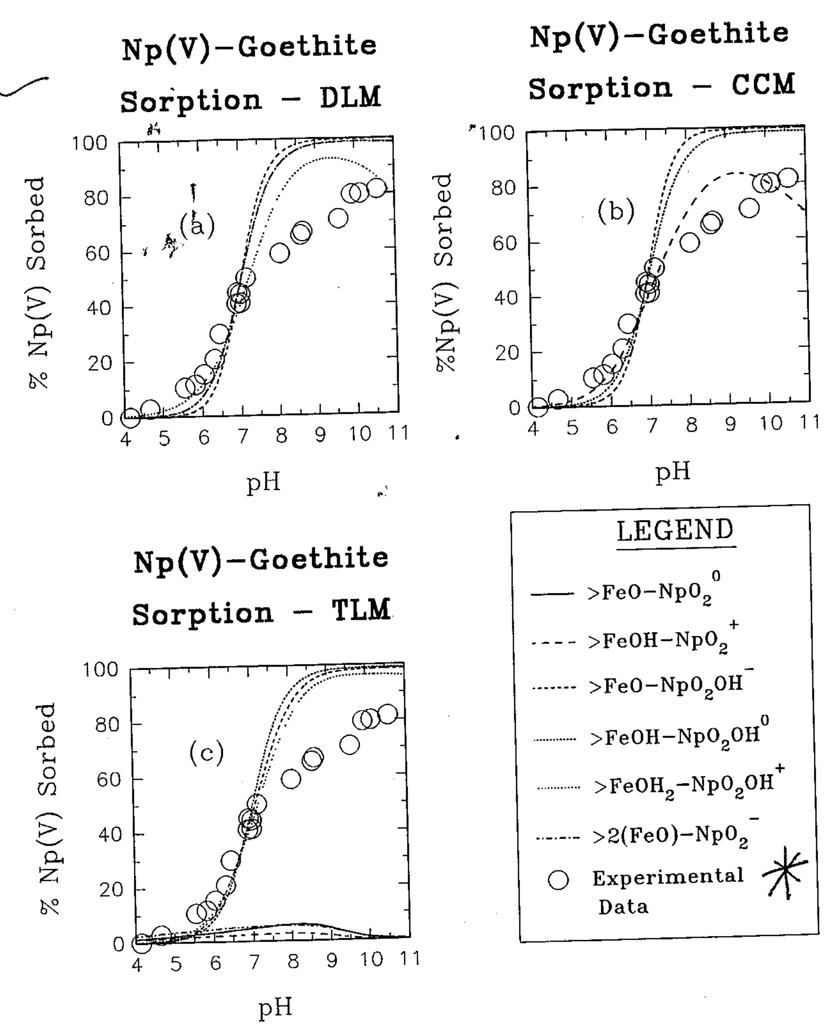
(Numbers written following reactions indicate numerical correction for log K value at ionic strength = 0, used in MINTEQA2 input.)

10/10/94 PM — SIGMAPLOT Graphs of MINTEQA2 Output

PM

A reduced-size copy of the SIGMAPLOT graphs for sorption of Np(V) onto goethite follows.

PM



* - See (*) on pg 13, this notebook
DM 10/13/94

PM

The graphs are saved on a floppy disk (a:\naknp\nknp31all.sp5) and on my PC at c:\FLOPPY\NAKNP\.

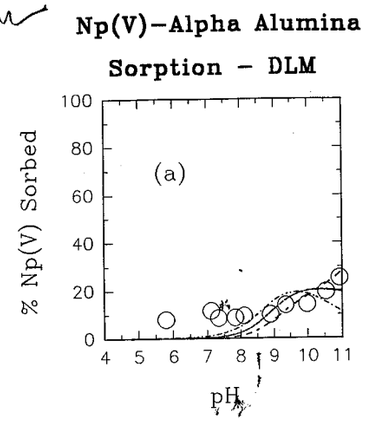
10/13/94PM

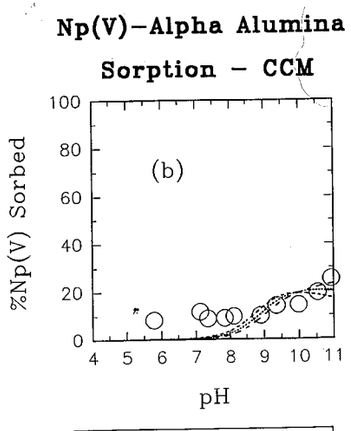
Np(V) sorption data on alpha alumina for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Nakayama and Sakamoto '91. The log K values calculated in FITEQL can be found in scientific notebook # 057, table Binding.N17, page 132. Below is a copy of the MINTEQA2 input file for TLM, species XO-NpO_2.

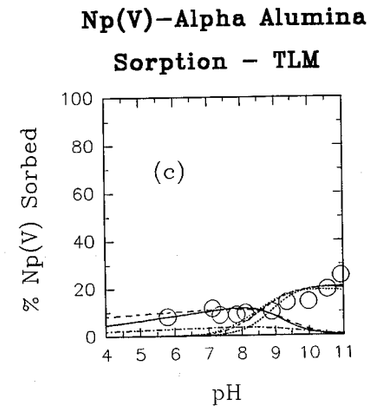
```
Np(V) Sorption on Alpha Alumina, XONpO2, TLM
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 29
  0.25
NAKNP43t.SST     552
3   1   6
1.000E+00   12.00 0.800 0.200 81
    330  0.000E-01   -4.00 y                    /H+1
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    552  6.000E-06   -5.22 y                    /NpO2+1
    813  0.000E-01    0.00 y                    /ADS1PSIo
    814  0.000E-01    0.00 y                    /ADS1PSIb
    815  0.000E-01    0.00 y                    /ADS1PSId
    811  4.600E-05   -4.34 y                    /ADS1TYP1

  3   1
    330      4.0000      0.0000                 /H+1
  6   3
    813      0.0000      0.0000                 /ADS1PSIo
    814      0.0000      0.0000                 /ADS1PSIb
    815      0.0000      0.0000                 /ADS1PSId

  2   5
8113300 XOH2+            0.0000    6.8000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 XO-              0.0000  -10.8000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115000 XONa             0.0000   -7.7300   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8114920 XOH2NO3          0.0000   10.1200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 492   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115520 XONpO2           0.0000   -4.7000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 552  -1.000 330  -1.000 813   1.000 814   0.000   0
 0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

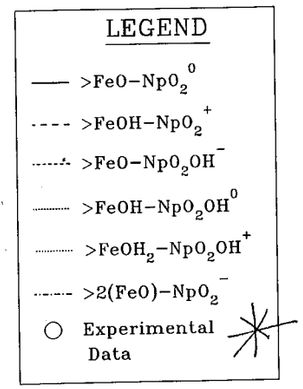
The file is saved on a floppy disk (a:\naknp\naknp43t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\NAKNP\.

A reduced-size copy of the SIGMAPLOT graphs for sorption of NP(V) onto alpha-alumina follows.









The graphs are saved on a floppy disk (a:\naknp\nknp43all.sp5) and on my PC at c:\FLOPPY\NAKNP\.

The experimental data were digitized from Nakayama and Sakamoto '91 (see Scientific Notebook #057 page 155 for complete reference) Figure 3a, Nat'l Goethite plot (Np(V) on goethite) and from Figure 4, α-Al_2O_3 plot (Np(V) on alpha alumina).
The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\NAKAYAMA\TLM*.T31 and *.T43.

10/17/94 PM MINTEQA2 PLOT - U(VI) on GOETHITE

PM U(VI) sorption data on goethite for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Kohler '92. The log K values calculated in FITEQL can be found in scientific notebook # 057, table Binding.U1, page 134. Below is a copy of the MINTEQA2 input file for TLM, species XO-UO_2^+.

PM

```
U(VI) Sorption on Goethite, XOUO2+, TLM

25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 33
  0.25
kohu41t.sst       893
3   1   6
1.000E+00    50.00 0.800 0.200 81
     330  0.000E-01   -2.00 y                    /H+1
     500  1.000E-01   -1.00 y                    /Na+1
     181  1.000E-01   -1.00 y                    /ClO4-
     893  1.000E-06   -6.00 y                    /UO2+2
     813  0.000E-01    0.00 y                    /ADS1PSIo
     814  0.000E-01    0.00 y                    /ADS1PSIb
     815  0.000E-01    0.00 y                    /ADS1PSId
     811  1.918E-04   -3.72 y                    /ADS1TYP1

  3   1
    330      2.0000      0.0000                  /H+1
  6   3
    813      0.0000      0.0000                  /ADS1PSIo
    814      0.0000      0.0000                  /ADS1PSIb
    815      0.0000      0.0000                  /ADS1PSId

  2   5
8113300 XOH2+            0.0000    6.0000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 XO-              0.0000  -10.0000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115000 XONa             0.0000   -7.6400   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8111810 XOH2ClO4         0.0000    8.7800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118930 XOUO2+           0.0000   -3.0900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 893  -1.000 330  -1.000 813   2.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

PM The file is saved on a floppy disk (a:\kohu\kohu41t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\KOHU\.

PM Surface reactions considered for U(VI) sorption on goethite -

corrections

PM $XOH + UO_2^{2+} = XOUO_2^+ + H^+$ +.33

$XOH + UO_2^{2+} = XOHUO_2^{2+}$ +.44

corrections

PM $XOH + UO_2^{2+} + H_2O = XO{\cdot}UO_2OH^0 + 2H^+$ +.22

$XOH + UO_2^{2+} + H_2O = XOHUO_2OH^+ + H^+$ +.33

$XOH + UO_2^{2+} + 2H_2O = XO{\cdot}UO_2(OH)_2^- + 3H^+$ +.11

$XOH + UO_2^{2+} + 2H_2O = XOH{\cdot}UO_2(OH)_2^0 + 2H^+$ +.22

$XOH + UO_2^{2+} - 2H_2O = XOH_2{\cdot}UO_2(OH)_2^+ + 4^-$ +.33

$XOH + UO_2^{2+} + 3H_2O = XOH{\cdot}UO_2(OH)_3^- + 3H^+$ +.11

$XOH + UO_2^{2+} + 3H_2O = XOH_2{\cdot}UO_2(OH)_3^0 + 2H^+$ +.22

$XOH + UO_2^{2+} + 4H_2O = XOH{\cdot}UO_2(OH)_4^{2-} + 4H^+$ 0

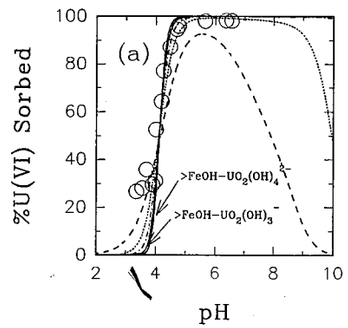
$XOH + UO_2^{2+} + 4H_2O = XOH_2{\cdot}UO_2(OH)_4^- + 3H^+$ +.11

PM Numbers written following reactions indicate numerical correction for log K value at ionic strength = 0, used in MINTEQA2 input.

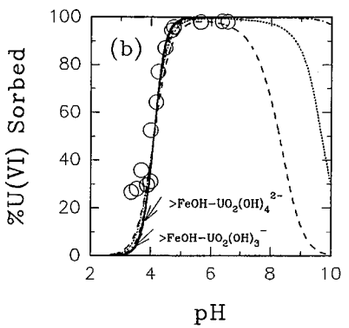
PM A reduced-size copy of the SIGMAPLOT graphs for sorption of U(VI) onto goethite follows.

PM

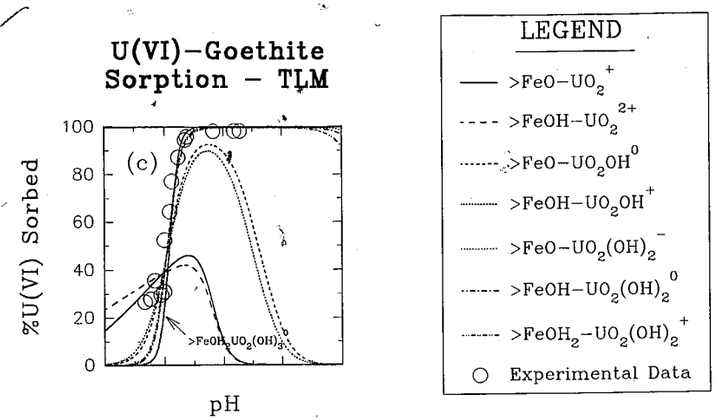
U(VI)–Goethite Sorption – DLM



U(VI)–Goethite Sorption – CCM



TLM next page →



The experimental data were digitized from Kohler '92 Figure 4, p_{CO2} plot. The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\KOHLER\TLM*.T41.

The graphs are saved on a floppy disk (a:\kohu\kou41all.sp5) and on my PC at c:\FLOPPY\KOHU\.

10/19/94 PM MINTEQA2 PLOT Pu(V) on γ ALUMINA

Pu(V) sorption data on gamma alumina for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Righetto et al '91. The log K values calculated in FITEQL can be found in scientific notebook # 123, table Binding5.P2, page 4. Below is a copy of the MINTEQA2 input file for TLM, species XO-PuO_2^0.

```
Sorption of Pu(V) on Gamma Alumina, XO-PuO2, TLM

25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 25
  0.25
rigpu8t.sst      642
3   1   6
2.000E-01  120.00 0.800 0.200 81
    330  0.000E-01   -5.00 y                  /H+1
    500  1.000E-01   -1.00 y                  /Na+1
    181  1.000E-01   -1.00 y                  /ClO4-
    642  2.000E-10   -9.70 y                  /PuO2+1
    813  0.000E-01    0.00 y                  /ADS1PSIo
    814  0.000E-01    0.00 y                  /ADS1PSIb
    815  0.000E-01    0.00 y                  /ADS1PSId
    811  9.205E-05   -4.04 y                  /ADS1TYP1
```


continued from previous page -

```
  3   1
    330      5.0000      0.0000                    /H+1
  6   3
    813      0.0000      0.0000                    /ADS1PSIo
    814      0.0000      0.0000                    /ADS1PSIb
    815      0.0000      0.0000                    /ADS1PSId

  2   5
8113300 XOH2+              0.0000    6.4000   0.000   0.000 0.00 0.00 0.00   0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 XO-                0.0000  -10.4000   0.000   0.000 0.00 0.00 0.00   0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115000 XONa               0.0000   -7.8100   0.000   0.000 0.00 0.00 0.00   0.00   0.0000
 0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8111810 XOH2ClO4           0.0000    8.3300   0.000   0.000 0.00 0.00 0.00   0.00   0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8116420 XOPUO2             0.0000   -2.7700   0.000   0.000 0.00 0.00 0.00   0.00   0.0000
 0.00 5   1.000 811   1.000 642  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

The file is saved on a floppy disk (a:\rigpu\rigpu8t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\RIGPU\.

Surface reactions considered for Pu(V) sorption on gamma alumina -

$$XOH + PuO_2^+ = XO\cdot PuO_2^0 + H^+ \qquad 0$$

$$XOH + PuO_2^+ = XOH\,PuO_2^+ \qquad +.11$$

$$XOH + PuO_2^+ + H_2O = XO\cdot PuO_2OH^- + 2H^+ \qquad -.11$$

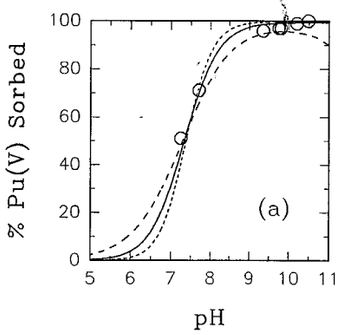
$$XOH + PuO_2^+ + H_2O = XOH\cdot PuO_2OH^0 + H^+ \qquad 0$$

$$XOH + PuO_2^+ + H_2O = XOH_2\cdot PuO_2OH^+ \qquad +.11$$

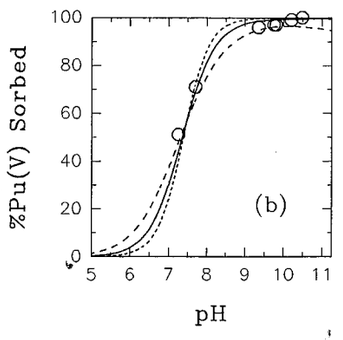
Numbers written following reactions indicate numerical correction for log K value at ionic strength = 0, used in MINTEQA2 input.

A reduced-size copy of the SIGMAPLOT graphs for sorption of Pu(V) onto gamma alumina follows.

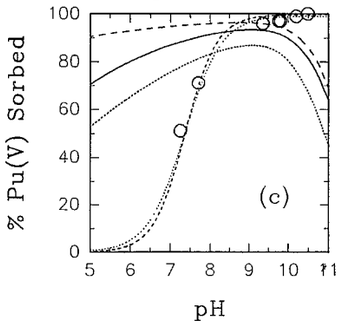
Pu(V)–Gamma Alumina Sorption – DLM



Pu(V)–Gamma Alumina Sorption – CCM



Pu(V)–Gamma Alumina Sorption – TLM



LEGEND

——— $>AlO-PuO_2^0$

- - - - $>AlOH-PuO_2^+$

····· $>AlO-PuO_2OH^-$

····· $>AlOH-PuO_2OH^0$

····· $>AlOH_2-PuO_2OH^+$

○ Experimental Data

The experimental data were digitized from Righetto et al '91 Figure 8, HA = 0 plot. The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\RIGHETTO\TLM\~~*.T81~~ AL203*.T81 10/19/94

The graphs are saved on a floppy disk (a:\rigpu\rigp8c.sp5) and on my PC at c:\FLOPPY\RIGPU\.

10/24/94PM MINTEQA2 PLOT Am(III) on γAl_2O_3

Am(III) sorption data on gamma alumina for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Righetto et al '88. The log K values calculated in FITEQL can be found in scientific notebook # 057, table Binding.A3, page 119. Below is a copy of the MINTEQA2 input file for TLM, species XO-Am^{2+}.

