Scientific Notebook #278

RADIONUCLIDE TRANSPORT

Project No. 20-1402-871

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The entries in this electronic scientific notebook #278 document activities conducted under the Key Technical Issue (KTI):

RADIONUCLIDE TRANSPORT

(Project No. 20-1402-871)

Individual(s) performing the activity: Roberto T. Pabalan

Objective:

Develop models for describing and predicting ion exchange equilibria between aqueous solutions and the zeolite mineral clinoptilolite.

Staff qualification requirements:

Geochemical modeling: Familiarity with thermodynamic models for ion exchange; ability to use and interpret results of geochemical models/codes.

Experimental work: Experience in design and conduct of ion exchange experiments.

Technical Approach:

Use experimental data from published literature and from CNWRA experiments to derive parameters for a Margules solid solution model for zeolites. Use data from published literature to calculated activity coefficients of aqueous ions using the Pitzer ion interaction model. The Margules model accounts for nonideal behavior of zeolite components. The Pitzer model accounts for nonideality in the aqueous phase.

Note that no new CNWRA experiments are currently being conducted as part of this study. CNWRA data are from experiments documented in Scientific Notebooks #001, #008, #015, #020, and #060.

Commercial software may be used in data manipulation and presentation, including SigmaPlot, Excel, and TableCurve. Publicly available geochemical codes, such as EQ3/6, may be used for calculating aqueous activity coefficients.

Technical Basis of the Study

Zeolite minerals are naturally-occurring aluminosilicate compounds with a characteristic three-dimensional pore system and large pore apertures that allow relatively easy exchange of cations between aqueous solutions and intracrystalline sites. Because of their favorable ion exchange selectivity for certain cations such as Cs^+, Sr^{2+}, and NH_4^+, zeolite minerals, particularly clinoptilolite, are of interest for use in the treatment of nuclear wastewaters, municipal and industrial wastewaters, and acid mine drainage waters, as well as in the remediation of sites contaminated with fission products such as ^{90}Sr and $^{135,137}Cs$ resulting from nuclear fallout. Additional interest arises from the potential siting of a high-level nuclear waste repository at Yucca Mountain, Nevada, which is underlain by diagenetically-altered, zeolite-rich (predominantly clinoptilolite) rhyolitic tuffs that could serve as barriers to radionuclide migration to the accessible environment.

Ion exchange equilibria is a function of solid and aqueous phase composition and aqueous solution concentration. Because these parameters can vary substantially for the chemical system of interest, it is essential to have chemical models that allow accurate description and prediction of ion exchange equilibria. In a previous study (Pabalan, 1994)[1], a thermodynamic approach that was found useful for this purpose combined the Pitzer electrolyte solution model with a Margules solid solution formulation. The former was used to describe nonideal behavior in the aqueous phase, whereas the latter accounted for nonideality effects in the zeolite solid. The thermodynamic approach was successful in describing and predicting ion exchange equilibria between clinoptilolite and aqueous solutions of Na^+/K^+ and Na^+/Ca^{2+} over wide ranges of solution composition and concentration (Pabalan, 1994).

In this study, additional data on ion exchange between clinoptilolite and aqueous solutions of Na^+/Sr^{2+}, K^+/Sr^{2+}, and K^+/Ca^{2+}, which were derived from previous CNWRA experiments, were

[1] Pabalan, R. T. 1994. Thermodynamics of ion-exchange between clinoptilolite and aqueous solutions of Na^+/K^+ and Na^+/Ca^{2+}. *Geochim. Cosmochim. Acta* **58**, 4573-4590.

interpreted. The data were used to derive Margules parameters, equilibrium constants, and Gibbs free energies for binary ion exchange reactions. Using the Pitzer equations for aqueous activity coefficients, predicted isotherms for ion exchange involving Na^+/Sr^{2+}, K^+/Sr^{2+}, and K^+/Ca^{2+} were derived as functions of solution composition and concentration. In addition, the use of zeolite composition to constrain the chemistry of the coexisting aqueous phase was investigated. This approach could be useful in providing chemical information on the chemistry of groundwaters in zeolitic, hydrologically unsaturated stratigraphic horizons, such as at Yucca Mountain, where sampling of the water is not practicable.

Summary of Experimental Procedures

The procedures used in CNWRA experiments are briefly summarized here.

Na^+/Sr^{2+} Ion Exchange

Ion exchange experiments involving Na^+/Sr^{2+} were conducted by equilibrating weighed amounts of Na-clinoptilolite powder with solutions containing Na^+ and Sr^{2+} at different equivalent concentration ratios, but at a constant total normality equal to 0.005, 0.05, or 0.50 N. The Na-clinoptilolite material, with grain size in the range of ~75–150 μm, was prepared from clinoptilolite-rich tuff samples (source locality: Death Valley Junction, California) obtained from Minerals Research Company (Clarkson, New York). Mineral impurities in the tuff were removed by heavy liquid (tetrabromoethane + *NN*-dimethyl formamide) separation, by treatment with a sodium acetate buffer (pH~5) to dissolve the carbonates, and by reacting with a sodium dithionite-citrate-bicarbonate mixture to dissolve iron oxides. The purified clinoptilolite was converted into the Na-form by ion exchange with NaCl solutions at 90°C, then dried in an oven at about 65 □C and later equilibrated with water vapor over saturated NaCl solution in a dessicator until constant mass was attained (~10 days). This last step was necessary to provide a constant zeolite water content prior to both chemical analysis and initiation of ion exchange experiments. A detailed description of clinoptilolite preparation and characterization is given in Pabalan (1994). The chemical compositions of the purified and Na-form clinoptilolite determined by inductively-coupled plasma emission spectrometry (ICPES) and gravimetric analysis are given in Table 1. The chemical formula of the Na-clinoptilolite was calculated to be

Table 1. Composition of clinoptilolite used in this study

Component	Weight percent[a]		
	Purified	Na-form	K-form
SiO_2	69.13	68.28	66.03
Al_2O_3	11.38	11.28	10.66
TiO_2	0.06	0.04	0.06
Fe_2O_3	0.47	0.40	0.39
MgO	0.27	0.16	0.16
CaO	0.09	0.02	0.01
Na_2O	4.83	6.36	0.0
K_2O	2.77	0.66	10.09
H_2O	—	15.21	12.70
TOTAL	89.00[b]	102.41	100.1

[a]Average of 4, 6, and 3 samples, respectively, of purified, Na-form, and K-form clinoptilolite
[b]The water content was not determined.

$(Na_{1.804}K_{.123})\cdot(Ca_{.003}Mg_{.035})\cdot(Al_{1.947}Fe^{3+}_{.044})\cdot(Si_{10.002}Ti_{0.004})O_{24}\cdot 7.43H_2O$. For comparison, the idealized formula of the Na-endmember clinoptilolite is $Na_2Al_2Si_{10}O_{24}\cdot 8H_2O$. The cation exchange capacity (CEC) of the Na-clinoptilolite calculated from its chemical composition is $2.04\pm0.02\times10^{-3}$ eq/g (Pabalan, 1994).

Aqueous mixtures of Na^+/Sr^{2+} at 0.50 N and with equivalent mole fractions of Sr^{2+} at 0.1 ,0.2, ... 1.0, were prepared by mass from reagent-grade NaCl and $SrCl_2\cdot 6H_2O$. Solutions at 0.05 N and 0.005N were prepared by factor of ten dilutions of the 0.50 N and 0.05 N mixtures, respectively. The initial total Sr concentration of each solution, which was calculated from the mass of $SrCl_2\cdot 6H_2O$ reagent used, was checked by atomic absorption (AA) analysis. To allow determination of the Sr^{2+} concentration in aqueous samples by liquid scintillation counting, each of the starting solutions was spiked with ^{90}Sr (50 pCi per gram of solution).

The mass of clinoptilolite used in the experiments ranged from 0.03 to 1.6 g, and the solution volumes ranged from 10 to 250 mL. The zeolite-mass to solution-volume ratios and the initial

aqueous compositions were optimized so that there are significant differences between the initial and final cation concentrations and a relatively evenly-spaced distribution of data points along the ion exchange isotherm. The clinoptilolite and aqueous solutions were reacted in capped polypropylene bottles that were agitated and thermostatted at 25 °C in a shaker water bath. Kinetics tests indicated that ion exchange equilibrium is closely approached in about two to three days. Samples of experimental solutions were taken after at least one week of reaction time.

To verify the reversibility of the ion exchange process, several isotherm points at 0.05 N were reversed by adding to the remaining solutions known volumes of a 0.05 N NaCl solution. The new mixtures were allowed to reequilibrate for at least one week, then samples were taken for analysis. The new data, together with the forward isotherm values for the selected solutions, allowed reverse isotherm points to be calculated.