```
Sorption of Am(III) on gamma alumina, XO-Am2+, TLM

25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 25
  0.25
rigam12t.sst   , 40
3   1   6
1.000E-02  120.00 0.800 0.200 81
    330  0.000E-01   -4.00 y                    /H+1
    500  1.000E-01   -1.00 y                    /Na+1
    181  1.000E-01   -1.00 y                    /ClO4-
     40  5.000E-10   -9.30 y                    /Am+3
    813  0.000E-01    0.00 y                    /ADS1PSIo
    814  0.000E-01    0.00 y                    /ADS1PSIb
    815  0.000E-01    0.00 y                    /ADS1PSId
    811  4.600E-06   -5.34 y                    /ADS1TYP1

  3   1
    330      4.0000       0.0000                /H+1
  6   3
    813      0.0000       0.0000                /ADS1PSIo
    814      0.0000       0.0000                /ADS1PSIb
    815      0.0000       0.0000                /ADS1PSId

  2   5
8113300 XOH2+              0.0000    6.4000   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 XO-                0.0000  -10.4000   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8111810 XOH2ClO4           0.0000    8.3300   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115000 XONa               0.0000   -7.8100   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8110400 XOAm+2             0.0000   -1.3600   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5   1.000 811   1.000  40  -1.000 330  -1.000 813   3.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

The file is saved on a floppy disk (a:\rigam\rigam12t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\RIGAM\.

Surface reactions considered for Am(III) sorption on gamma alumina -

corrections

$XOH + Am^{3+} \rightleftharpoons XO{\cdot}Am^{+2} + H^+$ .88

$XOH + Am^{3+} + H_2O \rightleftharpoons XO{\cdot}Am(OH)^+ + 2H^+$ .77

surface reactions continued — corrections

PM

$XOH + Am^{3+} + 2H_2O \rightleftharpoons XOHAm(OH)_2^+ + 2H^+$ ✓ .77

$XOH + Am^{3+} + 2H_2O \rightleftharpoons XO\cdot Am(OH)_2^\circ + 3H^+$ ✓ .66

$XOH + Am^{3+} + 3H_2O \rightleftharpoons XOAm(OH)_3^- + 4H^+$ ✓ .55

$XOH + Am^{3+} + 3H_2O \rightleftharpoons XOHAm(OH)_3^\circ + 3H^+$ .66

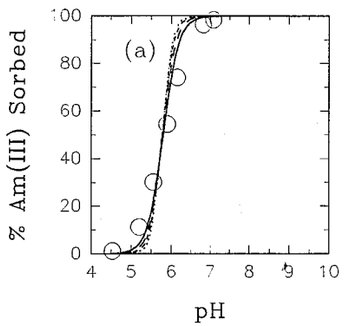
$XOH + Am^{3+} + 3H_2O \rightleftharpoons XOH_2Am(OH)_3^+ + 2H^+$ .77

PM Numbers written following reactions indicate numerical correction for log K value at ionic strength = 0, used in MINTEQA2 input.

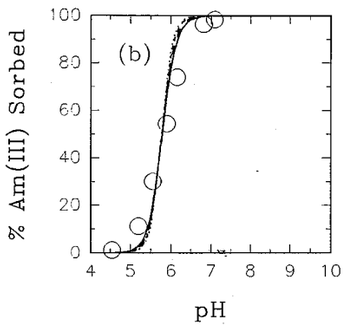
PM A reduced-size copy of the SIGMAPLOT graphs for sorption of ~~Pu(V)~~ onto gamma alumina follows.

Am(III) PM 10/24/94

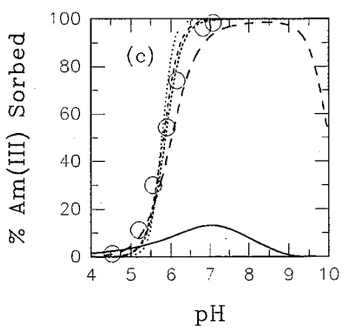
Am(III)–Gamma Alumina Sorption – DLM



Am(III)–Gamma Alumina Sorption – CCM



Am(III)–Gamma Alumina Sorption – TLM



LEGEND

——— >AlO–Am^{2+}

- - - >AlO–$AmOH^+$

------ >AlO–$Am(OH)_2^0$

..... >AlOH–$Am(OH)_2^+$

..... >AlO–$Am(OH)_3^-$

PM The experimental data were digitized from Righetto et al '88 Figure 1, Am(III) plot. The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\RIGHETTO\TLM\AL2O3*.T12.

The graphs are saved on a floppy disk (a:\rigam\rigam12t.sp5) and on my PC at c:\FLOPPY\RIGAM\.

10/31/94 PM MINTEQA2 PLOT Th(IV) on Al_2O_3

PM Th(IV) sorption data on gamma alumina for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Righetto et al '88. The log K values calculated in FITEQL can be found in scientific notebook # 057, table Binding.T1, page 133. Below is a copy of the MINTEQA2 input file for TLM, species XO-Th^{3+}.

PM

```
Th(IV) sorption on gamma alumina, XO-Th+3,TLM
 25.00 MOLAL  0.000  0.00000E-01
 0 0 1 0 3 0 0 0 1 2 1 1 1
 ACTIVITY   330 27
   0.25
 rigthl1t.sst      866
 3   1   6
 1.000E-02  120.00 0.800 0.200 81
     330  0.000E-01    -0.50 y                    /H+1
     500  1.000E-01    -1.00 y                    /Na+1
     181  1.000E-01    -1.00 y                    /ClO4-
     866  1.000E-11   -11.00 y                    /Th+4
     813  0.000E-01     0.00 y                    /ADS1PSIo
     814  0.000E-01     0.00 y                    /ADS1PSIb
     815  0.000E-01     0.00 y                    /ADS1PSId
     811  4.600E-06    -5.34 y                    /ADS1TYP1

 3   1
   330      0.5000      0.0000                    /H+1
 6   3
   813      0.0000      0.0000                    /ADS1PSIo
   814      0.0000      0.0000                    /ADS1PSIb
   815      0.0000      0.0000                    /ADS1PSId

 2   5
8113300 XOH2+              0.0000    6.4000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 XO-                0.0000  -10.4000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118660 XOTH+3             0.0000    2.0100   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 866  -1.000 330  -1.000 813   4.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8111810 XOH2CLO4           0.0000    8.3300   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115000 XONa               0.0000   -7.8100   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 500  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

PM The file is saved on a floppy disk (a:\rigth\rigth11t.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\RIGTH\.

Surface reactions considered for Th(IV) sorption on gamma alumina -

$XOH + Th^{+4} = XOTh^{+3} + H^+$ 1.65

$XOH + Th^{+4} + H_2O = XOThOH^{+2} + 2H^+$ 1.54

$XOH + Th^{+4} + 2H_2O = XOTh(OH)_2^+ + 3H^+$ 1.43

$XOH + Th^{+4} + 2H_2O = XOHTh(OH)_2^{2+} + 2H^+$ 1.54

$XOH + Th^{+4} + 3H_2O \rightleftharpoons XOTh(OH)_3^0 + 4H^+$ 1.32

$XOH + Th^{+4} + 3H_2O \rightleftharpoons XOHTh(OH)_3^+ + 3H^+$ 1.43

$XOH + Th^{+4} + 4H_2O \rightleftharpoons XOTh(OH)_4^- + 5H^+$ 1.21

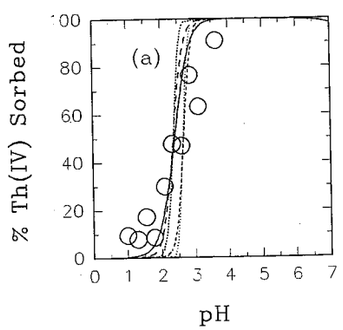
$XOH + Th^{+4} + 4H_2O \rightleftharpoons XOHTh(OH)_4^0 + 4H^+$ 1.32

$XOH + Th^{+4} + 4H_2O \rightleftharpoons XOH_2Th(OH)_4^+ + 3H^+$ 1.43

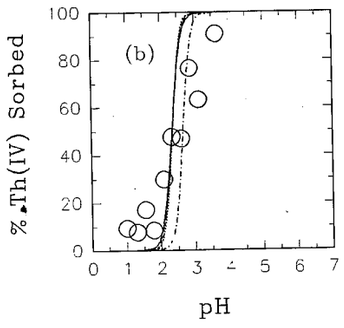
Numbers written following reactions indicate numerical correction for log K value at ionic strength = 0, used in MINTEQA2 input.

A reduced-size copy of the SIGMAPLOT graphs for sorption of Th(IV) onto gamma alumina follows.

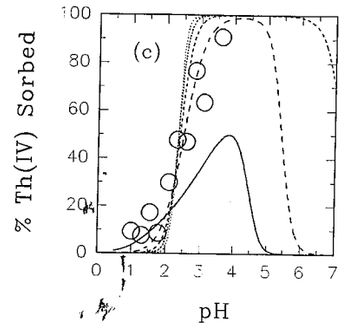
Th(IV)–Gamma Alumina Sorption – DLM

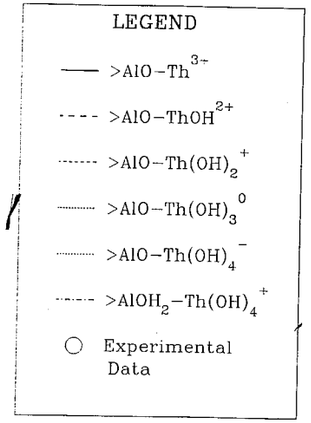


Th(IV)–Gamma Alumina Sorption – CCM



Th(IV)–Gamma Alumina Sorption – TLM





The experimental data were digitized from Righetto et al '88 Figure 1, Th(IV) plot. The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\RIGHETTO\TLM\AL2O3*.T11.

The graphs are saved on a floppy disk (a:\rigth\rigth11d.sp5) and on my PC at c:\FLOPPY\RIGTH\.

11/3/94 PM Waite FITEQL input U(VI) on Quartz

Reference for Waite Data:
Waite, T.D., T.E. Payne, J.A. Davis, and K. Sekine. 1993. Uranium Sorption Modeling - A Surface Complexation Approach. *5th CEC Natural Analogue Working Group Meeting and Alligator River Analogue Project (ARAP) Final Workshop.* H. von Maravic and J. Smellie, eds. Pre-print; to be published in the EUR series. Commission of the European Communities: 83-88.

The Waite data from fig. 2, no fluoride plot, will be entered into FITEQL files and the sorption binding constants for U(VI) on quartz determined. The data was digitized previously (refer to Scientific notebook 057, p. 109) and can be found at C:\floppy\digitizd\ on my PC. Copies of the FITEQL input files for species $XO\text{-}UO_2^+$ and $XOH\text{-}UO_2CO_3^0$, TLM model, follow.

(All FITEQL input files for this data can be found at
K:\TURNER\FITEQL\SORPTION\WAITE\
CCM*.CD2
DLM*.DD2
TLM*.TD2)

file | XOUO2.TDZ

```
              0
              1
              0
              1
              1
             90
              6          1          3          1
00001    0.2    1.66E00    XOH
00160   -1.0    0.00E00    PSI0
00161   -0.5    0.00E00    PSIB
00162   -0.1    0.00E00    PSID
00032   -6.0    1.00E-6    UO2+2
00140   -3.5    3.16E-4    CO2g
00033    0.0    0.00E00    UO2ads
00050    0.0    0.00E00    H+
00003   -1.0    0.00E00    K+
00005   -1.0    0.00E00    NO3-

00050     0.00   050   1
00032     0.00   032   1
00140     0.00   140   1
00100   -13.78   050  -1
03201    -5.43   032   1 050 -1
03202   -10.54   032   1 050 -2
03203   -19.22   032   1 050 -3
03204   -32.59   032   1 050 -4
03205    -2.49   032   2 050 -1
03206    -5.42   032   2 050 -2
03207   -12.37   032   3 050 -4
03208   -16.25   032   3 050 -5
03209   -31.49   032   3 050 -7
03210   -22.83   032   4 050 -7
03211    -8.77   032   1 140   1 050 -2
03212   -19.35   032   1 140   2 050 -4
03213   -30.81   032   1 140   3 050 -6
03214   -51.09   032   3 140   6 050-12
03215   -70.09   032  11 140   6 050-24
03216   -19.28   032   2 140   1 050 -5
03217   -18.11   032   3 140   1 050 -5
03218    -0.05   032   1 005   1
01401   -17.50   140   1 050 -2
01402    -7.61   140   1 050 -1
01403    -1.48   140   1
01050     0.79   001   1 160   1 050   1
01055     4.44   001   1 160   1 161 -1 050   1 005   1
00001     0.00   001   1
01100    -4.79   001   1 160 -1 050 -1
01103    -6.22   001   1 160 -1 161   1 050 -1 003   1
03301    -7.60   001   1 160 -1 161   2 050 -1 032   1 033   1

00004    0.03   100.0   1.0     0.2
0.1     1.0
          1
        3301
          11          1          1          0
          33
5.44e-10
6.23e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07
7.18e-07

8.01e-07
9.14e-07
9.64e-07
9.82e-07
          50
-3.39
-4.04
-4.36
-4.48
-4.72
-4.86
-5.04
-5.18
-5.43
-5.79
-6.22
          1          1
         33       0.08    1.0E-09
         50       0.05    0.0E-00
```

XOHUC1.TDZ

```
              0
              1
              0
              1
              1
             90
              6          2          3          1
00001    0.2    1.66E00    XOH
00160   -1.0    0.00E00    PSI0
00161   -0.5    0.00E00    PSIB
00162   -0.1    0.00E00    PSID
00032   -6.0    1.00E-6    UO2+2
00140   -3.5    3.16E-4    CO2g
00141    0.0    0.00E00    CO3ads
00033    0.0    0.00E00    UO2ads
00050    0.0    0.00E00    H+
00003   -1.0    0.00E00    K+
00005   -1.0    0.00E00    NO3-

00050     0.00   050   1
00032     0.00   032   1
00140     0.00   140   1
00100   -13.78   050  -1
03201    -5.43   032   1 050 -1
03202   -10.54   032   1 050 -2
03203   -19.22   032   1 050 -3
03204   -32.59   032   1 050 -4
03205    -2.49   032   2 050 -1
03206    -5.42   032   2 050 -2
03207   -12.37   032   3 050 -4
03208   -16.25   032   3 050 -5
03209   -31.49   032   3 050 -7
03210   -22.83   032   4 050 -7
03211    -8.77   032   1 140   1 050 -2
03212   -19.35   032   1 140   2 050 -4
03213   -30.81   032   1 140   3 050 -6
03214   -51.09   032   3 140   6 050-12
03215   -70.09   032  11 140   6 050-24
03216   -19.28   032   2 140   1 050 -5
03217   -18.11   032   3 140   1 050 -5
03218    -0.05   032   1 005   1
01401   -17.50   140   1 050 -2
01402    -7.61   140   1 050 -1
01403    -1.48   140   1
01050     0.79   001   1 160   1 050   1
01055     4.44   001   1 160   1 161 -1 050   1 005   1
00001     0.00   001   1
01100    -4.79   001   1 160 -1 050 -1
01103    -6.22   001   1 160 -1 161   1 050 -1 003   1
03301   -10.00   001   1 160   0 161   0 050 -2 032   1 033   1 140   1 141   1

00004    0.03   100.0   1.0     0.2
0.1     1.0
          1
        3301
          11          2          1          0
          33
5.44e-10
6.23e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07

7.18e-07
8.01e-07
9.14e-07
9.64e-07
9.82e-07
         141
5.44e-10
6.20e-08
1.91e-07
2.72e-07
4.12e-07
5.49e-07
7.18e-07
8.01e-07
9.14e-07
9.64e-07
9.82e-07
          50
-3.39
-4.04
-4.36
-4.48
-4.72
-4.86
-5.04
-5.18
-5.43
-5.79
-6.22
          2          1
         33       0.08    1.0E-09
        141       0.08    1.0E-09
         50       0.05    0.0E-00
```

```
quartz00
waite930
1.0E-600
2.31a/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000098
00000100
00000102
00000104
00000106
00000110
00000120
00000122
00000124
00000160
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00000156
00000158
00000159
00000161
00000162
00000163
00000166
00000167
00000168
00000170
00000171
 xouo2
00000180
00000182
00000184
00000185
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00000195
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310

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00000350
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00000520
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00000540
00000550
00000560
00000570
00000580
00000590
00000760
00000770
00000790
```

```
quartz00
waite930
1.0E-600
2.31a/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000097
00000098
00000099
00000100
00000102
00000104
00000106
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00000152
00000154
00000156
00000158
00000159
00000161
00000162
00000163
00000166
00000167
00000168
00000170
00000171
 xohuc1
00000180
00000182
00000184
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00000195
00000230
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00000270
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00000290
00000300