The initial and final solution concentrations of both Na^+ and Sr^{2+} were analyzed. The Na^+ concentrations were measured either by using an Orion ion-selective electrode (ISE) or by atomic absorption (AA) spectrometry (Perkin-Elmer Model 3100 AA analyzer). The Sr^{2+} concentrations were determined by liquid scintillation analysis (Cerenkov counting) of $^{90}Sr/^{90}Y$ using a Packard Tri-Carb Model 1900TR liquid scintillation analyzer (LSA) after secular equilibrium had been reached between ^{90}Sr and ^{90}Y in the aqueous samples. It was assumed that the ion exchange of ^{90}Sr is in direct proportion to all other Sr isotopes. The overall uncertainty in Sr^{2+} concentrations was estimated to be ±1 %, based on the LSA counting error. The uncertainty in measured Na^+ concentration was estimated to be ±2 %, based on the reproducibility of replicate analyses of experimental and standard solutions.

K^+/Ca^{2+} and K^+/Sr^{2+} Ion Exchange

The procedure used to study ion exchange involving K^+/Ca^{2+} and K^+/Sr^{2+} is generally similar to that used for the Na^+/Sr^{2+} experiment. Weighed amounts of K-clinoptilolite were equilibrated with known volumes of K^+/Ca^{2+} or K^+/Sr^{2+} solutions with different cationic ratios but a constant normality equal to 0.05 N. The aqueous mixtures of K^+/Ca^{2+} and K^+/Sr^{2+} were prepared from reagent-grade KCl, $CaCl_2 \cdot 2H_2O$, or $SrCl_2 \cdot 6H_2O$. The K^+/Sr^{2+} mixtures were spiked with ^{90}Sr (50 pCi per gram of solution). The K-clinoptilolite used in the experiments was prepared by exchanging Na-clinoptilolite with KCl solutions at 90 °C. Its composition determined by ICPES

and gravimetric analysis is given in Table 1. Its chemical formula and CEC are calculated to be $(K_{1.955})(Ca_{.002}Mg_{.036})(Al_{1.908}Fe^{3+}_{.045})(Si_{10.028}Ti_{.007})O_{24}\cdot 6.43H_2O$ and $2.06\pm0.03\times10^{-3}$ eq/g, respectively.

The K^+ and Ca^{2+} solution concentrations were determined using ISE analysis. Some aqueous samples were also taken for AA analysis, the results of which agreed very well with the ISE data. Overall uncertainties in the measured concentrations of K^+ and Ca^{2+} are estimated to be ±3 % and ±4 %, respectively, based on the reproducibility of replicate analyses of experimental and standard solutions. Sr^{2+} concentrations were determined using LSA as described previously.

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July 13, 1998

Summary of Experimental Results

The following are summaries of experimental data on ion exchange involving clinoptilolite and aqueous solutions of Na^+/Sr^{2+}, K^+/Ca^{2+}, and K^+/Sr^{2+} taken from the laboratory notebooks.

Na^+/Sr^{2+} Ion Exchange

Table 2. Summary of experimental data on Na^+/Sr^{2+} exchange at 0.05 N solution concentration

Exptl. soln	soln. volume (mL)	weight zeolite (g)	Sr initial ppm	Sr final ppm	Na initial ppm	Na final ppm
1	25	0.3102	219	16.5	1050	1154
2	25	0.1659	219	36.7	1050	1136
3	25	0.1032	219	79.4	1050	1122
4	25	0.2321	438	101.3	934	1096
5	25	0.1519	438	187.2	934	1070
6	25	0.1941	657	300.6	817	1002
7	25	0.2186	876	441.5	700	928
8	25	0.2658	1095	542.5	584	872
9	25	0.2809	1314	693.8	467	786
10	25	0.3182	1533	821.1	351	724
11	25	0.2756	1752	1092.7	236	590
12	25	0.3035	1971	1234.0	117	516
13	25	0.2867	2191	1431.7	0	394
14	25	0.2005	2191	1639.2	0	292
15	50	0.3088	2191	1779.7	0	229
16	50	0.2407	2191	1859.7	0	189
17	50	0.1893	2191	1921.6	0	147
18	50	0.1269	2191	1998.0	0	104
19	100	0.1361	2191	2073.8	0	57.4
20	100	0.0840	2191	2115.4	0	34.9

Table 3. Summary of experimental data on Na^+/Sr^{2+} exchange at 0.5 N solution concentration

Exptl. soln	soln. volume (mL)	weight zeolite (g)	Sr initial ppm	Sr final ppm	Na initial ppm	Na final ppm
1	10	1.6259	1096	146	10920	11300
2	10	1.4012	2190	528	10346	11000
3	10	1.9243	4381	1125	9196	10750
4	10	0.8024	4381	2466	9196	10000
5	10	0.9146	6571	3962	8047	9290
6	10	1.1063	8762	5219	6897	8570
7	10	0.5315	8762	6818	6897	7930
8	10	0.7589	10953	8004	5748	7250
9	10	0.6069	13143	10436	4598	6020
10	10	0.5759	15333	12656	3449	4910
11	10	0.6163	17524	14226	2299	3980
12	10	0.6093	19714	16231	1150	2940
13	10	0.7200	21905	17811	0	2250
14	10	0.4967	21905	19038	0	1650
15	25	0.8588	21905	19636	0	1180
16	25	0.5877	21906	20364	0	837
17	25	0.3931	21906	20781	0	562
18	50	0.4170	21906	21545	0	280
19	100	0.2460	21906	21726	0	109

Table 4. Summary of experimental data on Na^+/Sr^{2+} exchange at 0.005 N solution concentration

Exptl. soln	soln. volume (mL)	weight zeolite (g)	Sr initial ppm	Sr final ppm	Na initial ppm	Na final ppm
1	50	0.0957	22	0.1	104	118
2	100	0.1023	22	0.5	104	117
3	100	0.1621	44	0.7	92.3	116
4	100	0.1061	44	3.4	92.3	115
5	100	0.1363	66	4.4	80.3	114
6	100	0.1520	88	7.9	69.1	112
7	100	0.1746	110	13.0	57.3	110
8	100	0.1532	110	20.9	57.3	106

9	100	0.1628	131	32.8	46	99.9
10	100	0.1727	153	42.7	34.8	93.7
11	100	0.1831	175	55.9	23	87.1
12	100	0.1821	197	73.9	11.4	77.5
13	100	0.1704	219	99.4	0	62.9
14	100	0.1478	219	112.9	0	55.9
15	100	0.1280	219	126.6	0	48.9
16	100	0.1011	219	143.2	0	39
17	100	0.0729	219	165.4	0	29.1
18	250	0.1124	219	182.7	0	17.9
19	250	0.0574	219	202.0	0	9.6
20	250	0.0303	219	211.3	0	5.2

K^+/Sr^{2+} Ion Exchange

Table 5. Summary of experimental data on K^+/Sr^{2+} exchange at 0.05 N solution concentration.

Exptl. soln	soln. volume (mL)	weight zeolite (g)	Sr initial ppm	Sr final ppm	K initial ppm	K final ppm
1	50	0.3984	220	205	1850	1860
2	50	0.6713	439	391	1670	1690
3	50	1.1839	875	730	1280	1400
4	50	0.6228	1096	939	1070	1170
5	50	0.9764	1314	1127	862	1050
6	50	0.8678	1534	1280	652	885
7	50	0.8892	1753	1451	435	722
8	50	0.9647	1972	1568	220	607
9	50	0.6526	1972	1615	220	521
10	50	0.4423	1972	1701	220	431
11	50	0.2974	1972	1772	220	377
12	50	0.4861	2190	1865	0	313
13	50	0.3854	2190	1886	0	269
14	50	0.3085	2190	1898	0	233
15	50	0.2486	2190	1977	0	201
16	50	0.1992	2190	2000	0	177
17	50	0.1256	2190	2042	0	128
18	100	0.1939	2190	2097	0	104
19	250	0.1631	2190	2144	0	44.5
20	250	0.0925	2190	2151	0	27.3
21	250	0.0300	2190	2175	0	9

K^+/Ca^{2+} Ion Exchange

Table 6. Summary of experimental data on K^+/Ca^{2+} exchange at 0.05 N solution concentration.

Exptl. soln	soln. volume (mL)	wt zeolite (g)	Ca initial ppm	Ca final ppm	K initial ppm	K final ppm
1	10	0.4085	96.2	83.4	1730	1790
2	10	0.1399	96.2	92.1	1730	1790
3	10	0.1928	197	182	1560	1630
4	10	0.1909	289	268	1380	1390
5	10	0.1782	398	372	1190	1260
6	10	0.1852	488	458	1000	1090
7	10	0.1857	558	535	806	922
8	10	0.1972	674	606	603	735
9	10	0.1676	765	687	401	564
10	10	0.1545	848	766	200	399
11	10	0.1066	848	801	200	348
12	10	0.1023	961	868	0	214
13	25	0.1801	961	870	0	172
14	25	0.124	961	895	0	138
15	25	0.086	961	910	0	103
16	50	0.1174	961	888	0	84.5
17	50	0.0785	961	904	0	64.3
18	100	0.0835	961	913	0	41
19	250	0.0618	961	921	0	15.8

Results of these binary ion-exchange experiments can be represented conveniently by ion-exchange isotherms, which are plots of the equilibrium fraction of an exchanging ion in solution versus the equilibrium fraction of that same ion in the zeolite at constant temperature and total solution concentration. The isotherm is usually plotted in terms of the equivalent cationic fraction of the ion in solution, E_i, against that in the solid, $\bar{E}_i$. Values of E_i and $\bar{E}_i$ can be calculated from the zeolite mass (W, grams), the solution volume (V, liters), and the initial (i) and final (f) molar concentrations (M, moles/liter solution) of cation A using the equation:

$$\bar{E}_A = z_A(M_{A,i} - M_{A,f})V/(W \bullet CEC); \quad E_A = z_A M_{A,f}/TN \qquad (1)$$

where TN is the total cation normality of the aqueous solution. As mentioned previously, CEC of the Na-clinoptilolite is equal to 2.04×10^{-3} eq/g based on the zeolite composition, whereas the CEC of the K-clinoptilolite is $2.06\pm0.03\text{x}10^{-3}$ eq/g.

Various investigators have emphasized the need to analyze for *each* exchanging ion when constructing exchange isotherms because small errors in the analysis of an ion can cause large errors in the calculated isotherm points, particularly at the extrema of the isotherm plot. In this study, therefore, solution concentrations of the competing ion B (e.g., K^+ in K^+/Sr^{2+} experiments) were also analyzed in addition to the concentration of ion A. The data on B permitted values of E_A and $\bar{E}_A$ to be independently calculated from the equation:

$$\bar{E}_A = z_B(M_{B,f} - M_{B,i})V/(W \bullet CEC); \quad E_A = 1 - z_B M_{B,f} / TN. \qquad (2)$$

Note that to convert units in ppm (parts per million) to M (molarity), the conversion factor is:

$$M_i = ppm_i/atomic\text{-}mass_i/1000$$

The atomic masses of Na, K, Ca, and Sr are 22.990, 39.098, 40.08, and 87.62 g/mol, respectively.

For modeling purposes, the zeolite composition can also be represented in terms of the cationic mole fraction of *i* in the zeolite, $\bar{X}_i$, which can be calculated from:

$$\bar{X}_A = (\bar{E}_A / z_A) / [(\bar{E}_A / z_A) + ((1-\bar{E}_A) / z_B)]; \quad \bar{X}_B = (1-\bar{X}_A) \qquad (3)$$

using analytical data on cation A [Eqn. (1)] or cation B [Eqn. (2)].

Using the data listed in Tables 2 to 6, values of E_i, $\bar{E}_i$, and $\bar{X}_i$ were calculated. These are listed in the following Tables 7 to 11.

Table 7. Equivalent and cationic mole fractions for Na^+/Sr^{2+} exchange at 0.05 N solution concentration calculated from data in Table 2

Exptl. soln	$\bar{E}_{Sr}$ from Sr data	E_{Sr} from Sr data	$\bar{E}_{Sr}$ from Na data	E_{Sr} from Na data	$\bar{X}_{Sr}$ from Sr data	$\bar{X}_{Sr}$ from Na data
1	0.1826	0.0075	0.1787	-0.0039	0.1005	0.0981
2	0.3073	0.0168	0.2763	0.0117	0.1816	0.1603
3	0.3784	0.0363	0.3719	0.0239	0.2333	0.2284
4	0.4057	0.0463	0.3721	0.0465	0.2545	0.2285
5	0.4618	0.0855	0.4773	0.0692	0.3002	0.3134

6	0.5137	0.1372	0.5081	0.1283	0.3456	0.3405
7	0.5560	0.2016	0.5560	0.1927	0.3850	0.3850
8	0.5814	0.2477	0.5776	0.2414	0.4098	0.4060
9	0.6177	0.3167	0.6054	0.3162	0.4468	0.4341
10	0.6258	0.3749	0.6249	0.3702	0.4554	0.4544
11	0.6692	0.4988	0.6847	0.4867	0.5028	0.5206
12	0.6793	0.5633	0.7008	0.5511	0.5143	0.5394
13	0.7409	0.6536	0.7326	0.6572	0.5884	0.5780
14	0.7698	0.7483	0.7763	0.7460	0.6258	0.6344
15	0.7451	0.8125	0.7906	0.8008	0.5938	0.6537
16	0.7701	0.8490	0.8371	0.8356	0.6261	0.7199
17	0.7961	0.8773	0.8279	0.8721	0.6612	0.7063
18	0.8508	0.9121	0.8737	0.9095	0.7403	0.7758
19	0.9635	0.9467	0.8993	0.9501	0.9295	0.8170
20	1.0069	0.9657	0.8859	0.9696	1.0139	0.7951

Table 8. Equivalent and cationic mole fractions for Na^{+}/Sr^{2+} exchange at 0.5 N solution concentration calculated from data in Table 3

Exptl. soln	$\bar{E}_{Sr}$ from Sr data	E_{Sr} from Sr data	$\bar{E}_{Sr}$ from Na data	E_{Sr} from Na data	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from Na data
1	0.0654	0.0066	0.0498	0.0170	0.0338	0.0255
2	0.1328	0.0241	0.0996	0.0431	0.0711	0.0524
3	0.1893	0.0514	0.1722	0.0648	0.1046	0.0942
4	0.2671	0.1126	0.2136	0.1301	0.1541	0.1196
5	0.3192	0.1809	0.2899	0.1918	0.1899	0.1695
6	0.3584	0.2383	0.3224	0.2545	0.2183	0.1922
7	0.4094	0.3112	0.4144	0.3101	0.2574	0.2614
8	0.4348	0.3654	0.4221	0.3693	0.2778	0.2675
9	0.4991	0.4764	0.4996	0.4763	0.3325	0.3330
10	0.5202	0.5778	0.5411	0.5729	0.3515	0.3709
11	0.5988	0.6494	0.5816	0.6538	0.4273	0.4100
12	0.6397	0.7410	0.6266	0.7442	0.4703	0.4562
13	0.6362	0.8131	0.6663	0.8043	0.4665	0.4996
14	0.6458	0.8691	0.7083	0.8565	0.4768	0.5484
15	0.7392	0.8964	0.7324	0.8973	0.5862	0.5778
16	0.7339	0.9297	0.7592	0.9272	0.5797	0.6118
17	0.8004	0.9487	0.7621	0.9511	0.6672	0.6156
18	0.4847	0.9835	0.7159	0.9756	0.3199	0.5575
19	0.8185	0.9918	0.9448	0.9905	0.6928	0.8953

Table 9. Equivalent and cationic mole fractions for Na^+/Sr^{2+} exchange at 0.005 N solution concentration calculated from data in Table 4

Exptl. soln	$\bar{E}_{Sr}$ from Sr data	E_{Sr} from Sr data	$\bar{E}_{Sr}$ from Na data	E_{Sr} from Na data	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from Na data
1	0.1281	0.0004	0.1560	-0.0265*	0.0684	0.0846
2	0.2347	0.0025	0.2710	-0.0178*	0.1329	0.1567
3	0.2990	0.0031	0.3117	-0.0091*	0.1757	0.1847
4	0.4284	0.0154	0.4562	-0.0004*	0.2726	0.2955
5	0.5056	0.0201	0.5272	0.0083	0.3383	0.3579
6	0.5898	0.0360	0.6018	0.0257	0.4182	0.4304
7	0.6216	0.0594	0.6436	0.0431	0.4510	0.4745
8	0.6507	0.0955	0.6778	0.0779	0.4822	0.5126
9	0.6746	0.1499	0.7059	0.1309	0.5090	0.5455
10	0.7145	0.1950	0.7272	0.1849	0.5558	0.5713
11	0.7280	0.2550	0.7464	0.2423	0.5724	0.5955
12	0.7565	0.3373	0.7740	0.3258	0.6084	0.6313
13	0.7856	0.4536	0.7871	0.4528	0.6469	0.6489
14	0.8030	0.5156	0.8064	0.5137	0.6708	0.6756
15	0.8078	0.5779	0.8146	0.5746	0.6776	0.6872
16	0.8389	0.6537	0.8225	0.6607	0.7225	0.6985
17	0.8230	0.7550	0.8511	0.7468	0.6993	0.7408
18	0.9033	0.8341	0.8489	0.8443	0.8236	0.7375
19	0.8279	0.9222	0.8915	0.9165	0.7064	0.8043
20	0.7080	0.9648	0.9148	0.9548	0.5480	0.8430

*For plotting purposes these were set to zero.