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00000360
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00000380
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00000410
00000420
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00000470
00000480
00000490
00000500
00000510
00000520
00000530
00000540
00000550
00000560
00000570
00000580
00000590
00000760
00000770
00000780
00000790
```

FITEQL notes:

In the procedures section of Waite's paper, the mixtures used were mixed and monitored in open polypropylene tubes. This was accounted for in the FITEQL input files by considering $CO_2(g)$ and setting the $CO_2(g)$ concentration equal to 3.16E-4 M.

Pyro-SiO_2 site density, capacitance, and log K values were used in the quartz model. The specific surface area was set at 0.03 m^2/g.

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: quartz A_{sp}: 0.03 m^2/g Data Source: Waite 93 Concentration: [U(VI)] = 1e-6 M					Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): Abs Error (radionuclide): 1.0e-9			Ionic Strength (electrolyte): 0.1 M $KClO_4$ N_s = 2.31 sites/nm^2		
[quartz] = 100 g/L		DLM Log K_+ = Log K_- = -7.10			CCM Log K_1 = Log K_2 = -7.05			TLM Log K_1 = 0.79 Log K_2 = -4.79 Log K_{Co} = -6.22 Log K_{As} = 4.44		
		Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	XOUO2	-7.631	3.785	.02531	-7.977	1.544	.02830	-10.40	142.7	.1047
$XOH\text{-}UO_2^{2+}$	XOHUO2	-5.741	20.50	.02149	-6.379	3.780	.02705	-7.607	142.7	.1047
$XO\text{-}UO_2OH^0$	XOUO2OH	-9.545	1.406	.03161	-9.573*	.6012	.04042	-10.28	20.16	.02663
$XOH\text{-}UO_2OH^+$	XOHUO2OH	-7.631	3.785	.02531	-7.977	1.544	.02830	-7.795	59.59	.01984
$XO\text{-}UO_2(OH)_2^-$	XOUO2OH2	-11.48	3.731	.03465	-11.09	1.781	.03191	-12.32	1.515	.02988
$XOH\text{-}UO_2(OH)_2^0$	XOHUO2OH2	-9.545	1.406	.03161	-9.573*	.6012	.04042	-9.533	1.510	.02990
$XOH_2\text{-}UO_2(OH)_2^+$	XOH2UO2OH2	-7.631	3.785	.02531	-7.977	1.544	.02830	-6.743	1.518	.02982
$XOH\text{-}UO_2(OH)_3^-$	XOHUOOH3	-11.48	3.731	.03465	-1.109	1.781	.03191	-11.54	11.53	.04440
$XOH_2\text{-}UO_2(OH)_3^0$	XOH2UOH3	-9.545	1.406	.03161	-9.573*	.6012	.04042	-8.755	11.50	.04429
$XOH\text{-}UO_2(OH)_4^{2-}$	XOHUOOH4	-13.39	6.791	.03976	-12.58	1.525	.03442	-13.62	21.61	.06092
$XOH_2\text{-}UO_2(OH)_4^-$	XOH2UOH4	-11.48	3.731	.03465	-11.09	1.781	.03191	-10.83	21.58	.06098
$XOH\text{-}UO_2CO_3^0$	XOHUC1	-6.043	1.319	.02235	-6.037	1.539	.02077	-6.018	1.428	.02113
$XOH_2\text{-}UO_2(CO_3)_2^-$	XOH2UC2	-5.017	35.75	.02277	-4.569	27.16	.02055	-5.759	24.12	.01908
$XOH_2\text{-}UO_2(CO_3)_3^{3-}$	XOH2UC3	-6.947	98.31	.03181	-4.669	56.61	.02304	-8.273	48.89	.01740
$XOH_2\text{-}(UO_2)_2CO_3(OH)_3^-$	XOH2UCO	-8.847*	11.15	.05515	-8.975**	1.901	.1816	-8.656	18.96	.04576

BINDINGU.36

* ERROR FOR RADIONUCLIDE = 1E-8
** ERROR FOR BOTH RADIONUCLIDE AND CO_3ads =1E-8

Surface rxns for U(VI) on quartz are listed in this notebook, pages 14-15 PLUS the following rxn's, as CO_2 was present (corrections for log K values at ion. strength = 0 to be used in MINTEQA2 input, follow):

$XOH + UO_2^{2+} + CO_2 + H_2O = XOHUO_2CO_3^0 + 2H^+$		+.22
$XOH + UO_2^{2+} + 2CO_2 + 2H_2O = XOH_2UO_2(CO_3)_2^- + 3H^+$		+.11
$XOH + UO_2^{2+} + 3CO_2 + 3H_2O = XOH_2UO_2(CO_3)_3^{-3} + 5H^+$		-.11
$XOH + 2UO_2^{2+} + CO_2 + 4H_2O = XOH_2(UO_2)_2(CO_3)(OH)_3^0 + 4H^+$		+.44

11/8/94 PM

U(VI) sorption data on quartz for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Waite et al '93. The log K values calculated in FITEQL can be found in the above table BindingU.36.

11/4/94 DM

DM Below is a copy of the MINTEQA2 input file for TLM, species XO-UO_2^+ and species XOH-$UO_2CO_3^0$.

```
DM U(VI) sorption on quartz, XO-UO2+, TLM
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 20
  0.25
waitet.sst        893
3   1   6
1.000E+02  0.0300 0.800 0.200 81
    330  0.000E-01   -3.00 y                    /H+1
    410  1.000E-01   -1.00 y                    /K+1
    181  1.000E-01   -1.00 y                    /ClO4-
    893  1.000E-06   -6.00 y                    /UO2+2
    140  0.000E-01  -16.00 y                    /CO3-2
    813  0.000E-01    0.00 y                    /ADS1PSIo
    814  0.000E-01    0.00 y                    /ADS1PSIb
    815  0.000E-01    0.00 y                    /ADS1PSId
    811  1.660E+00    0.22 y                    /ADS1TYP1

  3   2
3301403    21.6603    -0.5300                  /CO2 (g)
    330     3.0000     0.0000                  /H+1
  6   3
    813     0.0000     0.0000                  /ADS1PSIo
    814     0.0000     0.0000                  /ADS1PSIb
    815     0.0000     0.0000                  /ADS1PSId

  2   5
8113300 xoh2+          0.0000    0.9000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 xo-            0.0000   -4.9000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8111810 xoh2clo4       0.0000    4.6600   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8114100 xoK            0.0000   -6.2200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 410  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118930 xouo2+         0.0000  -10.0700   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 893  -1.000 330  -1.000 813   2.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

U(VI) sorption on quartz, XOH-UO2CO3, TLM

25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 20
  0.25
waitet.sst        893
3   1   6
1.000E+02  0.0300 0.800 0.200 81
    330  0.000E-01   -3.00 y                    /H+1
    410  1.000E-01   -1.00 y                    /K+1
    181  1.000E-01   -1.00 y                    /ClO4-
    893  1.000E-06   -6.00 y                    /UO2+2
    140  0.000E-01  -16.00 y                    /CO3-2
    813  0.000E-01    0.00 y                    /ADS1PSIo
    814  0.000E-01    0.00 y                    /ADS1PSIb
    815  0.000E-01    0.00 y                    /ADS1PSId
    811  1.660E+00    0.22 y                    /ADS1TYP1

  3   2
3301403    21.6603    -0.5300                  /CO2 (g)
    330     3.0000     0.0000                  /H+1
  6   3
    813     0.0000     0.0000                  /ADS1PSIo
    814     0.0000     0.0000                  /ADS1PSIb
    815     0.0000     0.0000                  /ADS1PSId

  2   5
8113300 xoh2+          0.0000    0.9000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 xo-            0.0000   -4.9000   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

continued next page


```
8111810 xoh2clo4       0.0000    4.6600   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 181   1.000 330   1.000 813  -1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8114100 xoK            0.0000   -6.2200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 410  -1.000 330  -1.000 813   1.000 814   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118931 xohuc1         0.0000   12.3600   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 893   1.000 140   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

DM The file is saved on a floppy disk (a:\waite\waitet.tlm for input, .sst for spreadsheet-importable output) and on my PC at c:\FLOPPY\WAITE\.

CO_2 Equation Conversion to CO_3^{2-} Form:

DM To convert the surface reactions involving CO_2 to a form useable by MINTEQa2, the following procedure is used -

1 Take equation to be converted:

$$XOH + UO_2^{2+} + CO_2 + H_2O = XOHUO_2CO_3^0 + 2H^+$$

2 Add carbon dioxide / carbonate reaction so that the CO_2 is canceled (multiply stoichiometric coefficients if necessary):

$$XOH + UO_2^{2+} + CO_2 + H_2O = XOHUO_2CO_3^0 + 2H^+$$
$$+ \quad CO_3^{2-} + 2H^+ = H_2O + CO_2$$
$$XOH + UO_2^{2+} + CO_3^{2-} = XOHUO_2CO_3^0$$

3 Find the associated log K value by correcting the surface reaction's log K value to ionic strength 0 and adding the carbonate / carbon dioxide log K value (remember to multiply the CO_3^{2-} / CO_2 log K value as well if the equation 's stoichiometric coefficients were multiplied):

(CCM) log K for $XOHUO_2CO_3^0$ @ I = 0.1 = -6.04

" " " @ I = 0.0 = -5.78

" " CO_3^{2-} @ I = 0.0 = 18.16 +

12.38

Using this method, the other three carbonate equations become

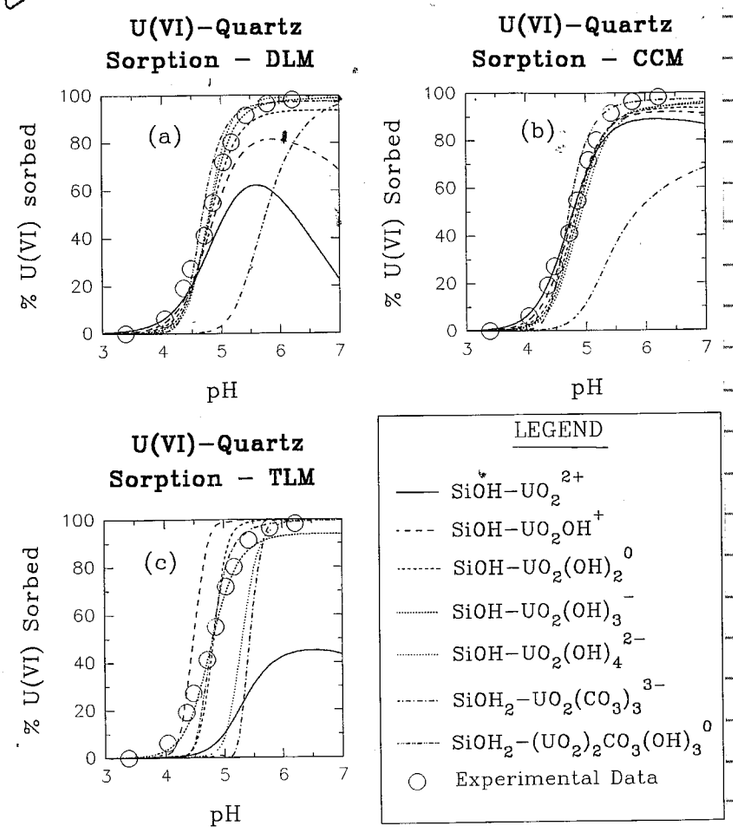
$XOH + UO_2^{2+} + 2CO_3^{2-} + H^+ = XOH_2UO_2(CO_3)_2^-$, log K = 31.86

$XOH + UO_2^{2+} + 3CO_3^{2-} + H^+ = XOH_2UO_2(CO_3)_3^{-3}$, log K = 49.70

$XOH + 2UO_2^{2+} + CO_3^{2-} + 3H_2O = XOH_2(UO_2)_2(CO_3)(OH)_3^0 + 2H^+$, log K = 9.62

DM A reduced-size copy of the SIGMAPLOT graphs for sorption of U(VI) onto quartz follows.

DM The graphs are saved on a floppy disk (a:\waite\waitec.sp5) and on my PC at c:\FLOPPY\WAITE\.



The experimental data were digitized from Waite et al '93 Figure 2, no fluoride plot. The data can be found in the FITEQL input files K:\TURNER\FITEQL\SORPTION\WAITE\TLM*.TDZ.

11/26/94 Sorption of U(VI) on Hydrated TiO2

FITEQL files for Lieser'88 data

The Lieser data (see notebook 057, p. 154 for journal reference) will be entered into FITEQL input files and the associated sorption binding constants determined.

Experimental data are from Lieser '88, Fig. 1, no NaCl plot (Ionic strength = 0). ← See "Lieser '88 Data" p 31 this notebook 12/29/97

TiO_2 anatase specific surface area and protonation/deprotonation K values were used to model the hydrous TiO_2.

12/1/94

All FITEQL input files for this data can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.C12
DLM*.D12
TLM*.T12.
A copy of the FITEQL input file for species XO-UO_2^+, tlm follows.

file XOUO2.T12

```
TiO2
Lieser88
2.10e-6M
2.3si/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098
00000100
00000102
00000110
00000120
00000124
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000139
00000140
00000145
00000150
xouo2
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240
0
1
0
0
1
90
5          1          1          1
00001  -3.32  4.79E-4  XOH
00160  -1.0   0.00E00  PSI0
00161  -0.5   0.00E00  PSIB
00162  -0.1   0.00E00  PSID
00032  -5.68  2.10E-6  UO2+2
00033   0.0   0.00E00  UO2ads
00050   0.0   0.00E00  H+

00050    0.00  050  1
00032    0.00  032  1
03201   -5.43  032  1 050 -1
03202  -10.54  032  1 050 -2
03203  -19.22  032  1 050 -3
03204  -32.59  032  1 050 -4
03205   -2.49  032  2 050 -1
03206   -5.42  032  2 050 -2
03207  -12.37  032  3 050 -4
03208  -16.25  032  3 050 -5
03209  -31.49  032  3 050 -7
03210  -22.83  032  4 050 -7
00100  -13.90  050 -1
01050    4.10  001  1 160  1 050  1
01100   -8.10  001  1 160 -1 050 -1
00001    0.00  001  1
03301    2.90  001  1 160 -1 161  2 050 -1 032  1 033  1


00004  125.0  1.0000  0.8   0.2
0.1    1.0
         1
      3301
        15          1          1          0
        33
1.39E-07
3.61E-07
2.95E-07
1.11E-06
1.83E-06
2.04E-06
2.07E-06
2.07E-06
2.04E-06
2.01E-06
1.97E-06
1.84E-06
1.72E-06
1.53E-06
1.10E-06
        50                                                    00000680
-2.10471
-2.51204
-2.66965
-3.37188
-4.47882
-5.61912
-6.39083
-6.87382

-8.01290
-8.65409
-8.82398
-9.12555
-9.81008
-10.01171
-10.50193
         1          1
        33       0.10    2.1E-09                              00001170
        50       0.05    0.0E-00                              00001180
                                                              00001190
```

12/6/94 DM

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{sp}: 125 m^2/g Data Source: Lieser et al, 88 Concentration: [U(VI)] = 2.1e-6 M					Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09			Ionic Strength (electrolyte): 0 N_s = 2.31 sites/nm^2		
		DLM Log K_+ = 5.37 Log K_- = -5.92 (TiO_2 anatase)			CCM Log K_+ = 5.24 Log K_- = -6.96			TLM Log K_1 = 4.10 Log K_2 = -8.10 Log $K_{1/2}$ = not used Log K_{ex} =		
		Log K	V_x	$\sigma_{\log K}$	Log K	V_x	$\sigma_{\log K}$	Log K	V_x	$\sigma_{\log K}$
$XO\text{-}UO_2^+$	xouo2	2.966E+00	1.311E+01	3.917E-02	2.791E+00	1.018E+01	5.077E-02	1.982E+00	1.016E+01	3.395E-02
$XOH\text{-}UO_2^{2+}$	xohuo2	7.810E+00	2.293E+01	3.833E-02	8.411E+00	8.715E+00	3.502E-02	7.318E+00	3.085E+01	3.257E-02
$XO\text{-}UO_2OH^0$	xouo21	-2.199E+00	1.488E+01	6.053E-02	-4.931E+00	2.465E+01	7.865E-02	-3.091E+00	1.236E+01	4.733E-02
$XOH\text{-}UO_2OH^+$	xohuo21	2.966E+00	1.311E+01	3.918E-02	2.790E+00	1.018E+01	5.079E-02	3.257E-02	4.838E+00	3.911E-02
$XO\text{-}UO_2(OH)_2^-$	xouo22	-1.102E+01	2.787E+01	8.192E-02	-1.185E+01	2.986E+01	8.333E-02	-1.215E+01	3.073E+01	8.115E-02
$XOH\text{-}UO_2(OH)_2^0$	xohuo22	-2.199E+00	1.488E+01	6.052E-02	-4.931E+00	2.465E+01	7.865E-02	-5.220E+00	2.495E+01	7.644E-02
$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo22	2.966E+00	1.311E+01	3.918E-02	2.790E+00	1.018E+01	5.079E-02	2.561E+00	1.048E+01	5.023E-02
$XOH\text{-}UO_2(OH)_3^-$	xohuo23	-1.102E+01	2.787E+01	8.192E-02	-1.185E+01	2.986E+01	8.333E-02	-1.264E+01	3.311E+01	7.625E-02
$XOH_2\text{-}UO_2(OH)_2^+$	xoh2uo23	-2.199E+00	1.488E+01	6.053E-02	-4.931E+00	2.465E+01	7.865E-02	-5.616E+00	2.781E+01	8.168E-02
$XOH\text{-}UO_2(OH)_4^{2-}$	xohuo24	-1.185E+01	1.923E+01	7.260E-02	-1.879E+01	3.424E+01	7.672E-02	-1.232E+01	1.630E+01	5.859E-02
$XOH_2\text{-}UO_2(OH)_4^-$	xoh2uo24	-1.102E+01	2.787E+01	8.192E-02	-1.185E+01	2.986E+01	8.333E-02	-1.285E+01	3.628E+01	9.022E-02
$XOH\text{-}UO_2CO_3^-$										
$XOH_2\text{-}UO_2(CO_3)_2^{3-}$										
$XOH_2\text{-}UO_2(CO_3)_3^{5-}$										

BINDING.U39

12/22/94 PM MINTEQA2 I/O for Lieser Data

U(VI) sorption data on hydrated TiO_2 for ccm, dlm, and tlm models was generated in MINTEQA2 using log K values calculated in FITEQL and experimental parameters from Lieser '88. The log K values calculated in FITEQL can be found in the above table.

Because this experiment was run with no background electrolyte, the MINTEQA2 input files for the $TiO\text{-}UO_2(OH)_2^-$, $TiOH\text{-}UO_2(OH)_2^0$, and $TiOH_2\text{-}UO_2(OH)_2^+$ were modified to exclude the charge component ADS1PSIb, component #814; without this change, the program cannot converge on a value for ADS1PSIb and the MINTEQA2 run is aborted for these species' calculations.

Below is a copy of the MINTEQA2 input file for TLM, species $TiOH\text{-}UO_2(OH)_2^0$.