Table 10. Equivalent and cationic mole fractions for Sr^{2+}/K^+ exchange at 0.05 N solution concentration calculated from data in Table 5

Exptl. soln	$\bar{E}_{Sr}$ from Sr data	E_{Sr} from Sr data	$\bar{E}_{Sr}$ from K data	E_{Sr} from K data	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from K data
1	0.0215	0.0934	0.0157	0.0485	0.0109	0.0079
2	0.0399	0.1785	0.0187	0.1355	0.0204	0.0094
3	0.0687	0.3333	0.0635	0.2839	0.0356	0.0328
4	0.1409	0.4288	0.1007	0.4015	0.0758	0.0530
5	0.1070	0.5145	0.1207	0.4629	0.0565	0.0642
6	0.1640	0.5841	0.1683	0.5473	0.0893	0.0919
7	0.1896	0.6626	0.2023	0.6307	0.1047	0.1126
8	0.2342	0.7157	0.2515	0.6895	0.1326	0.1438
9	0.3056	0.7373	0.2891	0.7335	0.1803	0.1690
10	0.3420	0.7766	0.2991	0.7795	0.2063	0.1758
11	0.3759	0.8088	0.3309	0.8072	0.2314	0.1983
12	0.3742	0.8515	0.4036	0.8399	0.2301	0.2529

13	0.4421	0.8609	0.4375	0.8624	0.2838	0.2800
14	0.5308	0.8663	0.4735	0.8808	0.3613	0.3102
15	0.4792	0.9027	0.5069	0.8972	0.3151	0.3395
16	0.5359	0.9128	0.5570	0.9095	0.3660	0.3860
17	0.6589	0.9324	0.6389	0.9345	0.4914	0.4694
18	0.5401	0.9572	0.6725	0.9468	0.3699	0.5066
19	0.7934	0.9788	0.8552	0.9772	0.6575	0.7470
20	1.1897	0.9820	0.9251	0.9860	1.4682	0.8606
21	1.3986	0.9929	0.9403	0.9954	2.3258	0.8874

Table 11. Equivalent and cationic mole fractions for Ca^{2+}/K^{+} exchange at 0.05 N solution concentration calculated from data in Table 6

Exptl. soln	$\bar{E}_{Ca}$ from Ca data	E_{Ca} from Ca data	$\bar{E}_{Ca}$ from K data	E_{Ca} from K data	$\overline{X}_{Ca}$ from Ca data	$\overline{X}_{Ca}$ from K data
1	0.0077	0.0832	0.0184	0.0844	0.0038	0.0093
2	0.0072	0.0919	0.0538	0.0844	0.0036	0.0276
3	0.0190	0.1816	0.0455	0.1662	0.0096	0.0233
4	0.0269	0.2675	0.0066	0.2890	0.0136	0.0033
5	0.0357	0.3713	0.0492	0.3555	0.0182	0.0252
6	0.0396	0.4571	0.0609	0.4424	0.0202	0.0314
7	0.0303	0.5339	0.0783	0.5284	0.0154	0.0408
8	0.0843	0.6048	0.0839	0.6240	0.0440	0.0438
9	0.1138	0.6856	0.1219	0.7115	0.0604	0.0649
10	0.1298	0.7645	0.1615	0.7959	0.0694	0.0878
11	0.1078	0.7994	0.1741	0.8220	0.0570	0.0953
12	0.2224	0.8663	0.2623	0.8905	0.1251	0.1509
13	0.3090	0.8683	0.2993	0.9120	0.1827	0.1760
14	0.3255	0.8932	0.3488	0.9294	0.1944	0.2113
15	0.3626	0.9082	0.3754	0.9473	0.2215	0.2311
16	0.7605	0.8862	0.4512	0.9568	0.6135	0.2913
17	0.8881	0.9022	0.5135	0.9671	0.7987	0.3454
18	1.4061	0.9112	0.6156	0.9790	2.3678	0.4447
19	3.9581	0.9192	0.8014	0.9919	-2.0214	0.6685

Verification of Excel spreadsheet calculations:

The values tabulated in Tables 7 to 11 were calculated with the aid of an Excel spreadsheet. To verify the Excel calculations, hand calculations were done using the raw data for Experimental Solution #1 listed in Table 2. These data were plugged into Eqns. (1), (2), and (3), and the values derived manually with a calculator were compared with those listed in Table 7. The following are the results of those hand calculations:

Table 2, Exptl soln #1

$$M_{Sr,i} = \frac{219}{87.62(1000)} = 2.4994E-03$$

$$M_{Sr,f} = \frac{16.5}{87.62(1000)} = 1.8831E-4$$

$V = 0.025\ L$

$W = 0.3102\ g$

$CEC = 2.04E-3\ eq/g$

Eqn (1)

$$E_{Sr} = 2(M_{Sr,i} - M_{Sr,f}) \cdot V/(W \cdot CEC)$$

$$= \frac{2(2.4994E-3 - 1.8831E-4) * .025}{0.3102 * 2.04E-3}$$

$E_{Sr} = 0.1826$ Table 7 value is 0.1826

Eqn (2)

$$E_{Sr} = 2(M_{Sr,f})/TN$$

$$= 2(1.8831E-4)/0.05$$

$E_{Sr} = 0.0075$ Table 7 value is 0.0075

Table 1, Exptl soln #1

$$M_{Na,i} = \frac{1050}{22.99(1000)} = 4.5672E-2$$

$$M_{Na,f} = \frac{1154}{22.99(1000)} = 5.0186E-2$$

Eqn (2)

$$E_{sr} = (M_{Na,f} - M_{Na,i}) \cdot V / (W \cdot C_{Sr})$$

$$= \frac{(5.0186E-2 - 4.5672E-2) * .025}{0.3102 * 2.04E-3}$$

$E_{sr} = 0.1787$ Table 7 value is 0.1787

Eqn (2)

$$E_{sr} = 1 - (M_{Na,f} / TN)$$

$$= 1 - (5.0186E-2 / 0.05)$$

$E_{sr} = -0.0039$ Table 7 value is -0.0039

Table 7, Exptl soln # 1

Using Sr data, $\bar{E}_{Sr} = 0.1826$

Eqn. (3) $\bar{X}_{Sr} = \dfrac{\bar{E}_{Sr}/2}{\bar{E}_{Sr}/2 + (1-\bar{E}_{Sr})}$

$= \dfrac{0.1826/2}{0.1826/2 + (1-0.1826)}$

$\bar{X}_{Sr} = 0.1005$ Table 7 value is 0.1005

Using Na data, $\bar{E}_{Sr} = 0.1787$

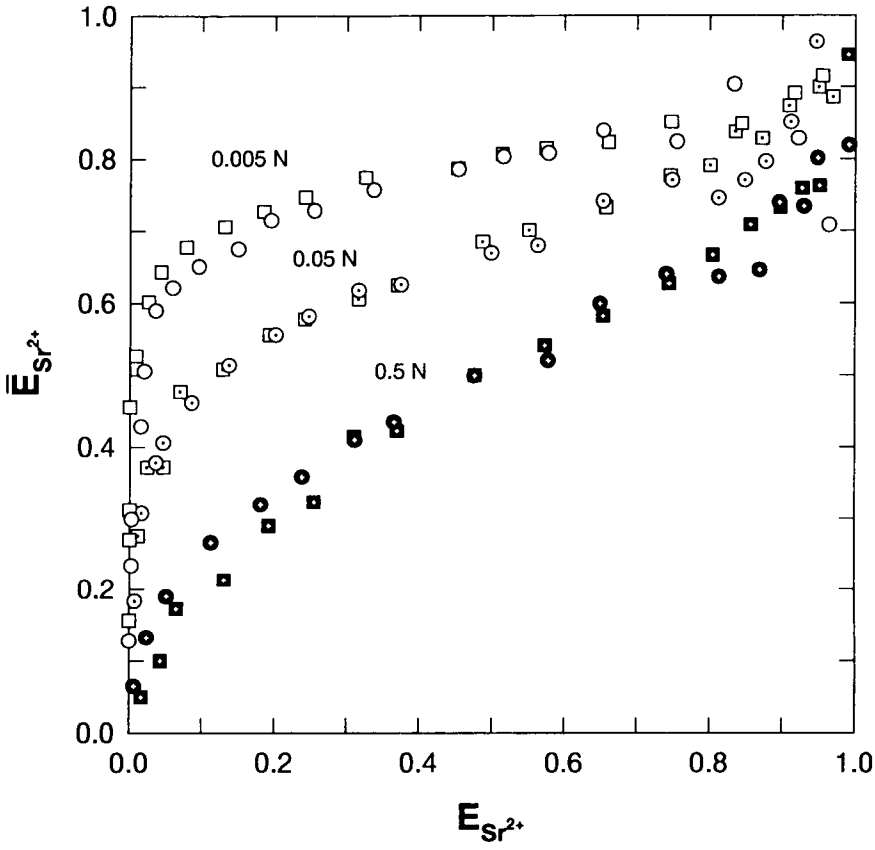
Eqn (3) $\bar{X}_{Sr} = \dfrac{0.1787/2}{0.1787/2 + (1-0.1787)}$

$\bar{X}_{Sr} = 0.0981$ Table 7 value is 0.0981

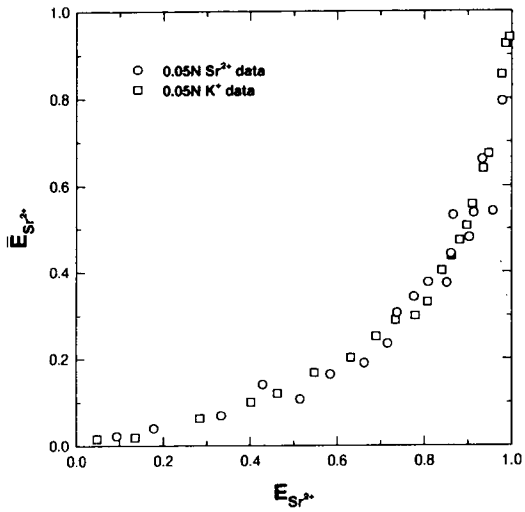
July 16, 1998

The following are isotherm plots of ion exchange data for the binary systems Na^+/Sr^{2+}, K^+/Sr^{2+}, and K^+/Ca^{2+}:

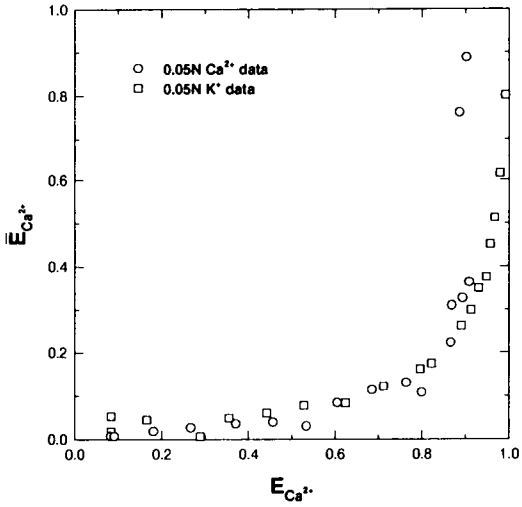
Na^+/Sr^{2+} Ion Exchange



K^+/Sr^{2+} Ion Exchange



K^+/Ca^{2+} Ion Exchange



July 20, 1998

THERMODYNAMIC MODEL FOR ION EXCHANGE

The following discussion of the model is taken from a manuscript being prepared by R. Pabalan and F. P. Bertetti:

3. THERMODYNAMIC MODEL

For a binary ion exchange reaction involving cations A^{z_A+} and B^{z_B+} with ionic charges z_{A+} and z_{B+}, respectively, the equilibrium reaction may be written as

$$z_B A^{z_A+} + z_A BL_{z_B} \rightleftharpoons z_A B^{z_B+} + z_B AL_{z_A} \tag{1}$$

where L is defined as a portion of zeolite framework holding a unit negative charge. The equilibrium constant, $K_{(A,B)}$, for Eq. (1) is given by

$$K_{(A,B)} = [(\bar{a}_A)^{z_B}(a_B)^{z_A}]/[(a_A)^{z_B}(\bar{a}_B)^{z_A}] \tag{2}$$

where a_A and a_B are aqueous activities of the cations, and $\bar{a}_A$ and $\bar{a}_B$ represent activities of the zeolite components. The zeolite may be considered as a solid solution of two components, AL_{z_A} and BL_{z_B}.[15-17] The number of moles of AL_{z_A} and BL_{z_B} is equal to the total number of moles $\bar{n}_A$ and $\bar{n}_B$, respectively, of ions A^{z_A+} and B^{z_B+} in the zeolite. Thus, the zeolite composition can be described in terms of

$$\bar{X}_A = \bar{n}_A/(\bar{n}_A + \bar{n}_B); \quad \bar{X}_B = \bar{n}_B/(\bar{n}_A + \bar{n}_B) \tag{3}$$

where $\bar{X}_A$ and $\bar{X}_B$ are the cationic mole fractions of A^{z_A+} and B^{z_B+}, respectively, in the solid.

Equation (2) may be expanded to give

$$K_{(A,B)} = [(\bar{X}_A)^{z_B}(M_B)^{z_A}]/[(\bar{X}_B)^{z_A}(M_A)^{z_B}] \cdot [(f_A)^{z_B}/(f_B)^{z_A}] \cdot [(\gamma_B)^{z_A}/(\gamma_A)^{z_B}] \tag{4}$$

or,

$$K_{(A,B)} = K_{v(A,B)}\,[(f_A)^{z_B}/(f_B)^{z_A}]; \quad K_{v(A,B)} = [(\bar{X}_A)^{z_B}(M_B)^{z_A}]/[(\bar{X}_B)^{z_A}(M_A)^{z_B}] \cdot [(\gamma_B)^{z_A}/(\gamma_A)^{z_B}] \tag{5}$$

where $K_{v(A,B)}$ is the Vanselow corrected selectivity coefficient for Eq. (1),[14,18] and M_A and M_B are the molarities of A^{z_A+} and B^{z_B+} in the aqueous phase. γ_A and γ_B are single-ion activity coefficients for the aqueous cations and account for nonideal behavior in the aqueous phase. The quantities f_A and f_B are rational activity coefficients for the zeolite components and account for nonideality in the zeolite phase. A convenient standard state for the zeolite solid solution is the appropriate homoionic zeolite component in equilibrium with an infinitely dilute solution of the same cation.[19,20] With that standard state, the criterion for ideal behavior in the solid solution is that $\bar{a}_i = \bar{X}_i$ for all $\bar{X}_i$. For the aqueous electrolyte

solution, the usual standard state is that of a hypothetical, one molar solution referenced to infinite dilution.

The above thermodynamic formulations are valid for conditions where electrolyte imbibition by the solid is negligible, which for zeolites is at solution concentrations approximately < 1.0 M,[21] and where changes in zeolite water activity are insignificant. For most cases of ion exchange equilibria, the water activity terms are not significant.[22] However, for ion exchange involving concentrated electrolyte solutions, terms can be included in the equations to account for the effects of sorbed or imbibed solvent and of imbibed salts.[19]

The standard Gibbs free energy, $\Delta G^{o}_{(A,B)}$, of the ion exchange reaction represented by Eq. (1) is given by

$$\Delta G^{o}_{(A,B)} = -RT \ln K_{(A,B)} \tag{6}$$

where R is the gas constant and T is temperature (Kelvin). If ion exchange experiments involving cations A^{z_A+}, B^{z_B+}, and C^{z_C+} pairwise were made, self-consistency of the derived thermodynamic constants and Gibbs energies can be assessed by applying the 'triangle rule',[23] which can be represented by

$$[K_{(A,B)}]^{z_C} \times [K_{(B,C)}]^{z_A} \times [K_{(C,A)}]^{z_B} = 1 \tag{7}$$

and

$$z_C \Delta G^{o}_{(A,B)} + z_A \Delta G^{o}_{(B,C)} + z_B \Delta G^{o}_{(C,A)} = 0 \tag{8}$$

where $K_{(i,j)}$ and $\Delta G^{o}_{(i,j)}$ are, respectively, the equilibrium constant and Gibbs free energy for ion exchange involving cations i and j. Note that $K_{(i,j)} = (K_{(j,i)})^{-1}$ and $\Delta G^{o}_{(i,j)} = -\Delta G^{o}_{(j,i)}$.

Thermodynamic parameters for ion exchange equilibria derived from isotherm data depend on the models used for the activity coefficients of aqueous species (γ_A, γ_B) and zeolite components (f_A, f_B). In this study, the Pitzer ion-interaction model was used to calculate aqueous activity coefficients. This model has the advantage of a large database of parameters at 25 °C and higher temperatures and has been successfully applied to thermodynamic calculations involving multicomponent mixtures over wide ranges of solution compositions, concentrations, and temperatures. Details of the model are given in the papers by Pitzer.[24-26] Ion-interaction parameters used in this study are listed in Table II.