```
U(VI) Sorption on hydrous TiO2, XOH-UO2(OH)2, TLM

25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 1 1 1
ACTIVITY   330 37
  0.25
liesert.sst      893
3   1   6
1.000E+00  125.00 0.800 0.200 81
     330  0.000E-01   -2.00 y                /H+1
     893  2.100E-06   -5.68 y                /UO2+2
     813  0.000E-01    0.00 y                /ADS1PSIo
     815  0.000E-01    0.00                  /ADS1PSId
     811  4.794E-04   -3.32 y                /ADS1TYP1
```


input file continued—

```
3   1
    330     2.0000     0.0000                    /H+1

6   2
    813     0.0000     0.0000                    /ADS1PSIo

    815     0.0000     0.0000                    /ADS1PSId

  2   3
8113300 xoh2+            0.0000    4.1000    0.000    0.000 0.00
 0.00 0.00    0.0000
  0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000
 0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0.000    0
 0  0.000    0    0.000    0    0.000    0
8113301 xo-              0.0000   -8.1000    0.000    0.000 0.00
 0.00 0.00    0.0000
  0.00 3    1.000 811   -1.000 330   -1.000 813    0.000    0    0.000
 0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0.000    0
 0  0.000    0    0.000    0    0.000    0
8118930 xohuo22          0.0000   -5.2200    0.000    0.000 0.00
 0.00 0.00    0.0000
  0.00 4    1.000 811    1.000 893   -2.000 330    2.000 002    0.000
 0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0.000    0
 0  0.000    0    0.000    0    0.000    0
```

PC NOTE:

My 486 66Mhz IBM compatible will not run MINTEQA2 from inside a WIN DOS window; Windows must be exited to free up enough memory for the I/O record buffer.
In WIN, the free conventional mem = 449 K
total = 1473 K.

Out of WIN, the free conventional mem = 457 K
total = 21,931 K.

12/29/94 PM

Lieser '88 Data:

Given that the g/L concentration = 1.0 and the A_{sp} (from TiO_2 anatase) = 125.0 m^2/g, then

$$[TiOH] = \frac{2.31*125.0*1.0*(1exp18)}{6.023exp23}$$

[TiOH] = 4.794e-4, and log[TiOH] = -3.319.

To transform the Lieser '88 data for use in FITEQL, the following equation was used:

$$S = \frac{K_d * \frac{C_s}{1000} * C_{tot}}{1 + (K_d * \frac{C_s}{1000})}$$

next page →

- continued from previous page -

2/29/94 PM

This is used to calculate the total U(VI) sorbed from the log of the sorption ratio values (R_s) plotted in the source paper.
R_s is assumed equal to K_d, $K_d = S/C_{tot}$, S = concentration of the metal that is bound to the surface, C_{tot} = total dissolved metal at equilibrium, and C_s = concentration of the solid (hydrous TiO_2, here) in g/L.

1/3/95 PM

PM

The MINTEQA2 files are saved on a floppy disk (b:\lieser\t\liesert.tlm or ...\d*.dlm or ...\c*.ccm for input, .sst for spreadsheet-importable output) and on my PC at c:\floppy\lieser\t\ or ...\d\ or ...\c\.

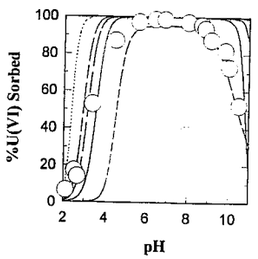
PM

A reduced-size copy of the SIGMAPLOT graphs for sorption of U(VI) onto hydrous TiO_2 follows.

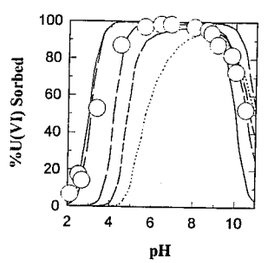
The graphs are saved on a floppy disk (a:\lieser\lieseral.spw) and on my PC at c:\floppy\lieser\.

PM

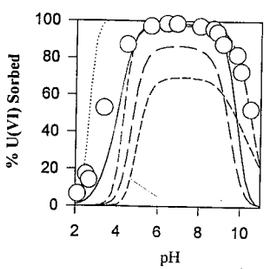
U(VI) Sorption on Hydrous TiO_2
DLM

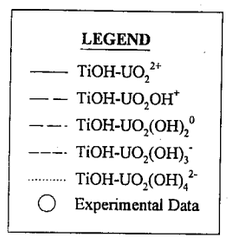


U(VI) Sorption on Hydrous TiO_2
CCM



U(VI) Sorption on Hydrous TiO_2
TLM





1/11/95 PM Lieser (1988) I=0 FITEQL output - modified

PM

The Lieser (1988) I=0 input files were modified. Dr. David Turner readjusted the log K values for the protonation/deprotonation reactions for TiO_2 anatase, CCM, which now are set to 6.75 and -5.71 for I=0. Also, the log K values for the chemical reactions were rechecked and corrected to I = 0 as necessary. The CCM and DLM input files now give ???????? as convergence values. The TLM files still give actual numerical values, as listed in the table below.

PM

	TLM Log K_+ = 4.10 Log K_- = -8.10 Log K_{cat} = not used Log K_{an} = " "		
	Log K	V_Y	$\sigma_{Log\ K}$
$XO\text{-}UO_2^+$	3.49	12.8	.0493
$XOH\text{-}UO_2^{2+}$	7.43	24.4	.0974
$XO\text{-}UO_2OH^\circ$	-5.20	25.0	.0772
$XOH\text{-}UO_2OH^+$	0.97	24.9	.0808
$XO\text{-}UO_2(OH)_2^-$	-11.25	24.9	.0795
$XOH\text{-}UO_2(OH)_2^\circ$	-2.65	8.9	.0485
$XOH_2\text{-}UO_2(OH)_2^+$	0.95	24.9	.0795
$XOH\text{-}UO_2(OH)_3^-$	-11.23	24.9	.0808
$XOH_2\text{-}UO_2(OH)_3^\circ$	-5.20	25.0	.0772
$XOH\text{-}UO_2(OH)_4^{2-}$	-16.97	24.4	.0973
$XOH_2\text{-}UO_2(OH)_4^-$	-11.15	24.8	.0847

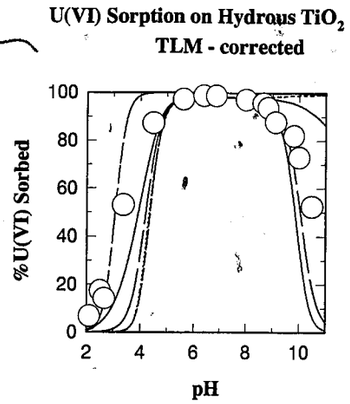
PM

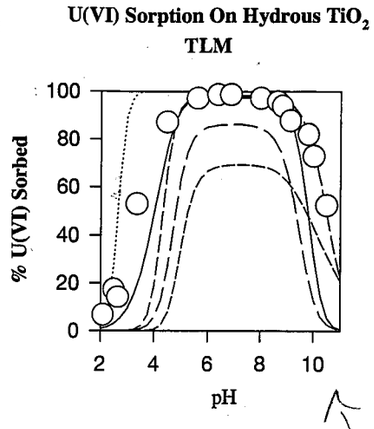
Due to memory allocation problems, my PC cannot run FITEQL using the FIT2DIM executable as the FORTRAN compiler when installed keeps Windows from loading. I ran the Lieser I=0 CCM input files with the compiler installed and with FIT2DIM, and got the following error message:

```
NDP error - invalid number, INTEGER overflow, or 0/0 (See Sectio:
4.2.1 in
 Lahey Programmer's Reference) in simq
Called by solvex
Called by fiteql2
```

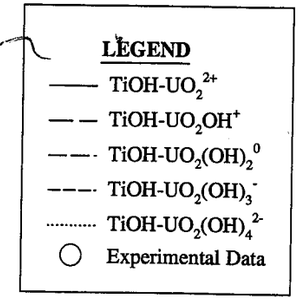
FIT2 will be used for future FITEQL input until FIT2DIM is accessible through my PC.

The corrected Log K values were entered into the Lieser.tlm MINTEQA2 file + the resulting % U(VI) sorbed plotted vs pH. These are saved at C:\floppy\lieser\lieseral.spw. The plots are shown on the next page





(same as TLM plot p 32 PM 1/11/95)



1/17/95 PM Lieser '88 Fig 1, I=0.5 FITEQL input

The Lieser data for figure 1, I = 0.5 M plot (see notebook 057, p. 154 for journal reference) will be entered into FITEQL input files and the associated sorption binding constants determined.

All FITEQL input files for Fig. 1, I = 0.5 M can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.C~~3b~~15
DLM*.D~~3b~~15
TLM*.T~~3b~~.15

and at C:\floppy\lieser\c\fig1i5\.c15
\d\ \.d15
\t\ \.t15.

PM 1/17/95

A copy of the FITEQL input file for species XOH_2-$UO_2(OH)_2^+$, tlm follows.

file XOH2UO22.T15

```
                                                                                TiO2
                                                                                Lieser88
                                                                                2.10e-5M
                                                                                2.3mi/nm
                                                                                00000050
                                                                                00000060
                                                                                00000070
                                                                                00000080
                                                                                00000090
                                                                                00000092
                                                                                00000094
                                                                                00000098
                                                                                00000100
                                                                                00000102
00001   -3.32   4.79E-4   XOH
00160   -1.0    0.00E00   PSI0
00161   -0.5    0.00E00   PSIB
00162   -0.1    0.00E00   PSID
00032   -5.68   2.10E-6   UO2+2
00033    0.0    0.00E00   UO2ads
00050    0.0    0.00E00   H+
00003   +0.3    0.00E00   Na+
00005   -0.3    0.00E00   Cl-

00050    0.00   050  1                                                         00000110
00032    0.00   032  1                                                         00000120
03201    -5.51  032  1 050 -1                                                  00000124
03202   -10.62  032  1 050 -2                                                  00000126
03203   -19.22  032  1 050 -3                                                  00000127
03204   -32.43  032  1 050 -4                                                  00000128
03205    -7.41  032  2 050 -1                                                  00000129
03206    -5.94  032  2 050 -2                                                  00000130
03207   -12.53  032  3 050 -4                                                  00000131
03208   -16.49  032  3 050 -5                                                  00000132
03209   -31.65  032  3 050 -7                                                  00000133
03210   -23.15  032  4 050 -7                                                  00000134
03211    +0.44  032  1 005  1                                                  00000135
03212    -2.03  032  1 005  2
00100   -13.70  050 -1                                                         00000139
01200     6.83  001  1 050  1 005 1                                           00000140
01300    -4.59  001  1 003  1 050 -1                                          00000145
01050     3.95  001  1 160  1 050  1                                          00000130
01100    -7.95  001  1 160 -1 050 -1                                          xoh2uo22
00001     0.00  001  1                                                        00000174
03307     1.00  001  1 160  1 161  0 050 -1 032  1 033  1                     00000175
                                                                             00000180
                                                                             00000185
00004  125.0  1.0000  0.8   0.2                                              00000190
0.5     1.0                                                                  00000195
          1                                                                  00000230
       3307                                                                  00000240
         13          1         1        0
         33
4.68E-07
1.61E-06
2.02E-06
2.05E-06
2.05E-06
2.06E-06
2.06E-06
2.07E-06
2.05E-06
1.98E-06
1.21E-06
9.83E-07
4.49E-07
         50                                                                  00000680
-2.66811
-3.86925
-5.39494
-5.50664
-5.71913
-6.46766
-7.23684
-7.43317
-7.81362
-8.12716
-9.01871
-9.60241
-10.01416
          1         1                                                       00001170
         33    0.10   2.1E-09                                               00001180
         50    0.05   0.0E-00                                               00001190
```

2/3/95 PM

Notes for Lieser FITEQL input files:

TiO_2 anatase specific surface area and protonation/deprotonation K values were used to model the hydrous TiO_2. NOTE: New values for the CCM log K_+ and log K_- were extrapolated; log K_+ = 6.60 and log K_- = -5.56 for I = 0.5 M.

The sorption binding constant table for figure 1, I = 0.5 M (BINDING.U38) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

table BINDING.U38

Uranium (VI) Sorption Binding Constants
Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{sp}: 125 m^2/g Data Source: Lieser et. al. (1988) Concentration: [U(VI)] = 2.1e-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09	Ionic Strength (electrolyte): 0.5 M NaCl N_s = 2.31 sites/nm^2 M/V = 1.00g/L

No CO_2 fig 1, I = 0.5 plot	DLM Log K_+ = 5.37 Log K_- = -5.92 (TiO_2 anatase)			CCM Log K_+ = 6.64 Log K_- = -5.60			TLM Log K_+ = 4.10 Log K_- = -8.10 Log K_{Cat} = -4.59 Log K_{An} = 7.13		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}UO_2^+$	3.34	11.5	.0566	n.c.			4.30	24.7	.0665
$XOH\text{-}UO_2^{2+}$	7.80	23.5	.0604	n.c.			7.38	57.8	.0615
$XO\text{-}UO_2OH^0$	-3.84	12.9	.0544	n.c.			-1.77	11.9	.0563
$XOH\text{-}UO_2OH^+$	3.34	11.5	.0566	n.c.			4.31	24.5	.0664
$XO\text{-}UO_2(OH)_2^-$	-11.89	21.3	.0378	n.c.			-11.54	21.4	.0409
$XOH\text{-}UO_2(OH)_2^0$	-3.84	12.9	.0544	n.c.			-1.80	12.1	.0556
$XOH_2\text{-}UO_2(OH)_2^+$	3.34	11.5	.0566	n.c.			4.34	24.3	.0672
$XOH\text{-}UO_2(OH)_3^-$	-11.89	21.3	.0378	n.c.			-11.56	21.8	.0406
$XOH_2\text{-}UO_2(OH)_3^0$	-3.84	12.9	.0544	n.c.			-1.81	12.3	.0559
$XOH\text{-}UO_2(OH)_4^{2-}$	-20.01	80.2	.0366	n.c.			-21.35	81.26	.0463
$XOH_2\text{-}UO_2(OH)_4^-$	-11.89	21.3	.0378	n.c.			-11.56	22.4	.0410

n.c. : FITEQL optimization did not converge.
log K values are at I = 0
table binding.u38

* t15 files were run on D. Turner's computer using the FIT2DM executable.

2/7/95

Fig 3 data is a curve- it has no plotted data points. 2/7/95

The Lieser data for figure 3, plot b will be entered into FITEQL input files and the associated sorption binding constants determined.

See this notebook pg. 48. 3 more fiteql corrections 4/4/95

All FITEQL input files for Fig. 3b can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.C3b
DLM*.D3b
TLM*.T3b.

and at C:\floppy\lieser\c\fig~~15~~3b\.c3b 2/7/95
\d\ \.d3b
\t\ \.t3b.

A copy of the FITEQL input file for species $XOH_2\text{-}UO_2(OH)_2^+$, tlm follows.

file XOH2UO22.T3b

```
                0                                                       TiO2
                1                                                       Lieser88
                0                                                       2.10e-6M
                0                                                       2.3si/nm
                1                                                       00000050
               90                                                       00000060
                6          1           1           1                   00000070
00001  -3.32  4.79E-4  XOH                                             00000080
00160  -1.0   0.00E00  PSI0                                            00000090
00161  -0.5   0.00E00  PSIB                                            00000092
00162  -0.1   0.00E00  PSID                                            00000094
00032  -5.68  2.10E-6  UO2+2                                          00000098
00140  -4.00  1.00E-4  CO3-2  * => see next page                       00000100
00033   0.0   0.00E00  UO2ads                                          00000102
00050   0.0   0.00E00  H+
00003  -0.1   0.00E00  Na+
00005  -0.3   0.00E00  Cl-                                             00000110
```

2/9/95

file XOH2UO22.T3b continued -