In the case of the solid phase, various models have been proposed to represent the activity coefficients of exchangeable ions or solid solutions.[13,27-32] A thermodynamic model that is useful in describing nonideal behavior in both solid and liquid solutions is the Margules formulation.[33] It has

been successfully applied to studies of ion exchange equilibria involving zeolite minerals.[13,34] Using the Margules model, the molar excess Gibbs free energy of mixing, g^{ex}, for a zeolite solid solution with two-components, AL_{z_A} and BL_{z_B}, can be represented by the equation

$$\frac{g^{ex}}{RT} = \bar{X}_A\bar{X}_B(\bar{X}_B W_A + \bar{X}_A W_B) \tag{9}$$

where W_A and W_B are empirical parameters that are functions only of temperature and pressure. From Eq. (9) and the Gibbs-Duhem relation, the zeolite activity coefficients, f_A and f_B, can be expressed in terms of W_A and W_B as

$$\ln f_A = \bar{X}_B^2[W_A+2\bar{X}_A(W_B-W_A)]; \quad \ln f_B = \bar{X}_A^2[W_B+2\bar{X}_B(W_A-W_B)]. \tag{10}$$

For solid solutions with three or more components, analogous expressions can be derived.[30,35]

The Vanselow selectivity coefficient, $K_{v(A,B)}$, for the ion exchange reaction represented by Eq. (1) can then be represented by:

$$\ln K_{v(A,B)} = \ln K_{(A,B)} + z_A\bar{X}_A^2[W_B+2\bar{X}_B(W_A-W_B)] - z_B\bar{X}_B^2[W_A+2\bar{X}_A(W_B-W_A)]. \tag{11}$$

Values of $K_{(A,B)}$, W_A, and W_B can be derived by nonlinear regression of Eq. (11) to isotherm data. If the zeolite phase behaves ideally, $f_A = f_B = 1$ and $g^{ex} = 0$ for all values of $\bar{X}_A$ and $\bar{X}_B$, and $K_{(A,B)} = K_{v(A,B)}$.

The following parameters are required by the Margules model: (i) ln K(A,B), (ii) W_A, and (iii) W_B. To derive these parameters, one needs to calculate values of the Vanselow selectivity coefficient, $K_{v(A,B)}$. As can be seen from Eqn. (5) of this section, one need values of the aqueous activity coefficients γ_A and γ_B in order to calculate $K_{v(A,B)}$. Values of γ_A and γ_B can be calculated using the Pitzer equations for aqueous activity coefficients. These equations are discussed in detail in the following references:

K. S. Pitzer, *J. Phys. Chem.* **77**, 268 (1973).

K. S. Pitzer, *Rev. Mineral.* **17**, 97 (1987).

K. S. Pitzer, in *Activity Coefficients in Electrolyte Solutions*, 2nd ed., K. S. Pitzer, ed. (CRC Press, Boca Raton, Florida, 1991), Chap. 3.

To calculate the aqueous activity coefficients, the program SOLCALC was used. This program was developed by R.T. Pabalan during his postdoctoral work at U.C. Berkeley and was used in calculating mineral solubilities in aqueous electrolyte mixtures up to high temperature and pressure. The program was written in FORTRAN 77 and was originally compiled to run on a VAX 8700 mainframe computer. SOLCALC is not under TOP-018 configuration control at this time. Steps are currently being taken to place this code under configuration control.

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July 23, 1998

The first step taken to place SOLCALC under TOP-018 is to recompile the source code to run under the WINDOWS NT operation system. The source code was compiled using the LAHEY Fortran 77 compiler. Because of differences in the VAX and LAHEY compilers, a lot of error messages were encountered during the first attempts in compiling the SOLCALC code. Changes were made iteratively to the source code until no fatal error messages were received.

A few tests were done to test the results of the SOLCALC calculations. Solubility calculations were made at 25 C for various electrolyte mixtures. The resulting output was compared with printed output from previous runs that were done at the University of California at Berkeley. Because the model parameters that were used in the UC Berkeley runs may not be exactly the same as the parameters used in the current runs (several parameter options are available in SOLCALC), the output may not be exactly the same, but the calculated solubilities in the two sets of runs should be within several percent of each other.

In the next few pages are comparisons of the output of the two sets of runs.

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August 3, 1998

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SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00
NUMBER CORRESPONDING TO SATURATED SOLID      36
NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3
          THE NUMBER OF ITERATIONS IS     23

              EQUATION        LOG K
                 36          -1.2277
              CATION #        TOTAL
                  3           0.5000
              IONIC STRENGTH =    7.6677
          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.16674E+01      0.44129E+00       0.37785E+01       -.0008
CATION # 3   0.44413E-01      0.88826E-01       0.50000E+00       0.0000
ANION #  2   0.46993E-01      0.19669E-01       0.23892E+01       -.0008
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00
NUMBER CORRESPONDING TO SATURATED SOLID      36
NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3
          THE NUMBER OF ITERATIONS IS     38

              EQUATION        LOG K
                 36          -1.2277
              CATION #        TOTAL
                  3           2.0000
              IONIC STRENGTH =   14.2041
          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.17995E+01      0.43508E+00       0.41361E+01       0.0009
CATION # 3   0.85540E+00      0.12770E+00       0.20000E+01       0.0000
ANION #  2   0.10655E+00      0.26192E-01       0.40680E+01       0.0009
```

(a)

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SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00
NUMBER CORRESPONDING TO SATURATED SOLID      36
NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3
          THE NUMBER OF ITERATIONS IS     25

              EQUATION        LOG K
                 36          -1.2277
              CATION #        TOTAL
                  3           0.50000000
              IONIC STRENGTH =    7.72752076
          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.16726E+01      0.43805E+00       0.3818347E+01     0.0008
CATION # 3   0.45081E-01      0.90162E-01       0.5000000E+00     0.0000
ANION #  2   0.47359E-01      0.19658E-01       0.2409174E+01     0.0008
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00
NUMBER CORRESPONDING TO SATURATED SOLID      36
NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3
          THE NUMBER OF ITERATIONS IS     34

              EQUATION        LOG K
                 36          -1.2277
              CATION #        TOTAL
                  3           2.00000000
              IONIC STRENGTH =   13.70448244
          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.16221E+01      0.42654E+00       0.3802988E+01     -.0008
CATION # 3   0.23380E+00      0.11690E+00       0.2000000E+01     0.0000
ANION #  2   0.11477E+00      0.29418E-01       0.3901494E+01     -.0008
```

(b)

Mirabilite ($Na_2SO_4 \cdot 10H_2O$) solubility in $MgSO_4$+Na_2SO_4 solutions: (a) old and (b) new output.

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

        TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID      17

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

        THE NUMBER OF ITERATIONS IS    21

            EQUATION        LOG K

               17          -7.6054

            CATION #        TOTAL

               1           1.0000

            IONIC STRENGTH =   3.6491

          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.47751E+00     0.47751E+00     0.10000E+01     0.0000
CATION # 2   0.67037E+00     0.46789E+00     0.14327E+01     0.0008
ANION #  2   0.33089E-01     0.27203E-01     0.12164E+01     0.0000
```

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

        TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID      17

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

        THE NUMBER OF ITERATIONS IS    19

            EQUATION        LOG K

               17          -7.6054

            CATION #        TOTAL

               1           4.5000

            IONIC STRENGTH =   8.4006

          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.19302E+01     0.42898E+00     0.45000E+01     0.0000
CATION # 2   0.39791E+00     0.36160E+00     0.11004E+01     -.0008
ANION #  2   0.35991E-01     0.12853E-01     0.28002E+01     0.0000
```

(a)

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

        TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID      17

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

        THE NUMBER OF ITERATIONS IS    9

            EQUATION        LOG K

               17          -7.6054

            CATION #        TOTAL

               1           1.00000000

            IONIC STRENGTH =   3.62701690

          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.47825E+00     0.47825E+00     0.1000000E+01     0.0000
CATION # 2   0.66399E+00     0.46826E+00     0.1418011E+01     -.0008
ANION #  2   0.33541E-01     0.27743E-01     0.1209006E+01     0.0000
```

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

        TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID      17

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

        THE NUMBER OF ITERATIONS IS    16

            EQUATION        LOG K

               17          -7.6054

            CATION #        TOTAL

               1           4.50000000

            IONIC STRENGTH =   8.34650729

          ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.19343E+01     0.42984E+00     0.4500000E+01     0.0000
CATION # 2   0.38506E+00     0.36179E+00     0.1064338E+01     -.0009
ANION #  2   0.37765E-01     0.13574E-01     0.2782169E+01     0.0000
```

(b)

Glaserite [$Na_2K_6(SO_4)_4$] solubility in K_2SO_4+Na_2SO_4 solutions: (a) old and (b) new output.