```
00050    0.00  050  1                                                  00000120
00032    0.00  032  1                                                  00000124
00140    0.00  140  1
03201   -5.51  032  1 050 -1                                          00000126
03202  -10.62  032  1 050 -2                                          00000127
03203  -19.22  032  1 050 -3                                          00000128
03204  -32.43  032  1 050 -4                                          00000129
03205   -2.41  032  2 050 -1                                          00000130
03206   -5.94  032  2 050 -2                                          00000131
03207  -12.53  032  3 050 -4                                          00000132
03208  -16.49  032  3 050 -5                                          00000133
03209  -31.65  032  3 050 -7                                          00000134
03210  -23.15  032  4 050 -7                                          00000135
03212    8.41  032  1 140  1                                          00000139
03213   15.77  032  1 140  2                                          00000140
03214   21.58  032  1 140  3                                          00000141
03215   -2.10  032  2 140  1 050 -3                                   00000144
03216   28.43  032 11 140  6 050-12                                   00000144
03318   -1.09  032  3 140  1 050 -3                                   00000144
03311   -0.44  032  1 005  1
03312   -2.03  032  1 005  2
00100  -13.70  050 -1                                                00000139
01200    6.83  001  1 050  1 005 1
01300   -4.59  001  1 003  1 050 -1                                   00000140
01050    3.95  001  1 160  1 050  1                                   00000145
01100   -7.95  001  1 160 -1 050 -1                                   00000130
00001    0.00  001  1                                                xoh2uo22
03307    1.00  001  1 160  1 161  0 050 -1 032  1 033  1             00000174
                                                                     00000175
00004  125.0  1.0000  0.8   0.2                                       00000180
0.5    1.0                                                           00000185
          1                                                          00000190
       3307                                                          00000195
         19          1           1           0                     00000230
         33                                                         00000240
2.05E-07
5.52E-07
8.03E-07
1.67E-06
1.79E-06
1.73E-06
1.85E-06
1.94E-06
2.01E-06
2.05E-06
2.04E-06
2.07E-06
2.07E-06
1.99E-06
1.98E-06
1.77E-06
1.59E-06
1.59E-06
1.73E-06
          50                                                         00000680
-2.26353
-2.67041
-3.04042
-3.97454
-4.08256
-4.33589
-4.37746
-4.79038
-5.10104
-5.64784
-5.75014
-6.19451
-6.90316
-7.32142
-7.49044
-7.89169
-8.38533
-8.90088
-9.58948
          1           1                                            00001170
         33    0.10  2.1E-09                                        00001180
         50    0.05  0.0E-00                                        00001190
```

* see pg 38 this notebook 2/9/95

The sorption binding constant table for figure 3b (BINDING.U39) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{sp}: 125 m^2/g Data Source: Lieser et. al. (1988) Concentration: [U(VI)] = 2.1e-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09	Ionic Strength (electrolyte): 0.5 M NaCl N_s = 2.31 sites/nm^2 M/V = 1.00g/L

Tot CO_3^- =1.0e-4 M fig 3b	DLM Log K_+ = 5.37 Log K_- = -5.92 (TiO_2 anatase)			CCM Log K_+ = 6.64 Log K_- = -5.60			TLM Log K_+ = 4.10 Log K_- = -8.10 Log K_{Cat} = -4.59 Log K_{An} = 7.13		
	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$	Log K	V_Y	$\sigma_{Log K}$
$XO\text{-}UO_2^+$	12.71	4.5	.0514	n.c.			14.06	4.5	.0544
$XOH\text{-}UO_2^{2+}$	17.29	2.3	.0398	n.c.			17.14	8.9	.0358
$XO\text{-}UO_2OH^0$	7.94	7.4	.0677	n.c.			10.83	8.4	.0777
$XOH\text{-}UO_2OH^+$	12.71	4.5	.0514	n.c.			14.06	4.6	.0542
$XO\text{-}UO_2(OH)_2^-$	3.08	9.3	.0844	n.c.			4.21	16.9	.2014
$XOH\text{-}UO_2(OH)_2^0$	7.94	7.4	.0677	n.c.			10.83	8.5	.0777
$XOH_2\text{-}UO_2(OH)_2^+$	12.71	4.5	.0514	n.c.			14.09	4.5	.0543
$XOH\text{-}UO_2(OH)_3^-$	3.08	9.3	.0844	n.c.			4.21	16.9	.2003
$XOH_2\text{-}UO_2(OH)_3^0$	7.94	7.4	.0677	n.c.			10.86	8.4	.0777
$XOH\text{-}UO_2(OH)_4^{2-}$	-4.36	16.8	.1908	n.c.			0.29	17.0	.2297
$XOH_2\text{-}UO_2(OH)_4^-$	3.08	9.3	.0843	n.c.			4.32	16.9	.2025
$XOH\text{-}UO_2CO_3^0$	n.c.			n.c.			n.c.		
$XOH_2\text{-}UO_2(CO_3)_3^-$	n.c.			n.c.			n.c.		
$XOH_2\text{-}(UO_2)_3CO_3(OH)_3^0$	n.c.			n.c.			n.c.		

log K values are at I = 0 n.c. FITEQL optimization did not converge. Table bindingU.39

Notes for Lieser FITEQL input files:
Total carbonate was reported in the journal article, and so CO_3^{-2} was used as a component, and the associated reactions were written in terms of CO_3^{-2}, e.g.

$UO_2^{2+} + CO_3^{2-} = UO_2CO_3^0$, not $UO_2^{2+} + CO_2 + H_2O = UO_2CO_3^0 + 2H^+$

The Lieser data for figure 3, plot c will be entered into FITEQL input files, and the associated sorption binding constants determined.

All FITEQL input files for Fig. 3c can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.c3c
DLM*.d3c
TLM*.t3c.
and at C:\floppy\lieser\c\fig3c*.c3c
\d\ *.d3c
\t\ *.t3c.

A copy of the FITEQL input file for species XOH_2-$UO_2(OH)_2^+$, tlm follows.

file XOH2UO22.t3c

```
                0
                1
                0
                0
                1
               90
                6          1                3          1
00001   -3.32    4.79E-4   XOH
00160   -1.0     0.00E00   PSI0
00161   -0.5     0.00E00   PSIB
00162   -0.1     0.00E00   PSID
00032   -5.68    2.10E-6   UO2+2
00140   -3.00    1.00E-3   CO3-2
00033    0.0     0.00E00   UO2ads
00050    0.0     0.00E00   H+
00003   -0.3     0.00E00   Na+
00005   -0.3     0.00E00   Cl-

00050     0.00   050   1
00032     0.00   032   1
00140     0.00   140   1
03201    -5.51   032   1 050 -1
03202   -10.62   032   1 050 -2
03203   -19.22   032   1 050 -3
03204   -32.43   032   1 050 -4
03205    -2.41   032   2 050 -1
03206    -5.94   032   2 050 -2
03207   -12.53   032   3 050 -4
03208   -16.49   032   3 050 -5
03209   -31.65   032   3 050 -7
03210   -23.15   032   4 050 -7
03212     8.41   032   1 140  1
03213    15.77   032   1 140  2
03214    21.58   032   1 140  3
03215    -2.10   032   2 140  1 050 -3
03216    28.43   032  11 140  6 050-12
03318    -1.09   032   3 140  1 050 -3
03311    -0.44   032   1 005  1
03312    -2.03   032   1 005  2
00100   -13.70   050  -1
01200     6.83   001   1 050  1 005 1
01300    -4.59   001   1 003  1 050 -1
01050     3.95   001   1 160  1 050  1
01100    -7.95   001   1 160 -1 050 -1
00001     0.00   001   1
03307     1.00   001   1 160  1 161  0 050 -1 032  1 033  1

00004   125.0   1.0000   0.8    0.2
0.5     1.0
          1
       3307
         20          1          1          0
         33
2.07E-07
5.52E-07
8.13E-07
1.67E-06
1.8E-06
1.73E-06
1.85E-06
1.94E-06
2.01E-06
2.05E-06
2.04E-06
2.07E-06
2.03E-06
1.99E-06
1.99E-06
1.75E-06
1.4E-06
9.24E-07
9.38E-07
1.11E-06
         50
-2.25817
-2.67041
-3.04231
-3.98
-4.08625
-4.33585

7102
Lieser88
2.10e-6M
2.3#1/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098

00000100
00000102

00000110
00000120
00000124

00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000139
00000140
00000141
00000144
00000144
00000144

00000139

00000140
00000145
00000130
xoh2uo22
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240

00000680
```


file XOH2UO22 continued -

```
-4.37567
-4.80309
-5.09563
-5.64786
-5.75553
-6.18724
-6.95915
-7.15195
-7.32317
-7.69667
-8.20145
-8.9855
-9.38224
-9.86136
          1          1
         33       0.10   2.1E-09
         50       0.05   0.0E-00
```

00001170
00001180
00001190

The sorption binding constant table for figure 3c (BINDING.U40) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{sp}: 125 m^2/g Data Source: Lieser et. al. (1988) Concentration: [U(VI)] = 2.1e-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09			Ionic Strength (electrolyte): 0.5 M NaCl N_s = 2.31 sites/nm^2 M/V = 1.00g/L		
Tot CO_3^{-2} = 1e-3 M fig 3c	DLM Log K_1 = 5.37 Log K_{-1} = -5.92 (TiO_2 anatase)			CCM Log K_1 = 6.64 Log K_{-1} = -5.60			TLM Log K_{-1} = 4.10 Log K_{-2} = -8.10 Log K_{Cu} = -4.59 Log K_{Ca} = 7.13		
	Log K	V_T	$\sigma_{Log\ K}$	Log K	V_T	$\sigma_{Log\ K}$	Log K	V_T	$\sigma_{Log\ K}$
XO-UO_2^+	6.99	79.8	.0458	n.c.			11.94	51.3	.0460
XOH-UO_2^{2+}	14.62	65.6	.0482	n.c.			20.23	8.2	.0335
XO-UO_2OH^0	10.97	27.1	.0679	n.c.			2.04	86.2	.0566
XOH-UO_2OH^+	6.99	79.8	.0458	n.c.			11.90	51.5	.0451
XO-$UO_2(OH)_2^-$	6.11	28.9	.0846	n.c.			-7.46	90.4	.0789
XOH-$UO_2(OH)_2^0$	10.97	27.1	.0679	n.c.			2.01	86.3	.0559
XOH_2-$UO_2(OH)_2^+$	6.99	79.8	.0458	n.c.			11.91	51.6	.0457
XOH-$UO_2(OH)_3^-$	6.11	28.9	.0846	n.c.			-7.48	90.5	.0785
XOH_2-$UO_2(OH)_2^0$	10.97	27.1	.0679	n.c.			2.02	86.2	.0566
XOH-$UO_2(OH)_4^{2-}$	-1.38	35.8	.1834	n.c.			-16.63	92.0	.1059
XOH_2-$UO_2(OH)_4^-$	6.11	20.0	.0846	n.c.			n.c.		
XOH-$UO_2CO_3^0$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_2^-$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{-3}$	n.c.			n.c.			n.c.		
XOH_2-$(UO_2)_3CO_3(OH)_3^0$	n.c.			n.c.			n.c.		

n.c. FITEQL optimization did not converge. Table binding.U40 Log K values corrected to I = 0.

The Lieser data for figure 3, plot d will be entered into FITEQL input files, and the associated sorption binding constants determined.

All FITEQL input files for Fig. 3d can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.c3d
DLM*.d3d
TLM*.t3d.
and at C:\floppy\lieser\c\fig3d*.c3d
\d\ *.d3d
\t\ *.t3d.

A copy of the FITEQL input file for species XOH_2-$UO_2(OH)_2^+$, tlm follows.

file XOH2UO22.t3d

```
                0
                1
                0
                0
                1
               50
          6          2          3          1
00001   -3.32   4.79E-4  XOH
00160   -1.0    0.00E00  PSIO
00161   -0.5    0.00E00  PSIB
00162   -0.1    0.00E00  PSID
00032   -5.68   2.10E-6  UO2+2
00140   -2.00   1.00E-2  CO3-2
00033    0.0    0.00E00  UO2ads
00050    0.0    0.00E00  H+
00003   -0.3    0.00E00  Na+
00005   -0.3    0.00E00  Cl-

00050    0.00   050  1
00032    0.00   032  1
00140    0.00   140  1
03201   -5.51   032  1 050 -1
03202  -10.62   032  1 050 -2
03203  -19.22   032  1 050 -3
03204  -32.43   032  1 050 -4
03205   -2.41   032  2 050 -1
03206   -5.94   032  2 050 -2
03207  -12.53   032  3 050 -4
03208  -16.49   032  3 050 -5
03209  -31.65   032  3 050 -7
03210  -23.15   032  4 050 -7
03212    8.41   032  1 140  1
03213   15.77   032  1 140  2
03214   21.58   032  1 140  3
03215   -2.10   032  2 140  1 050 -3
03216   28.43   032 11 140  6 050-12
03318   -1.09   032  3 140  1 050 -3
03319   -0.44   032  1 005  1
03320   -2.03   032  1 005  2
00100  -13.70   050 -1
01200    6.83   001  1 050  1 005  1
01300   -4.59   001  1 003  1 050 -1
01050    3.95   001  1 160  1 050  1
01100   -7.95   001  1 160 -1 050 -1
00001    0.00   001  1
03307    1.00   001  1 160  1 161  0 050 -1 032  1 033  1

00004  125.0  1.0000  0.8   0.2
0.5    1.0
          1
       3307
         24          1          1          0
         33
9.85E-08
2.65E-07
6.75E-07
9.71E-07
1.39E-06
1.38E-06
1.55E-06
1.71E-06
1.88E-06
1.96E-06
1.91E-06
1.95E-06
2.06E-06
2.06E-06
2.01E-06
1.91E-06
1.96E-06
1.5E-06
1.28E-06
9.57E-07
6.56E-07
5.86E-07
5.99E-07
6.51E-07
          50
-1.90878
-2.40713
-2.8879
-3.27613
-3.47212
-3.6363
-3.90116
-4.19163
-4.55917
-4.6773
-4.90494
-4.98531
-5.01458
-5.46719
-5.62493
-7.07212
-7.31636
-7.83636
-8.05262
-8.49898
-8.79939
-9.3578
-9.78323
-10.1912
          1          1
         33       0.10    2.1E-09
         50       0.05    0.0E-00
```

```
TiO2
Lieser88
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00000070
00000080
00000090
00000092
00000094
00000098

00000100
00000102

00000110
00000120
00000124

00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000139
00000140
00000141
00000144
00000144
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00000139

00000140
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00000130
xoh2uo22
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240

00000680

00001170
00001180
00001190
```

5pt pg 48
4/4/95 PM

table BINDING.U41 for plot 3d

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{sp}: 125 m^2/g Data Source: Lieser et. al. (1988) Concentration: [U(VI)] = 2.1e-6 M				Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09			Ionic Strength (electrolyte): 0.5 M NaCl N_s = 2.31 sites/nm² M/V = 1.00g/L		
Tot CO_3^{-} =2e-3 M fig 3d	DLM Log K_+ = 5.37 Log K_- = -5.92 (TiO_2 anatase)			CCM Log K_+ = 6.64 Log K_- = -3.60			TLM Log K_1 = 4.10 Log K_{-1} = -8.10 Log K_{CO_3} = -4.59 Log K_{+1} = 7.13		
	Log K	V_y	$\sigma_{\log K}$	Log K	V_y	$\sigma_{\log K}$	Log K	V_y	$\sigma_{\log K}$
XO-UO_2^{+}	7.43	76.9	.0285	n.c.			12.24	59.4	.0263
XOH-UO_2^{2+}	15.00	69.0	.0315	n.c.			21.05	7.9	.0263
XO-UO_2OH^{0}	11.52	111.0	.0725	n.c.			2.02	87.8	.0423
XOH-UO_2OH^{+}	7.43	76.9	.0285	n.c.			12.22	59.5	.0258
XO-$UO_2(OH)_2^{-}$	6.54	112.4	.0888	n.c.			-8.25	92.0	.0638
XOH-$UO_2(OH)_2^{0}$	11.52	111.0	.0725	n.c.			2.00	87.9	.0420
XOH_2-$UO_2(OH)_2^{+}$	7.43	76.9	.0285	n.c.			12.23	59.5	.0262
XOH-$UO_2(OH)_3^{-}$	6.54	112.4	.0888	n.c.			-8.28	92.0	.0634
XOH_2-$UO_2(OH)_3^{0}$	12.52	111.0	.0725	n.c.			2.01	87.8	.0423
XOH-$UO_2(OH)_4^{2-}$	1.54	113.3	.1054	n.c.			-18.40	93.2	.0891
XOH_2-$UO_2(OH)_4^{-}$	6.54	112.4	.0888	n.c.			-8.26	91.9	.0638
XOH-$UO_2CO_3^{0}$	n.c			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{-}$	n.c			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{5-}$	n.c			n.c.			n.c.		
XOH_2-$(UO_2)_3CO_3(OH)_3^{+}$	n.c.			n.c.			n.c.		

n.c. FITEQL optimization did not converge. table binding.u41 Log K values corrected to I = 0.

The Lieser data for figure 3, plot e will be entered into FITEQL input files, and the associated sorption binding constants determined.

All FITEQL input files for Fig. 3e can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.c3e
DLM*.d3e
TLM*.t3e.

and at C:\floppy\lieser\c\fig3e*.c3e
\d\ *.d3e
\t\ *.t3e.

A copy of the FITEQL input file for one of the carbonate-incorporating species, XOH-$UO_2CO_3^{0}$, tlm follows.

file XOHUCl.t3e

```
                0
                1
                0
                0
                1
               50
          6          2          3          1
00001   -3.32   4.79E-4  XOH
00160   -1.0    0.00E00  PSIO
00161   -0.5    0.00E00  PSIB
00162   -0.1    0.00E00  PSID
00032   -5.68   2.10E-6  UO2+2
00140   -2.00   1.00E-2  CO3-2
00033    0.0    0.00E00  UO2ads
00141    0.0    0.00E00  CO3ads
00050    0.0    0.00E00  H+
00003   -0.3    0.00E00  Na+
00005   -0.3    0.00E00  Cl-

00050    0.00   050  1
00032    0.00   032  1
00140    0.00   140  1
01401    9.73   140  1 050  1
01402   15.78   140  1 050  2
01403    0.67   140  1 003  1
01404    9.18   140  1 050 -1 003  1
03201   -5.51   032  1 050 -1
03202  -10.62   032  1 050 -2
03203  -19.22   032  1 050 -3
03204  -32.43   032  1 050 -4
03205   -2.41   032  2 050 -1
03206   -5.94   032  2 050 -2
03207  -12.53   032  3 050 -4
03208  -16.49   032  3 050 -5
03209  -31.65   032  3 050 -7
03210  -23.15   032  4 050 -7
03212    8.41   032  1 140  1
03213   15.77   032  1 140  2
03214   21.58   032  1 140  3
03215   -2.10   032  2 140  1 050 -3
03216   28.43   032 11 140  6 050-12
03318   -1.09   032  3 140  1 050 -3
03319   -0.44   032  1 005  1
03320   -2.03   032  1 005  2
00100  -13.70   050 -1
01200    6.83   001  1 050  1 005  1
01300   -4.59   001  1 003  1 050 -1
01050    3.95   001  1 160  1 050  1
01100   -7.95   001  1 160 -1 050 -1
00001    0.00   001  1
03332    5.00   001  1 160  0 161  0 050  0 032  1 033  1 140  1 141  1

00004  125.0  1.0000  0.8   0.2
0.5    1.0
          1
       3312
         11          2          1          0
         33
1.68E-07
3.6E-07
1.42E-06
2.02E-06
1.92E-06
1.48E-06
1.03E-06
3.42E-07
1.87E-07
2.11E-07
2.9E-07
          141
1.68E-07
3.6E-07
1.42E-06
2.02E-06
1.92E-06
1.48E-06
1.03E-06
3.42E-07
1.87E-07
2.11E-07
2.9E-07
          50
-2.17973
-2.53659
-3.73766
-5.49672
-6.19244
-6.80131
-7.48989
-8.17757
-8.74449
-8.99383
-10.0968
          1          1
         33       0.10    2.1E-09
        141       0.10    1.2E-09
         50       0.05    0.0E-00
```

```
TiO2
Lieser88
2.10e-6M
2.3#i/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098

00000100
00000102

00000110
00000120
00000124

00000146
00000147
00000146
00000147
00000126
00000127
00000128
00000129
00000130
00000131
00000132
00000133
00000134
00000135
00000139
00000140
00000141
00000144
00000144
00000144

00000139

00000140
00000145
00000130
xoh2uo21
00000174
00000175
00000180
00000185
00000190
00000195
00000230
00000240

00000250

00000680

00001170
00001180
00001180
00001190
```

The sorption binding constant table for figure 3e (BINDING.U42) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2	Rel Error (pH): 0.05	Ionic Strength (electrolyte): 0.5 M NaCl
A_{sp}: 125 m^2/g	Abs Error (pH): 0.0	N_s = 2.31 sites/nm^2
Data Source: Lieser et. al. (1988)	Rel Error (radionuclide): 0.10	M/V = 1.00g/L
Concentration: [U(VI)] = 2.1e-6 M	Abs Error (radionuclide): 2.1e-09	

Tot CO_3^- =1e-2 M fig 3e	DLM			CCM			TLM		
	Log K_1 = 5.37 Log K_{-1} = -5.92 (TiO_2 anatase)			Log K_1 = 6.64 Log K_{-1} = -5.60			Log K_1 = 4.10 Log K_{-1} = -8.10 Log K_{Cu} = -4.59 Log K_{An} = 7.13		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	8.97	69.1	.0283	n.c.			13.61	57.6	.0254
XOH-UO_2^{2+}	16.10	70.10	.0297	n.c.			22.44	21.7	.0313
XO-UO_2OH^0	.73	87.4	.0500	n.c.			3.56	86.7	.0487
XOH-UO_2OH^+	8.97	69.1	.0283	n.c.			13.60	57.7	.0252
XO-$UO_2(OH)_2^-$	7.29	2.1e+3	.1495	n.c.			-6.76	90.4	.0705
XOH-$UO_2(OH)_2^0$	12.58	2.1e+3	.1580	n.c.			3.54	86.7	.0485
XOH_2-$UO_2(OH)_2^+$	8.97	69.1	.0283	n.c.			13.60	57.7	.0253
XOH-$UO_2(OH)_3^-$	7.29	2.1e+3	.1495	n.c.			-6.77	90.4	.0701
XOH_2-$UO_2(OH)_3^0$	12.58	2.1e+3	.1580	n.c.			3.54	86.7	.0487
XOH-$UO_2(OH)_4^{2-}$	2.09	2.1e+3	.1525	n.c.			-16.94	90.7	.0904
XOH_2-$UO_2(OH)_4^-$	7.29	2.1e+3	.1495	n.c.			-6.77	90.4	.0705
XOH-$UO_2CO_3^0$	n.c			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_2^{2-}$	n.c			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c			n.c.			n.c.		
XOH_2-$(UO_2)_2CO_3(OH)_3^+$	n.c.			n.c.			n.c.		

n.c. FITEQL optimization did not converge. Table binding.U42 Log K values corrected to I = 0.

2/13/95 PM

The Lieser data for figure 3, plot f will be entered into FITEQL input files, and the associated sorption binding constants determined.

All FITEQL input files for Fig. 3f can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.c3f
DLM*.d3f
TLM*.t3f.
and at C:\floppy\lieser\c\fig3e*.c3f
\d\ *.d3f
\t\ *.t3f.

A copy of the FITEQL input file for one of the carbonate-incorporating species, XOH-$UO_2CO_3^0$, tlm follows.

file XOHUC1.t3f

```
 0
 1
 0
 0
 1
 50
  6          2          3          1
00001  -3.32   4.79E-4   XOH
00160  -1.0    0.00E00   PSIO
00161  -0.5    0.00E00   PSIB
00162  -0.1    0.00E00   PSID
00032  -5.68   2.10E-6   UO2+2
00140  -1.52   3.00E-2   CO3-2
00033   0.0    0.00E00   UO2ads
00141   0.0    0.00E00   CO3ads
00050   0.0    0.00E00   H+
00003  -0.3    0.00E00   Na+
00005  -0.3    0.00E00   Cl-

TiO2
Lieser88
2.10e-6M
2.3sl/nm
00000050
00000060
00000070
00000080
00000090
00000092
00000094
00000098

00000100
00000101
00000102


00000110
```


file XOHUC1.t3f continued

```
00050    0.00  050  1                                                    00000120
00032    0.00  032  1                                                    00000124
00140    0.00  140  1
01401    9.73  140  1 050  1                                            00000146
01402   15.78  140  1 050  2                                            00000147
01403    0.67  140  1 003  1                                            00000146
01404    9.18  140  1 050  1 003  1                                     00000147
03201   -5.51  032  1 050 -1                                           00000126
03202  -10.62  032  1 050 -2                                           00000127
03203  -19.22  032  1 050 -3                                           00000128
03204  -32.43  032  1 050 -4                                           00000129
03205   -2.41  032  2 050 -1                                           00000130
03206   -5.94  032  2 050 -2                                           00000131
03207  -12.53  032  3 050 -4                                           00000132
03208  -16.49  032  3 050 -5                                           00000133
03209  -31.65  032  3 050 -7                                           00000134
03210  -23.15  032  4 050 -7                                           00000135
03212    8.41  032  1 140  1                                           00000139
03213   15.77  032  1 140  2                                           00000140
03214   21.58  032  1 140  3                                           00000141
03215   -2.10  032  2 140  1 050 -3                                     00000144
03216   28.43  032 11 140  6 050-12                                    00000144
03318   -1.09  032  3 140  1 050 -3                                     00000144
03319   -0.44  032  1 005  1                                           00000144
03320   -2.03  032  1 005  2
00100  -13.70  050 -1                                                  00000139
01200    6.83  001  1 050  1 005  1
01300   -4.59  001  1 003  1 050 -1                                    00000140
01050    3.95  001  1 160  1 050  1                                     00000145
01100   -7.95  001  1 160 -1 050 -1                                    00000130
00001    0.00  001  1                                                  00000174
03312    5.00  001  1 160  0 161  0 050  0 032  1 033  1 140  1 141  1 xohuc2c1  00000175
                                                                       00000180
00004  125.0  1.0000  0.8  0.2                                         00000185
0.5    4.0                                                             00000190
         1                                                             00000195
       1112                                                            00000230
        7 9        2          1          0                           00000240
         33
2E-06
1.8E-06
1.13E-06
6.97E-07
8.66E-07
9.12E-07
8.88E-07
7.5E-07
8.35E-07
          141                                                          00000250
2E-06
1.8E-06
1.13E-06
6.97E-07
8.66E-07
9.12E-07
8.88E-07
7.5E-07
8.35E-07
          50                                                           00000680
-5.28814
-5.99919


-6.56585
-6.69759
-7.0235
-7.7955
-8.2893
-9.18963
-9.99621
          1          1
         33       0.10    2.1E-09                                     00001170
        141       0.10    1.2E-09                                     00001180
         50       0.05    0.0E-00                                     00001180
                                                                      00001190
```

The sorption binding constant table for figure 3f (BINDING.U43) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2	Rel Error (pH): 0.05	Ionic Strength (electrolyte): 0.5 M NaCl
A_{sp}: 125 m^2/g	Abs Error (pH): 0.0	N_s = 2.31 sites/nm^2
Data Source: Lieser et. al. (1988)	Rel Error (radionuclide): 0.10	M/V = 1.00g/L
Concentration: [U(VI)] = 2.1e-6 M	Abs Error (radionuclide): 2.1e-09	

Tot CO_3^- =3e-2 M fig 3f	DLM			CCM			TLM		
	Log K_1 = 5.37 Log K_{-1} = -5.92 (TiO_2 anatase)			Log K_1 = 6.64 Log K_{-1} = -5.60			Log K_1 = 4.10 Log K_{-1} = -8.10 Log K_{Cu} = -4.59 Log K_{An} = 7.13		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	n.c.			n.c.			n.c.		
XOH-UO_2^{2+}	n.c.			n.c.			n.c.		
XO-UO_2OH^0	n.c.			n.c.			n.c.		
XOH-UO_2OH^+	n.c.			n.c.			n.c.		
XO-$UO_2(OH)_2^-$	n.c.			n.c.			n.c.		
XOH-$UO_2(OH)_2^0$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(OH)_2^+$	n.c.			n.c.			n.c.		
XOH-$UO_2(OH)_3^-$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(OH)_3^0$	n.c.			n.c.			n.c.		
XOH-$UO_2(OH)_4^{2-}$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(OH)_4^-$	n.c.			n.c.			n.c.		
XOH-$UO_2CO_3^0$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_2^{2-}$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c.			n.c.			n.c.		
XOH_2-$(UO_2)_2CO_3(OH)_3^+$	n.c.			n.c.			n.c.		

n.c. FITEQL optimization did not converge. Table binding.U43

The Lieser data for figure 3, plot g will be entered into FITEQL input files, and the associated sorption binding constants determined.

All FITEQL input files for Fig. 3g can be found at K:\TURNER\FITEQL\SORPTION\LIESER\CCM*.c3g
DLM*.d3g
TLM*.t3g.

and at C:\floppy\lieser\c\fig3g*.c3g
\d\ *.d3g
\t\ *.t3g.

A copy of the FITEQL input file for one of the carbonate-incorporating species, XOH-$UO_2CO_3^0$, tlm follows.

file XOHUC1.t3g

```
                0                                                       TiO2
                1                                                       Lieser88
                0                                                       2.10e-6M
                0                                                       2.3e1/mm
                1                                                       00000050
               90                                                       00000060
                6          2          3          1                     00000070
00001   -3.32   4.79E-4   XOH                                          00000080
00160   -1.0    0.00E00   PSIO                                         00000090
00161   -0.5    0.00E00   PSIB                                         00000092
00162   -0.1    0.00E00   PSID                                         00000094
00032   -5.68   2.10E-6   UO2+2                                        00000098
00140   -1.00   1.00E-1   CO3-2
00033    0.0    0.00E00   UO2ads                                       00000100
00141    0.0    0.00E00   CO3ads                                       00000101
00050    0.0    0.00E00   H+                                           00000102
00003   -0.3    0.00E00   Na+
00005   -0.3    0.00E00   Cl-                                          00000110

00050    0.00   050  1                                                00000120
00032    0.00   032  1                                                00000124
00140    0.00   140  1
01401    9.73   140  1 050  1                                         00000146
01402   15.78   140  1 050  2                                         00000147
01403    0.67   140  1 003  1                                         00000146
01404    9.18   140  1 050  1 003  1                                  00000147
03201   -5.51   032  1 050 -1                                         00000126
03202  -10.52   032  1 050 -2                                         00000127
03203  -19.22   032  1 050 -3                                         00000128
03204  -32.43   032  1 050 -4                                         00000129
03205   -2.41   032  2 050 -1                                         00000130
03206   -5.94   032  2 050 -2                                         00000131
03207  -12.53   032  3 050 -4                                         00000132
03208  -16.49   032  3 050 -5                                         00000133
03209  -31.65   032  3 050 -7                                         00000134
03210  -23.15   032  4 050 -7                                         00000135
03212    8.41   032  1 140  1                                         00000139
03213   15.77   032  1 140  2                                         00000140
03214   21.58   032  1 140  3                                         00000141
03215   -2.10   032  2 140  1 050 -3                                  00000144
03216   28.43   032 11 140  6 050-12                                  00000144
03318   -1.09   032  3 140  1 050 -3                                  00000144
03319   -0.44   032  1 005  1
03320   -2.03   032  1 005  2
00100  -13.70   050 -1                                               00000139
01200    6.83   001  1 050  1 005  1
01300   -4.59   001  1 003  1 050 -1
01050    3.95   001  1 160  1 050  1                                  00000140
01100   -7.95   001  1 160 -1 050 -1                                  00000145
00001    0.00   001  1                                                00000130
03312    5.00   001  1 160  0 161  0 050  0 032  1 033  1 140  1 141  1  xohuo2c1
                                                                       00000174
                                                                       00000175
00004  125.0  1.0000  0.8   0.2                                       00000180
0.5    1.0                                                           00000185
         1                                                           00000190
      3312                                                           00000195
        26          2          1          0                         00000230
        33                                                           00000240
9.89E-08
2.66E-07
6.71E-07
9.67E-07
1.39E-06
1.37E-06
1.55E-06
1.73E-06
1.87E-06
1.95E-06
1.91E-06
1.95E-06
1.94E-06
1.58E-06
1.4E-06
8.03E-07
1.03E-06
1.26E-06
1.36E-06
1.66E-06
1.91E-06
1.95E-06

2E-06
1.98E-06
1.99E-06
2E-06
        141                                                            00000250
9.89E-08
2.66E-07
6.71E-07
9.67E-07
1.39E-06
1.37E-06
1.55E-06
1.73E-06
1.87E-06
1.95E-06
1.91E-06
1.95E-06
1.94E-06
1.58E-06
1.4E-06
8.03E-07
1.03E-06
1.26E-06
1.36E-06
1.66E-06
1.91E-06
1.95E-06
2E-06
1.98E-06
1.99E-06
2E-06
```


file XOHUC1.t3g, continued

```
                50                                                     00000680
-1.91421
-2.40173
-2.88066
-3.27069
-3.46331
-3.63265
-3.89575
-4.19164
-4.55634
-4.67363
-4.91407
-4.98895
-5.48997
-5.71513
-5.88472
-6.10893
-6.31087
-6.41738
-6.519
-6.69682
-7.06125
-7.58509
-8.10079
-8.39388
-9.19115
-9.90738
        1          1
       33    0.10   2.1E-09                                            00001170
      141    0.10   1.2E-09                                            00001180
       50    0.05   0.0E-00                                            00001180
                                                                       00001190
```

The sorption binding constant table for figure 3g (BINDING.U44) follows. It has been saved at C:\floppy\lieser on my PC and on the K:\ drive.

Uranium (VI) Sorption Binding Constants Monodentate, mononuclear compounds

Solid: hydrated TiO_2 A_{SP}: 125 m^2/g Data Source: Lieser et. al. (1988) Concentration: [U(VI)] = 2.1e-6 M	Rel Error (pH): 0.05 Abs Error (pH): 0.0 Rel Error (radionuclide): 0.10 Abs Error (radionuclide): 2.1e-09	Ionic Strength (electrolyte): 0.5 M NaCl N_S = 2.31 sites/nm^2 M/V = 1.00g/L

Tot CO_3 =1e-1 M fig 3g	DLM			CCM			TLM		
	Log K_1 = 5.37 Log K_{-1} = -5.92 (TiO_2 anatase)			Log K_1 = 6.64 Log K_{-1} = -5.60			Log K_1 = 4.10 Log K_{-1} = -8.10 Log K_{Cat} = -4.59 Log K_{An} = 7.13		
	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$	Log K	V_Y	$\sigma_{Log\ K}$
XO-UO_2^+	10.85	91.9	.0682	n.c.			15.53	90.4	.0503
XOH-UO_2^{2+}	17.86	92.2	.0767	n.c.			24.22	53.8	.0274
XO-UO_2OH^0	2.61	92.5	.0911	n.c.			5.40	92.5	.0903
XOH-UO_2OH^+	10.85	91.9	.0682	n.c.			15.52	90.4	.0503
XO-$UO_2(OH)_2^-$	11.29	2.06e4	.0831	n.c.			-4.64	92.6	.1000
XOH-$UO_2(OH)_2^0$	16.41	2.06e4	.0710	n.c.			5.40	92.5	.0902
XOH_2-$UO_2(OH)_2^+$	10.85	91.9	.0682	n.c.			15.52	90.4	.0504
XOH-$UO_2(OH)_3^-$	11.29	2.06e4	.0831	n.c.			-4.64	92.6	.0999
XOH_2-$UO_2(OH)_3^0$	16.41	2.06e4	.0710	n.c.			5.39	92.5	.0903
XOH-$UO_2(OH)_4^{2-}$	n.c.			n.c.			-14.67	92.6	.1120
XOH_2-$UO_2(OH)_4^-$	11.29	2.06e4	.0831	n.c.			-4.65	92.6	.1000
XOH-$UO_2CO_3^0$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_2^-$	n.c.			n.c.			n.c.		
XOH_2-$UO_2(CO_3)_3^{3-}$	n.c.			n.c.			n.c.		
XOH_2-$(UO_2)_3CO_3(OH)_3^0$	n.c.			n.c.			n.c.		

n.c. FITEQL optimization did not converge. Table binding.U44 Log K values corrected to I = 0

3/1/95 Preparation of Data Folders

Folders are being prepared for the following data sources:

1) Righetto et. al. (1988), Am -γAl_2O_3, Th -γAl_2O_3, and Np -$Al_2O_3\gamma$;

2) Righetto et. al. (1991), Np -SiO_2, Th -SiO_2, Am -SiO_2, and Pu -γAl_2O_3;

3) Waite et. al. (1993), U -quartz;

4) Sanchez et. al. (1985), Pu -goethite;

5) Venkataramani and Gupta (1991), U -magnetite;

6) Lieser et. al. (1988), U -hydrated TiO_2.

The folders will contain:

1) a Xerox copy of the relevant graph from the article, labelled with the author and year, the concentration of the radionuclide, the concentration of the mineral solid, and the ionic strength of the electrolyte;

2) a data table listing the pH value, % species adsorbed, and the concentration in moles of the species adsorbed at each data point;

3) one example of the FITEQL input file from each of the three models (CCM, DLM, and TLM) for each data set, labelled with the figure number, characteristic that is being varied (e.g., pH or solid concentration), model type, and relevant chemical equation for the sorbed species;

4) the log K table with the FITEQL results corrected to ionic strength = 0;

5) the plot of the MINTEQA2 results, if complete.

3/17/95 The completed folders were given to Dr. David Turner.

3/23/95 Renaming of Log K Tables

The log K tables from the shared computer drive K into my Windows system appear to be named like this:

```
binding^.~a2
binding^.~a5
binding^.~ah
binding^.~ak
binding^.~an
binding^.~aq
binding^.~at
binding^.~aw
```