Sylvite (KCl) in CaCl2 solution 5/17

```
*
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3

          THE NUMBER OF ITERATIONS IS    13

              EQUATION        LOG K

                 53           0.8999

              CATION #        TOTAL

                  3           1.0000

              IONIC STRENGTH =   6.4043

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 2  0.14887E+01       0.43728E+00         0.34043E+01       -.0008
CATION # 3  0.56322E+00       0.56322E+00         0.10000E+01       0.0000
ANION #  1  0.53342E+01       0.98703E+00         0.54043E+01       -.0008
*
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3

          THE NUMBER OF ITERATIONS IS    16

              EQUATION        LOG K

                 53           0.8999

              CATION #        TOTAL

                  3           2.0000

              IONIC STRENGTH =   8.1683

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 2  0.78274E+00       0.33333E+00         0.21683E+01       0.0008
CATION # 3  0.16472E+01       0.82358E+00         0.20000E+01       0.0000
ANION #  1  0.10987E+02       0.17812E+01         0.61683E+01       0.0008
```

(a)

```
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3

          THE NUMBER OF ITERATIONS IS    12

              EQUATION        LOG K

                 53           0.8999

              CATION #        TOTAL

                  3           1.00000000

              IONIC STRENGTH =   6.32067252

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 2  0.14255E+01       0.42927E+00         0.3320673E+01     -.0009
CATION # 3  0.51438E+00       0.51438E+00         0.1000000E+01     0.0000
ANION #  1  0.55708E+01       0.10470E+01         0.5320673E+01     -.0009
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY       3

          THE NUMBER OF ITERATIONS IS    10

              EQUATION        LOG K

                 53           0.8999

              CATION #        TOTAL

                  3           2.00000000

              IONIC STRENGTH =   8.06562901

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 2  0.67695E+00       0.32772E+00         0.2065629E+01     -.0006
CATION # 3  0.14945E+01       0.74725E+00         0.2000000E+01     0.0000
ANION #  1  0.11730E+02       0.19339E+01         0.6065629E+01     -.0006
```

(b)

Sylvite (KCl) solubility in KCl+$CaCl_2$ solutions: (a) old and (b) new output.

```
* RUN SOL
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID     20

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4

          THE NUMBER OF ITERATIONS IS     8

              EQUATION        LOG K

                 20           1.5704

              CATION #        TOTAL

                  4           1.0000

              IONIC STRENGTH =   7.3712

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.41309E+01      0.94503E+00        0.43712E+01       -.0010
CATION # 4   0.11119E+01      0.11119E+01        0.10000E+01        0.0000
ANION #  1   0.90027E+01      0.14130E+01        0.63712E+01       -.0010
*
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID     20

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4

          THE NUMBER OF ITERATIONS IS     9

              EQUATION        LOG K

                 20           1.5704

              CATION #        TOTAL

                  4           2.0000

              IONIC STRENGTH =   8.8474

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.26528E+01      0.93165E+00        0.28474E+01       -.0006
CATION # 4   0.20674E+01      0.10337E+01        0.20000E+01        0.0000
ANION #  1   0.14019E+02      0.20473E+01        0.68474E+01       -.0006
```

(a)

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID     20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4

          THE NUMBER OF ITERATIONS IS     8

              EQUATION        LOG K

                 20           1.5704

              CATION #        TOTAL

                  4           1.00000000

              IONIC STRENGTH =   7.37314180

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.40685E+01      0.93034E+00        0.4373142E+01     0.0008
CATION # 4   0.10442E+01      0.10442E+01        0.1000000E+01     0.0000
ANION #  1   0.91404E+01      0.14342E+01        0.6373142E+01     0.0008

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   25.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID     20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4

          THE NUMBER OF ITERATIONS IS     9

              EQUATION        LOG K

                 20           1.5704

              CATION #        TOTAL

                  4           2.00000000

              IONIC STRENGTH =   8.83653474

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION # 1   0.25969E+01      0.91551E+00        0.2836535E+01     0.0006
CATION # 4   0.19288E+01      0.96442E+00        0.2000000E+01     0.0000
ANION #  1   0.14320E+02      0.20947E+01        0.6836535E+01     0.0006
```

(b)

Halite (NaCl) solubility in NaCl+$MgCl_2$ solutions: (a) old and (b) new output.

```
TYP SOLCALC.OUT
   SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   25.00     PRESS(BARS) =     1.00
   NUMBER CORRESPONDING TO SATURATED SOLID      54
   NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4
            THE NUMBER OF ITERATIONS IS     9

                EQUATION        LOG K
                   54          -7.4484
                CATION #        TOTAL
                   4            0.0045
                IONIC STRENGTH = 0.941
              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR
CATION # 2   0.36402E+00       0.59175E+00       0.61515E+00       0.0958
CATION # 4   0.37589E-03       0.83531E-01       0.45000E-02       0.0000
ANION #  2   0.26834E-01       0.85987E-01       0.31208E+00       0.0958
* RUN SOLCALC
   CATION ARRAY: Na=1, K=2, Mg=3, Ca=4, H=5

   SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   25.00     PRESS(BARS) =     1.00
   NUMBER CORRESPONDING TO SATURATED SOLID      54
   NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4
            THE NUMBER OF ITERATIONS IS     5

                EQUATION        LOG K
                   54          -7.4484
                CATION #        TOTAL
                   4            0.0100
                IONIC STRENGTH = 0.644
              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR
CATION # 2   0.25071E+00       0.62239E+00       0.40282E+00       0.0813
CATION # 4   0.98165E-03       0.98165E-01       0.10000E-01       0.0000
ANION #  2   0.24075E-01       0.11388E+00       0.21141E+00       0.0813
```

(a)

```
   SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   25.00     PRESS(BARS) =     1.00
   NUMBER CORRESPONDING TO SATURATED SOLID      54
   NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4
            THE NUMBER OF ITERATIONS IS    31

                EQUATION        LOG K
                   54          -7.4484
                CATION #        TOTAL
                   4            0.00450000
                IONIC STRENGTH =   0.94566175
              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR
CATION # 2   0.36558E+00       0.59112E+00       0.6184412E+00       0.0009
CATION # 4   0.37470E-03       0.83266E-01       0.4500000E-02       0.0000
ANION #  2   0.26828E-01       0.85517E-01       0.3137206E+00       0.0009
   SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   25.00     PRESS(BARS) =     1.00
   NUMBER CORRESPONDING TO SATURATED SOLID      54
   NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      4
            THE NUMBER OF ITERATIONS IS    29