```
binding^.~az
binding^.~i1
binding^.~i4
binding^.~ij
binding^.~im
binding^.~ip
```

etc.

I will rename them in my system and shorten the file names so that they will remain recognizable when I call them up.

3/28/95 List of Renamed Tables

The new file names are bind**RM.#**, where **R** is the first letter of the radionuclide (e.g., a for americium) and **M** for the first letter of the mineral (e.g., s for silica) and the # stands for the number of the file - there are eight americium files, so the americium file names run 1 through 8. Note that within a radionuclide/mineral group, the tables aren't numbered in any particular order.

The renamed files are at K:\turner\ktables\ktable2\ bind**RM.#** and at C:\floppy\ktables on my PC.
key to names:

R =
a americium, # = 1-8
c carbon, 1
n neptunium, 1-13
p plutonium, 1-5
t thorium, 1-3
u uranium, 1-40

M =
a alumina
b boehmite
f ferrihydrite
g goethite
k kaolinite
l lepridocrocite
m magnetite
s silica
t hydrous titanium dioxide

A listing of the renamed files is on the next page.

PM

Print File List
3/29/95 10:25AM

File List - c:\floppy\ktables*.*

[..]	[DIR]							
bindaa.1	14,203	12/2/94	binduf.1	16,400	3/23/95	bindum.31	9,270	3/23/95
bindaa.2	11,022	3/23/95	binduf.10	10,534	3/23/95	bindum.32	9,278	3/23/95
bindaa.3	14,113	3/23/95	binduf.11	10,795	3/23/95	bindut.33	8,421	3/10/95
bindaa.4	14,201	12/2/94	binduf.12	27,840	3/23/95	bindut.34	9,726	3/28/95
bindaa.5	33,936	2/22/95	binduf.13	16,620	3/23/95	bindut.35	11,577	3/28/95
bindas.6	9,730	3/23/95	binduf.14	10,548	3/23/95	bindut.36	11,577	3/28/95
bindas.7	9,727	3/23/95	binduf.2	10,514	3/23/95	bindut.37	11,570	3/28/95
bindas.8	8,594	3/23/95	binduf.3	30,553	2/8/95	bindut.38	11,566	3/28/95
bindcf.1	6,814	3/23/95	binduf.4	10,547	3/23/95	bindut.39	11,322	3/28/95
bindna.1	9,030	12/2/94	binduf.5	10,071	3/28/95	bindut.40	11,571	3/28/95
bindna.2	26,133	3/23/95	binduf.6	10,515	3/23/95	tblindx.lst	44,344	3/28/95
bindnb.3	35,883	2/17/95	binduf.7	30,937	2/8/95			
bindnb.4	29,369	3/23/95	binduf.8	10,426	7/11/94			
bindnf.5	8,179	3/23/95	binduf.9	10,766	3/23/95			
bindnf.6	8,179	3/23/95	bindug.15	12,496	3/23/95			
bindnf.7	8,254	12/20/94	bindug.16	10,708	3/23/95			
bindng.8	26,086	3/23/95	bindug.17	9,276	3/23/95			
bindnk.9	10,949	3/23/95	bindug.18	12,306	3/23/95			
bindnl.10	26,215	3/23/95	bindug.19	13,697	3/23/95			
bindnm.11	8,811	3/23/95	bindug.20	11,005	3/23/95			
bindnm.12	26,103	3/23/95	bindug.21	10,592	3/23/95			
bindns.13	8,419	3/23/95	bindug.22	10,356	3/23/95			
bindpa.1	7,672	3/23/95	bindug.23	10,501	3/23/95			
bindpg.2	9,812	3/23/95	bindug.24	12,436	3/23/95			
bindpg.3	7,657	3/23/95	bindug.25	9,974	3/27/95			
bindpg.4	7,656	3/23/95	bindug.26	10,598	3/23/95			
bindpg.5	9,868	3/23/95	binduk.27	23,767	3/23/95			
bindta.1	8,738	3/23/95	bindum.28	9,290	3/23/95			
bindts.2	9,087	3/23/95	bindum.29	9,307	3/23/95			
bindts.3	10,021	2/13/95	bindum.30	11,462	11/18/94			

PM

An index file listing the filename.ext, radionuclide-mineral, author reference, concentration of the radionuclide, ionic strength, solid concentration, and any other pertinent variables is presently at k:\turner\ktables\ tblindx.lst and at c:\floppy\ktables on my PC.

4/4/95 PM

The Lieser files 3b+ all needed more equations added, which changed the numerical values coming out of FITEQL. The following four equations were added:

PM

Reaction	log $K^{I=0}$	log $K^{I=0.5}$
$CO_3^{2-} + H^+ \Leftrightarrow HCO_3^-$	10.33	9.73
$CO_3^{2-} + 2H^+ \Leftrightarrow H_2CO_3^-$	16.68	15.78
$CO_3^{2-} + Na^+ \Leftrightarrow NaCO_3^-$	1.27	0.67
$CO_3^{2-} + 2Na^+ \Leftrightarrow Na_2CO_3^-$	10.08	9.18

These corrections were used in all Lieser files. Previously, only the files describing systems with carbonate incorporated into the surface species included these equations.

In FITEQL, they're written:

PM
```
01401     9.73  140   1 050   1
01402    15.78  140   1 050   2
01403     0.67  140   1 003   1
01404     9.18  140   1 050   1 003   2
```

The corrected files are found in the old files' place, + the corrected tables are in c:\floppy\ktables*.*.

4/11/95 PM Sorption Related Files

All sorption-related files on my PC will be transferred on to floppy disk, listed by name in a Word Perfect file, + given to Dr. Dave Turner.

5/10/95 Applicable Range of K Value - MINTEQA2 Model

PM To gauge the applicable range of a given K value, MINTEQA2 was used to model a system where the radionuclide (U(VI)) concentration was varied between 10^{-16} and 10^{-5} mol/L as the pH was held constant at 6, 7, or 8.

☆ See pg. 53 + this notebook 5/11/95 for listing PM

The sorbed species considered was XO-$UO_2(OH)_2^-$, with the following parameters:

model	DLM
N_s	2.31 sites/m^2
A_{sp}	50 m^2/g (goethite)
log K	-10.19 I=0
K_+	7.35
K_-	-9.17
C_t	0.01 M total carbon
M/V	1 g/L
[XOH]	1.918e-4

the MINTEQA2 input file follows:

File U165.inp.

```
U(VI) sorption on goethite, DLM, XO-UO2(OH)2-
pH = 6
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 2 1 1
TOTAL CONC 893 12
  1.000E-15  1.000E-14  1.000E-13  1.000E-12  1.000E-11  1.000E-10
  1.000E-09  1.000E-08  1.000E-07  1.000E-06  1.000E-05
uvari.sst        893
4   1   7
1.000E+00   50.00 0.000 0.000 81
    330  0.000E-01   -6.00 y                    /H+1
    500  5.000E-01   -0.30 y                    /Na+1
    180  5.000E-01   -0.30 y                    /Cl-1
    893  1.000E-16  -16.00 y                    /UO2+2
    140  1.000E-02   -2.00 y                    /CO3-2
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  1.918E-04   -3.32 y                    /ADS1TYP1

  3   1
    330      6.0000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 xoh2+            0.0000    7.3500   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 xo-              0.0000   -9.1700   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118931 xuo2oh2-         0.0000  -10.1900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 893   2.000   2  -3.000 330  -1.000 813   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

U(VI) sorption on goethite, DLM, XO-UO2(OH)2-
pH = 7
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 2 1 1
TOTAL CONC 893 12
  1.000E-15  1.000E-14  1.000E-13  1.000E-12  1.000E-11  1.000E-10
  1.000E-09  1.000E-08  1.000E-07  1.000E-06  1.000E-05
uvari.sst        893
4   1   7
1.000E+00   50.00 0.000 0.000 81
    330  0.000E-01   -7.00 y                    /H+1
    500  5.000E-01   -0.30 y                    /Na+1
```


File continued

```
    180  5.000E-01   -0.30 y                    /Cl-1
    893  1.000E-16  -16.00 y                    /UO2+2
    140  1.000E-02   -2.00 y                    /CO3-2
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  1.918E-04   -3.32 y                    /ADS1TYP1

  3   1
    330      7.0000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 xoh2+            0.0000    7.3500   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 xo-              0.0000   -9.1700   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118931 xuo2oh2-         0.0000  -10.1900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 893   2.000   2  -3.000 330  -1.000 813   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

U(VI) sorption on goethite, DLM, XO-UO2(OH)2-
pH = 8
25.00 MOLAL  0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 2 2 1 1
TOTAL CONC 893 12
  1.000E-15  1.000E-14  1.000E-13  1.000E-12  1.000E-11  1.000E-10
  1.000E-09  1.000E-08  1.000E-07  1.000E-06  1.000E-05
uvari.sst        893
4   1   7
1.000E+00   50.00 0.000 0.000 81
    330  0.000E-01   -8.00 y                    /H+1
    500  5.000E-01   -0.30 y                    /Na+1
    180  5.000E-01   -0.30 y                    /Cl-1
    893  1.000E-16  -16.00 y                    /UO2+2
    140  1.000E-02   -2.00 y                    /CO3-2
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  1.918E-04   -3.32 y                    /ADS1TYP1

  3   1
    330      8.0000      0.0000                 /H+1
  6   1
    813      0.0000      0.0000                 /ADS1PSIo

  2   3
8113300 xoh2+            0.0000    7.3500   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 xo-              0.0000   -9.1700   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8118931 xuo2oh2-         0.0000  -10.1900   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 5   1.000 811   1.000 893   2.000   2  -3.000 330  -1.000 813   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

The MINTEQA2 output was converted from % U sorbed to mol/g + plotted vs mol/L in solution. A table showing the data is on the following page. All data files & plots were put on floppy disk & given to Dr. Dave Turner.

sorption of U(VI) on goethite, pH = 6,7,8
[U] = 1E-16 to 1E-5

pH	% srb	$(U)_{tot}$ mol/L	srb mol/g	
6	92.3	1.00e-16	9.23e-17	
6	92.3	1.00e-15	9.23e-16	
6	92.3	1.00e-14	9.23e-15	
6	92.3	1.00e-13	9.23e-14	
6	92.3	1.00e-12	9.23e-13	
6	92.3	1.00e-11	9.23e-12	
6	92.3	1.00e-10	9.23e-11	
6	92.3	1.00e-09	9.23e-10	
6	92.3	1.00e-08	9.23e-09	
6	92.3	1.00e-07	9.23e-08	
6	92.1	0.000001	9.21e-07	
6	90.3	0.00001	0.000009	
7	72.1	1.00e-16	7.21e-17	
7	72.1	1.00e-15	7.21e-16	
7	72.1	1.00e-14	7.21e-15	
7	72.1	1.00e-13	7.21e-14	
7	72.1	1.00e-12	7.21e-13	
7	72.1	1.00e-11	7.21e-12	
7	72.1	1.00e-10	7.21e-11	
7	72.1	1.00e-09	7.21e-10	
7	72.1	1.00e-08	7.21e-09	
7	72	1.00e-07	7.20e-08	
7	71.7	0.000001	7.17e-07	
7	68.4	0.00001	0.000007	
8	39.2	1.00e-16	3.92e-17	
8	39.2	1.00e-15	3.92e-16	
8	39.2	1.00e-14	3.92e-15	
8	39.2	1.00e-13	3.92e-14	
8	39.2	1.00e-12	3.92e-13	
8	39.2	1.00e-11	3.92e-12	
8	39.2	1.00e-10	3.92e-11	
8	39.2	1.00e-09	3.92e-10	
8	39.2	1.00e-08	3.92e-09	
8	39.1	1.00e-07	3.91e-08	
8	39	0.000001	3.90e-07	
8	37.2	0.00001	0.000004	

5/11/95 PM listing of files on floppy disk

The following WP listing (master.lst) notes which files were taken from my PC & saved on floppy disks. The disks will be turned over to Dr. Dave Turner.

yellow disk

{dtatabls}
{rigpu}
{..}
ntbkfldr.txt
rig88am.tbl
rig88np.tbl
rig88th.tbl
rig91am.tbl
rig91np.tbl
rig91pu.tbl
rig91th.tbl
san85iva.tbl
san85pu.tbl
san85vb.tbl
san85vc.tbl
tableadj.num
ven.dat
ven.dta
ven.prn
ven.qat
ven91hi.tbl
wai.prn
wai93.tbl
wait.prn
[..]
rig8.dta
rigp8c.com
rigp8c.sp5
rigp8c.sst
rigpu8d.dlm
rigpu8d.sst
rigpu8t.sst
rigpu8t.tlm

[DIR]		
2,195	3/29/95	9:35AM
21,670	3/1/95	1:52PM
23,337	3/1/95	2:56PM
21,929	3/2/95	9:13AM
22,510	3/2/95	1:20PM
22,496	3/2/95	10:47AM
21,026	3/2/95	1:53PM
21,824	3/2/95	9:57AM
21,796	3/6/95	11:23AM
22,109	3/6/95	11:07AM
21,499	3/6/95	12:41PM
21,923	3/6/95	1:20PM
6,995	1/25/95	1:22PM
5,958	3/7/95	1:31PM
405	3/7/95	1:13PM
570	3/7/95	1:31PM
2,363	3/7/95	1:22PM
25,158	3/8/95	10:01AM
110	3/8/95	1:33PM
21,543	3/8/95	1:42PM
118	3/8/95	1:38PM
[DIR]		
11,231	10/17/94	1:45PM
8,571	10/13/94	8:59AM
32,760	10/24/94	10:27AM
7,020	10/13/94	9:03AM
8,571	10/21/94	11:33AM
6,750	10/21/94	11:37AM
6,750	10/21/94	12:34PM
12,721	10/21/94	12:33PM

yellow disk

{text}
{waite}
{..}
fitdir.txt
montprep.txt
qarefa.wp
steve.nts
wkfloon.txt
[..]
c
d
t
binding.u36
qtzascii.prn
qtzexpt.dta
qtzexpt.prn
quartz.prn
read.me
ref.txt
tripl.bat
waitec.com
waitec.sp5
waited.dlm
waitet.tlm

[DIR]		
2,777	5/11/95	9:38AM
7,840	5/11/95	9:38AM
42,947	8/19/94	11:13AM
1,086	5/11/95	9:38AM
25,505	5/11/95	9:38AM
[DIR]		
[DIR]	5/11/95	9:35AM
[DIR]	5/11/95	9:35AM
[DIR]	5/11/95	9:36AM
11,787	11/17/94	8:41AM
162	11/4/94	8:47AM
383	10/27/94	11:42AM
291	11/4/94	9:09AM
4,292	5/18/94	9:14AM
1,239	5/11/95	1:44PM
2,935	11/17/94	2:49PM
40	11/16/94	2:54PM
23,626	11/23/94	9:39AM
49,912	11/28/94	2:48PM
23,625	11/23/94	9:41AM
39,692	11/22/94	2:52PM

3m disk

minteqal
minteqa2
qpro
[..]
unn00__c
unn05__
unn05__c
unn05_c
unn05_cb
unn06__
unn06__c
unn06_c
uon00__c

[DIR]	12/13/94	11:18AM
[DIR]	12/13/94	11:18AM
[DIR]	12/13/94	10:41AM
[DIR]		
9,075	7/12/92	3:03PM
1,174	6/26/92	4:04PM
1,450	6/26/92	5:01PM
9,075	7/9/92	3:32PM
1,312	7/14/92	10:57AM
1,174	6/25/92	3:06PM
1,450	6/26/92	4:22PM
9,075	7/9/92	2:30PM
9,075	7/12/92	3:11PM

uon00__c.wp	23,398	7/12/92 4:40PM
uon05__	1,174	6/26/92 3:52PM
uon05__c	1,450	6/26/92 4:47PM
uon05_c	9,058	7/9/92 3:35PM
uon06__	1,174	6/25/92 3:28PM
uon06__c	1,450	6/26/92 4:34PM
uon06_c	9,068	7/9/92 3:38PM
[..]	[DIR]	
p1n10__	587	6/18/92 1:55PM
p1n11__	587	6/18/92 1:49PM
p1n11_a	5,032	6/19/92 2:02PM
p4n11__	587	6/18/92 1:26PM
p4n11_a	5,032	6/18/92 4:56PM
p4n11_b	1,258	6/19/92 9:13AM
p4n11_c	551	6/19/92 11:03AM
p4n11_d	629	6/19/92 11:13AM
p4n11_e	5,032	6/19/92 11:37AM
t4n13__	587	6/18/92 4:14PM
t4n13__c	725	6/19/92 2:14PM
u2n15-2	656	6/18/92 11:21AM
u2n15-3	656	6/17/92 5:01PM
u2n15__	587	6/17/92 11:22AM
u2n16-3	656	6/18/92 11:38AM
u2n16__	587	6/17/92 2:58PM
uco2dlm3.inp	1,837	6/15/92 10:06AM
unn00__	715	7/6/92 11:02AM
unn00__c	853	7/6/92 11:21AM
unn05__	1,174	6/26/92 4:04PM
unn05__c	8,803	7/6/92 9:22AM
unn06__	1,174	6/25/92 3:06PM
unn06__c	9,074	6/24/92 10:56AM
uon00__	716	7/6/92 11:26AM
uon00__c	863	7/6/92 11:28AM
uon05__	1,174	6/26/92 3:52PM
uon05_c	9,076	7/6/92 9:19AM
uon06_c	8,874	7/6/92 8:35AM
uphco016	9,304	8/25/92 9:13AM
uphco251	1,391	8/13/92 5:52PM
uphco256	29,419	8/11/92 11:31AM
[..]	[DIR]	
analyze.wql	4,270	11/16/93 3:56PM
csna0lm.wql	6,475	7/1/92 9:12AM
flamme2b.wql	18,134	6/5/92 2:40PM
flamme2c.wql	8,463	6/5/92 2:55PM
hsifig1.wkl	9,853	5/27/92 1:01PM
hsifig10.wql	5,672	5/28/92 8:48AM
hsifig11.wql	6,362	5/28/92 8:54AM
hsifig12.wql	5,669	5/28/92 9:07AM
hsifig13.wql	5,314	5/28/92 9:11AM
hsifig18.wql	4,286	5/28/92 9:16AM
hsifig2.wkl	7,075	5/27/92 1:10PM
hsifig20.wql	4,799	5/28/92 9:25AM
hsifig25.wql	11,186	5/28/92 9:40AM
hsifig27.wql	20,341	5/28/92 5:06PM
hsifig28.wql	5,109	5/28/92 4:10PM
hsifig29.wql	6,193	5/29/92 9:00AM
hsifig30.wql	5,119	5/29/92 9:06AM
hsifig31.wql	4,906	5/29/92 9:13AM
hsifig32.wql	4,788	5/29/92 10:07AM
hsifig35.wql	12,935	5/29/92 1:36PM
hsifig36.wql	4,417	5/29/92 3:41PM
hsifig37.wql	4,562	6/4/92 10:20AM
hsifig38.wql	5,518	6/4/92 10:21AM
hsifig47.wql	11,517	5/29/92 4:07PM
hsifig48.wql	4,519	5/29/92 4:23PM
hsifig49.wql	8,878	5/29/92 4:36PM
hsifig61.wql	8,360	5/29/92 5:04PM
hsifig62.wql	5,161	6/2/92 8:35AM
hsifig63.wql	10,097	6/2/92 9:27AM
huntf-1a.wkl	8,005	5/26/92 5:03PM
huntf-1b.wkl	6,535	5/27/92 9:30AM
huntf-2a.wkl	9,049	5/27/92 8:45AM
huntf-2b.wkl	6,544	5/27/92 9:34AM
huntf-3a.wql	7,142	5/27/92 11:03AM
huntf-3b.wql	8,526	5/27/92 11:01AM
huntf-4a.wql	8,432	5/27/92 11:31AM
huntf-4b.wkl	10,117	6/3/92 1:51PM
hypcoa.wql	8,239	6/11/92 3:30PM
install.wql	1,766	9/27/91 3:01AM
ishihf-3.wql	7,923	6/2/92 9:40AM
ishihf-4.wql	5,479	6/2/92 9:58AM
ishihf-5.wql	4,191	6/2/92 10:05AM
ishihwp.wql	12,694	6/3/92 3:59PM
katayf15.wql	7,902	6/2/92 10:23AM
ksat1.wql	16,910	11/11/93 4:16PM
ksat5080.wql	16,910	11/11/93 4:15PM
lieserl.wkl	5,137	11/29/94 2:42PM
lieserl.wka	5,137	11/29/94 2:42PM
lieserl.wql	5,137	11/29/94 2:42PM
lieserl.wrk	5,137	11/29/94 2:42PM
master.wql	69,500	2/12/92 4:00AM
nakayf3a.wql	19,511	6/26/92 2:09PM
nakayf3b.wql	11,060	6/26/92 2:21PM
nakayf4.wql	9,418	6/26/92 2:31PM
notauze.wql	5,354	6/26/92 1:50PM
optimizr.wql	6,215	2/12/92 4:00AM
register.wql	5,537	2/12/92 4:00AM
righf-1.wql	15,585	6/5/92 4:13PM
righf-2.wql	11,494	6/5/92 5:05PM
righf-3.wql	13,959	6/8/92 10:03AM
righf-5.wql	7,427	6/8/92 10:05AM
sample.wql	5,084	2/12/92 4:00AM
sancfla.aci	748	3/6/95 9:55AM
sancfla.wql	10,496	6/2/92 11:31AM
sancflc.wql	9,892	6/2/92 11:43AM
sancf4a.wql	4,968	6/2/92 12:42PM
sancf4b.wql	4,859	6/2/92 12:58PM
sancglb.wql	9,215	6/2/92 11:36AM
sanch.wql	28,294	6/4/92 11:51AM
sanfla.wkq	4,868	3/6/95 10:05AM
sibwta.wql	4,999	12/30/93 11:00AM
srna_005.wql	10,769	6/26/92 3:39PM
srna_05.wql	17,583	6/26/92 3:37PM
srnal_0.wql	11,636	6/26/92 3:33PM
srnaiso.wql	28,328	6/26/92 3:12PM
vochtf4.wql	5,938	6/2/92 10:55AM
vochtf5.wql	4,393	6/2/92 11:16AM

orange disk

analog	{DIR}	5/8/95	11:24AM
fiteql	{DIR}	5/8/95	11:28AM
[..]	{DIR}		
analog1.123	34,807	5/31/94	1:59PM
analog1.inp	48,145	5/31/94	8:54AM
analog1.sp5	45,208	5/31/94	10:22AM
analog2.123	46,981	5/31/94	2:00PM
analog2.inp	64,995	5/31/94	1:56PM
analog2.sp5	57,656	5/31/94	3:16PM
analog5.123	17,400	5/20/94	10:14AM
analog5.inp	38,509	5/27/94	8:49AM
analog8.sp5	64,824	5/26/94	9:10AM
analog8.spw	127,494	2/1/95	11:55AM
[..]	{DIR}		
fit2.exe	129,072	12/12/87	6:15PM

yellow disk

kohu	{DIR}	5/8/95	11:05AM
ktables	{DIR}	5/8/95	10:47AM
[..]	{DIR}		
kohu41.dta	2,543	10/14/94	1:56PM
kohu41c.ccm	18,856	10/14/94	1:29PM
kohu41c.sp5	33,796	10/14/94	2:18PM
kohu41c.sst	19,602	10/14/94	1:39PM
kohu41d.dlm	18,855	10/14/94	2:33PM
kohu41d.sp5	34,300	10/17/94	8:17AM
kohu41d.sst	19,602	10/14/94	2:43PM
kohu41t.sp5	30,708	10/19/94	2:22PM
kohu41t.sst	19,602	10/17/94	9:00AM
kohu41t.tlm	27,902	10/17/94	8:50AM
kou41a11.sp5	65,532	10/24/94	10:10AM
kudata41.sp5	2,788	10/12/94	9:56AM
utmplat1.sp5	18,916	10/18/94	2:50PM
[..]	{DIR}		
bindaa.1	14,203	12/2/94	5:56PM
bindaa.2	11,022	3/23/95	8:56AM
bindaa.3	14,113	3/23/95	10:23AM
bindaa.4	14,201	12/2/94	5:56PM
bindaa.5	33,936	2/22/95	10:15AM
bindaa.6	9,730	3/23/95	8:48AM
bindaa.7	9,727	3/23/95	9:20AM
bindas.8	8,594	3/23/95	9:22AM
bindef.1	6,814	3/23/95	9:55AM
binding.am3	14,998	3/8/94	8:35AM
binding.np5	9,625	3/8/94	8:49AM
binding.pu4	14,921	3/8/94	8:30AM
binding.pu5	14,638	3/8/94	8:34AM
binding.th4	14,945	3/8/94	8:37AM
binding.u6	10,112	3/28/95	1:11PM
bindna.1	9,030	12/2/94	6:03PM
bindna.2	26,133	3/23/95	9:26AM
bindnb.3	35,883	2/17/95	4:39PM
bindnb.4	29,369	3/23/95	9:24AM
bindnf.5	8,179	3/23/95	10:05AM
bindnf.6	8,179	3/23/95	9:03AM
bindnf.7	8,254	12/20/94	4:03PM
bindng.8	26,086	3/23/95	9:04AM
bindnk.9	10,949	3/23/95	10:06AM
bindnl.10	26,215	3/23/95	9:01AM
bindnm.11	8,811	3/23/95	9:00AM
bindnm.12	26,103	3/23/95	10:03AM
bindns.13	8,419	3/23/95	9:30AM
bindpa.1	7,672	3/23/95	11:21AM
bindpg.2	9,812	3/23/95	11:22AM
bindpg.3	7,657	3/23/95	11:10AM
bindpg.4	7,686	3/23/95	10:54AM
bindpg.5	9,868	3/23/95	11:34AM
bindta.1	8,738	3/23/95	9:33AM
bindts.2	9,087	3/23/95	10:08AM
bindts.3	10,021	2/13/95	5:16PM
binduf.1	16,400	3/23/95	8:43AM
binduf.10	10,534	3/23/95	11:20AM
binduf.11	10,736	3/23/95	11:17AM
binduf.12	27,840	3/23/95	10:11AM
binduf.13	16,620	3/23/95	9:14AM
binduf.14	10,548	3/23/95	9:45AM
binduf.2	10,514	3/23/95	8:45AM
binduf.3	30,553	2/8/95	3:32PM
binduf.4	10,547	3/23/95	9:11AM
binduf.5	10,071	3/28/95	12:46PM
binduf.6	10,515	3/23/95	11:30AM
binduf.7	30,937	2/8/95	3:15PM
binduf.8	10,426	7/11/94	10:55AM
binduf.9	10,766	3/23/95	10:38AM
binduq.15	12,496	3/23/95	10:16AM
binduq.16	10,708	3/23/95	9:07AM
binduq.17	9,276	3/23/95	9:08AM
binduq.18	12,306	3/23/95	11:28AM
binduq.19	13,697	3/23/95	11:27AM
binduq.20	11,005	3/23/95	11:16AM
binduq.21	10,592	3/23/95	11:13AM
binduq.22	10,356	3/23/95	10:39AM
binduq.23	10,501	3/23/95	10:41AM
binduq.24	12,436	3/23/95	11:07AM
binduq.25	9,974	3/27/95	9:44AM
binduq.26	10,598	3/23/95	9:35AM
binduk.27	23,767	3/23/95	11:38AM
bindum.28	9,290	3/23/95	11:24AM
bindum.29	9,307	3/23/95	10:51AM
bindum.30	11,462	11/18/94	5:55PM
bindum.31	9,270	3/23/95	11:15AM
bindum.32	9,278	3/23/95	11:14AM
bindut.33	8,421	3/10/95	9:35AM
bindut.34	9,726	3/28/95	1:23PM
bindut.35	11,577	3/28/95	1:23PM
bindut.36	11,577	3/28/95	1:24PM
bindut.37	11,570	3/28/95	1:25PM
bindut.38	11,566	3/28/95	1:25PM
bindut.39	11,322	3/28/95	1:26PM
bindut.40	11,571	3/28/95	1:26PM
tblindx.lst	44,344	3/28/95	1:40PM

maroon disk

lieser	{DIR}	5/8/95	1:00PM
naknp	{DIR}	5/8/95	1:15PM
payne	{DIR}	5/8/95	1:17PM
rigam	{DIR}	5/8/95	1:18PM
rigth	{DIR}	5/8/95	1:21PM
[..]	{DIR}		
t	{DIR}	5/8/95	1:00PM
figlcl0.prn	339	11/30/94	8:55AM
figlcl5.prn	390	8/19/93	10:17AM
figlclo.wk1	339	11/30/94	8:55AM
figlclo.wkq	339	11/30/94	8:55AM
figlclo.wql	339	11/30/94	8:55AM
fig3b.prn	570	8/19/93	10:26AM
fig3c.prn	600	8/19/93	10:29AM
fig3d.prn	720	8/19/93	10:31AM
fig3d.wkq	7,669	2/1/95	9:13AM
fig3e.prn	228	2/3/95	10:00AM
fig3e.wkq	4,651	2/3/95	9:57AM
fig3f.prn	182	2/6/95	1:14PM
fig3f.wkq	4,189	2/6/95	1:10PM
fig3g.prn	521	2/7/95	10:38AM
fig3g.wkq	8,130	2/7/95	10:31AM
form.wks	1,527	1/26/95	8:48AM
lie05.wkq	4,784	1/16/95	2:51PM
lie15.spw	61,957	3/22/95	9:37AM
lie15.sst	20,201	3/22/95	8:50AM
lie15.xfm	40	2/15/95	1:58PM
lie15d.inp	18,854	3/22/95	8:27AM
lie15t.inp	27,984	3/22/95	10:05AM
lie15t.sst	20,196	3/22/95	10:14AM
lie3b.prn	392	1/17/95	10:08AM
lie3b.wkq	6,268	1/16/95	1:44PM
lie3bt.spw	7,232	2/24/95	1:30PM
lie3c.prn	406	1/26/95	10:04AM
lie3c.wkq	5,951	1/26/95	9:29AM
lie3cd.inp	19,613	2/22/95	8:32AM
lie3cd.spw	58,955	2/27/95	4:59PM
lie3ct.inp	28,749	2/28/95	9:56AM
lie3ct.sst	20,206	2/28/95	10:11AM
lie3d.prn	485	2/1/95	9:26AM
lie881.tbl	23,554	3/17/95	9:39AM
lie882.tbl	29,155	3/17/95	10:56AM
lie883.tbl	31,738	3/17/95	11:20AM
liesedat.wkq	7,469	2/13/95	8:58AM
liesedta.wkq	7,469	1/12/95	1:14PM
lieser.prn	376	1/12/95	4:02PM
lieserl.wql	5,137	11/29/94	2:42PM
lieseral.spw	78,126	3/10/95	10:54AM
liet.spw	7,232	2/16/95	11:02AM
rs.sp5	7,012	11/29/94	9:48AM
utio2.wp	4,849	1/12/95	11:25AM

[..]	{DIR}		
data1lc.sp5	2,820	10/10/94	1:41PM
datac31.dta	3,200	10/10/94	1:35PM
naknp3lc.ccm	10,285	10/14/94	10:17AM
naknp3lc.sp5	22,212	10/14/94	10:43AM
naknp3lc.sst	9,396	10/14/94	10:22AM
naknp3ld.dlm	10,285	10/14/94	11:06AM
naknp3ld.sp5	22,180	10/14/94	11:26AM
naknp3ld.sst	9,396	10/14/94	11:12AM
naknp3lt.sp5	22,180	10/17/94	10:49AM
naknp3lt.sst	9,396	10/17/94	10:38AM
naknp3lt.tlm	15,241	10/17/94	10:32AM
naknp43c.ccm	10,302	10/13/94	2:26PM
naknp43c.sp5	22,572	10/14/94	10:46AM
naknp43d.dlm	10,285	10/13/94	3:04PM
naknp43d.sp5	22,964	10/14/94	10:53AM
naknp43t.sp5	22,136	10/17/94	11:13AM
naknp43t.sst	9,396	10/17/94	11:07AM
naknp43t.tlm	15,253	10/17/94	11:02AM
nknp31a1.sp5	41,196	10/21/94	8:23AM
nknp43a1.sp5	41,416	10/24/94	9:41AM
[..]	{DIR}		
xao.bat	373	10/3/94	11:27AM
xoh2uo22.d73	5,494	10/3/94	11:29AM
xoh2uo23.d73	5,492	10/3/94	11:32AM
xoh2uo24.d73	5,494	10/3/94	11:34AM
xohuo2.d73	5,492	10/3/94	11:37AM
xohuo21.d73	5,492	10/3/94	11:41AM
xohuo22.d73	5,493	1/25/94	4:47PM
xohuo23.d73	5,492	10/3/94	1:56PM
xohuo24.d73	5,493	1/25/94	4:47PM
xouo2.d73	5,493	1/25/94	4:47PM
xouo21.d73	5,493	1/25/94	4:47PM
xouo22.d73	5,493	1/25/94	4:47PM
[..]	{DIR}		
raml2dta.sp5	2,628	10/26/94	11:36AM
rigaml2c.ccm	11,999	10/26/94	1:48PM
rigaml2c.sst	9,450	10/26/94	1:53PM
rigaml2d.dlm	11,999	10/27/94	9:31AM
rigaml2d.sst	9,450	10/27/94	9:36AM
rigaml2t.dta	1,231	10/26/94	11:34AM
rigaml2t.sp5	35,188	10/31/94	9:44AM
rigaml2t.sst	9,450	10/26/94	11:14AM
rigaml2t.tlm	17,809	10/26/94	11:07AM
[..]	{DIR}		
rigth11.dta	1,723	10/28/94	9:52AM
rigth11c.ccm	15,425	10/28/94	11:14AM
rigth11c.sst	13,122	10/28/94	11:22AM
rigth11d.dlm	13,711	10/28/94	9:35AM
rigth11d.sp5	41,264	10/31/94	9:34AM
rigth11d.sst	11,664	10/28/94	9:41AM
rigth11t.sst	11,664	10/28/94	1:44PM
rigth11t.tlm	20,353	10/28/94	1:36PM

green disk

lieser	{DIR}	5/8/95	11:41AM
[..]	{DIR}		
c	{DIR}	5/8/95	11:45AM
d	{DIR}	5/8/95	11:50AM
t	{DIR}	5/8/95	12:56PM

black disk

model	{DIR}	12/13/94	10:08AM
oldrig	{DIR}	5/11/95	9:11AM
[..]	{DIR}		
amsif5	{DIR}	12/13/94	10:09AM
ccm	{DIR}	12/13/94	10:08AM
dlm	{DIR}	12/13/94	10:09AM
npsif5	{DIR}	12/13/94	10:10AM
thsif5	{DIR}	12/13/94	10:09AM
tlm	{DIR}	12/13/94	10:09AM
[..]	{DIR}		
acdz.bat	301	2/8/94	11:00AM
athcdz1.go	27,006	2/7/94	3:31PM
axoh2th4.cgo	5,988	2/8/94	11:04AM
axohth2.cgo	5,988	2/8/94	1:37PM
axohth3.cgo	5,988	2/8/94	11:06AM
axohth4.cgo	5,988	2/8/94	1:39PM
axoth.cgo	5,989	2/8/94	11:08AM
axoth1.cgo	5,988	2/8/94	11:19AM
axoth2.cgo	5,988	2/8/94	1:41PM
axoth3.cgo	5,988	2/8/94	11:18AM
axoth4.cgo	5,988	2/8/94	11:22AM
r9lamc1.sp5	18,228	6/1/94	2:27PM
r9lamc2.sp5	16,440	6/1/94	2:49PM
r9lamd1.sp5	20,276	6/1/94	2:58PM
r9lamd2.sp5	16,440	6/1/94	3:01PM
r9lamt1.sp5	17,924	6/1/94	3:03PM
r9lamt2.sp5	17,340	3/29/94	2:48PM
rig91th1.sp5	17,252	3/25/94	8:47AM
rigsio2.wql	6,951	2/9/94	10:36AM

Project 20-5704-472 - Sorption modeling for HLW
DRWRS Performance Assessment closed due to CNWRA
reorganization - effective 1/20/16