                EQUATION        LOG K
                   54          -7.4484
                CATION #        TOTAL
                   4            0.01000000
                IONIC STRENGTH =   0.64826432
              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR
CATION # 2   0.25202E+00       0.62149E+00       0.4055095E+00       0.0010
CATION # 4   0.97669E-03       0.97669E-01       0.1000000E-01       0.0000
ANION #  2   0.24059E-01       0.11308E+00       0.2127548E+00       0.0010
```

(b)

Syngenite (K_2SO_4) solubility in K_2SO_4+$CaSO_4$ solutions: (a) old and (b) new output.

Comparison of new and old output indicates that new and old values agree well. Thus, SOLCALC can be used for calculating activity coefficients of aqueous ions. ***However, a problem was encountered in multiple calculations (i.e., successive calculations in a single run) when NaCl is involved. The first calculation is okay, but the succeeding calculation gives incorrect results. For some reason, the incorrect NaCl parameters are used after the first run. This problem will be fixed later, but multiple calculations in a single run should not be done when NaCl is involved.****

The Pitzer model parameters used for calculating aqueous activity coefficients in this study are listed in the following table:

Table 12. Ion-interaction parameters used in this study to calculate aqueous activity coefficients using the Pitzer equations*

Single Electrolyte Parameters*			
Electrolyte	$\beta^{(0)}$	$\beta^{(1)}$	C^{ϕ}
NaCl	0.0765	0.2664	0.00127
KCl	0.04835	0.2122	-0.00084
$CaCl_2$	0.3159	1.614	-0.00034
$SrCl_2$	0.2858	1.6673	-0.00130
$NaNO_3$	0.0068	0.1783	-0.00072
KNO_3	-0.0816	0.0494	0.00660
$Ca(NO_3)_2$	0.2108	1.409	-0.02014

Mixture parameters			
$\theta_{Na,K} = -0.012$	$\theta_{Na,Ca} = 0.07$	$\theta_{Na,Sr} = 0.051$	$\theta_{K,Sr} = 0.0149$
$\psi_{Na,K,Cl} = -0.0018$	$\psi_{Na,Ca,Cl} = -0.007$	$\psi_{Na,Sr,Cl} = -0.0021$	$\psi_{K,Sr,Cl} = -0.0201$
$\psi_{Na,K,NO_3} = -0.0012$	$\psi_{Na,Ca,NO_3} = -0.007$		

*Values were taken from Pitzer,[26] except for $\theta_{Na,Sr}$, $\theta_{K,Sr}$, ψ_{Na,Ca,NO_3}, $\psi_{Na,Sr,Cl}$, and $\psi_{K,Sr,Cl}$. The value of ψ_{Na,Ca,NO_3} is based on the activity coefficient data of Smith et al.[45] Values of $\theta_{Na,Sr}$ and $\psi_{Na,Sr,Cl}$ were taken from Reardon and Armstrong,[46] and those of $\theta_{K,Sr}$ and $\psi_{K,Sr,Cl}$ were taken from Kim and Frederick.[47]

References:
45. S. N. Smith, S. Sarada S, and R. Palepu, *Can. J. Chem.* **71**, 384 (1993).
46. E. J. Reardon and D. K. Armstrong, *Geochim. Cosmochim. Acta* **51**, 63 (1987).
47. H. T. Kim and W. J. Frederick, Jr., *J. Chem. Eng. Data* **33**, 278 (1988).

August 5, 1998

The following are values of Vanselow selectivity coefficient, $K_{v(A,B)}$, calculated from the ion exchange data:

Table 13. Cationic mole fractions and Vanselow selectivity coefficients for Na^+/Sr^{2+} exchange at 0.05 N solution concentration

Exptl. soln	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from Na data	ln $K_{v(Sr,Na)}$ from Sr data	ln $K_{v(Sr,Na)}$ from Na data
1	0.1005	0.0981	0.8863	
2	0.1816	0.1603	0.8490	1.0391
3	0.2333	0.2284	0.4191	0.8261
4	0.2545	0.2285	0.2972	0.1146
5	0.3002	0.3134	-0.1088	0.2194
6	0.3456	0.3405	-0.4236	-0.3664
7	0.3850	0.3850	-0.7309	-0.6640
8	0.4098	0.4060	-0.9112	-0.8911
9	0.4468	0.4341	-1.1339	-1.2055
10	0.4554	0.4544	-1.4301	-1.4083
11	0.5028	0.5206	-1.8766	-1.6969
12	0.5143	0.5394	-2.2043	-1.9735
13	0.5884	0.5780	-2.3503	-2.4451
14	0.6258	0.6344	-2.8726	-2.7906
15	0.5938	0.6537	-3.7600	-3.2091
16	0.6261	0.7199	-4.0177	-3.1152
17	0.6612	0.7063	-4.2135	-3.7742
18	0.7403	0.7758	-4.2761	-3.8749
19	0.9295	0.8170	-2.4788	-4.6494
20	1.0139	0.7951		-5.9171

Table 14. Cationic mole fractions and Vanselow selectivity coefficients for Na^+/Sr^{2+} exchange at 0.5 N solution concentration

Exptl. soln	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from Na data	ln $K_{v(Sr,Na)}$ from Sr data	ln $K_{v(Sr,Na)}$ from Na data
1	0.0338	0.0255	2.3895	1.1346
2	0.0711	0.0524	1.8891	0.9241
3	0.1046	0.0942	1.5345	1.1459
4	0.1541	0.1196	1.1183	0.6003
5	0.1899	0.1695	0.7787	0.5300
6	0.2183	0.1922	0.5690	0.2671
7	0.2574	0.2614	0.3675	0.4003
8	0.2778	0.2675	0.1752	0.0866
9	0.3325	0.3330	-0.1372	-0.1338
10	0.3515	0.3709	-0.6470	-0.5010

11	0.4273	0.4100	-0.6921	-0.8245
12	0.4703	0.4562	-1.1775	-1.2900
13	0.4665	0.4996	-1.9452	-1.6453
14	0.4768	0.5484	-2.6636	-2.0304
15	0.5862	0.5778	-2.4861	-2.5604
16	0.5797	0.6118	-3.3393	-3.0547
17	0.6672	0.6156	-3.3829	-3.8510
18	0.3199	0.5575	-7.8584	-5.6510
19	0.6928	0.8953	-6.9036	-4.1962

Table 15. Cationic mole fractions and Vanselow selectivity coefficients for Na^+/Sr^{2+} exchange at 0.005 N solution concentration

Exptl. soln	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from Na data	ln $K_{v(Sr,Na)}$ from Sr data	ln $K_{v(Sr,Na)}$ from Na data
1	0.0684	0.0846	0.8880	
2	0.1329	0.1567	-0.1811	
3	0.1757	0.1847	-0.0394	
4	0.2726	0.2955	-0.9626	
5	0.3383	0.3579	-0.8351	0.1966
6	0.4182	0.4304	-0.9779	-0.5481
7	0.4510	0.4745	-1.3369	-0.8432
8	0.4822	0.5126	-1.7060	-1.2814
9	0.5090	0.5455	-2.1216	-1.7177
10	0.5558	0.5713	-2.2049	-2.0276
11	0.5724	0.5955	-2.5227	-2.2869
12	0.6084	0.6313	-2.7990	-2.5729
13	0.6469	0.6489	-3.2134	-3.1941
14	0.6708	0.6756	-3.4054	-3.3573
15	0.6776	0.6872	-3.7437	-3.6478
16	0.7225	0.6985	-3.8985	-4.1494
17	0.6993	0.7408	-4.9277	-4.4963
18	0.8236	0.7375	-4.5764	-5.6212
19	0.7064	0.8043	-7.3649	-6.2754
20	0.5480	0.8430		-7.0545

Table 16. Cationic mole fractions and Vanselow selectivity coefficients for K^+/Sr^{2+} exchange at 0.05 N solution concentration

Exptl. soln	$\overline{X}_{Sr}$ from Sr data	$\overline{X}_{Sr}$ from K data	ln $K_{v(Sr,K)}$ from Sr data	ln $K_{v(Sr,K)}$ from K data
1	0.0109	0.0079	-4.2420	-3.8128
2	0.0204	0.0094	-4.4406	-4.8551
3	0.0356	0.0328	-4.8928	-4.6760
4	0.0758	0.0530	-4.6125	-4.8601
5	0.0565	0.0642	-5.4546	-5.0027
6	0.0893	0.0919	-5.3628	-5.0939
7	0.1047	0.1126	-5.7140	-5.3940
8	0.1326	0.1438	-5.8335	-5.5133
9	0.1803	0.1690	-5.6015	-5.6597
10	0.2063	0.1758	-5.7784	-6.0438
11	0.2314	0.1983	-5.9514	-6.1709
12	0.2301	0.2529	-6.5170	-6.1986
13	0.2838	0.2800	-6.3041	-6.3518
14	0.3613	0.3102	-5.9195	-6.4726
15	0.3151	0.3395	-6.8727	-6.6095
16	0.3660	0.3860	-6.7991	-6.6026
17	0.4914	0.4694	-6.5938	-6.7908
18	0.3699	0.5066	-8.2466	-6.9975
19	0.6575	0.7470	-7.8804	-7.0024
20	1.4682	0.8606	-8.0283	-6.6551
21	2.3258	0.8874	-11.5323	-8.4267

Table 17. Cationic mole fractions and Vanselow selectivity coefficients for K^+/Ca^{2+} exchange at 0.05 N solution concentration

Exptl. soln	$\overline{X}_{Ca}$ from Ca data	$\overline{X}_{Ca}$ from K data	ln $K_{v(Ca,K)}$ from Ca data	ln $K_{v(Ca,K)}$ from K data
1	0.0038	0.0093	-5.1510	-4.2738
2	0.0036	0.0276	-5.3369	-3.1469
3	0.0096	0.0233	-5.2317	-4.1921
4	0.0136	0.0033	-5.4817	-7.0600
5	0.0182	0.0252	-5.8191	-5.3826
6	0.0202	0.0314	-6.2099	-5.6598
7	0.0154	0.0408	-6.9535	-5.8926
8	0.0440	0.0438	-6.2972	-6.4340
9	0.0604	0.0649	-6.5305	-6.6565
10	0.0694	0.0878	-7.0575	-7.1089
11	0.0570	0.0953	-7.6469	-7.3163
12	0.1251	0.1509	-7.6022	-7.7826
13	0.1827	0.1760	-7.1194	-8.0296
14	0.1944	0.2113	-7.4771	-8.2190
15	0.2215	0.2311	-7.5968	-8.6827
16	0.6135	0.2913	-4.7239	-8.6936

17	0.7987	0.3454	-3.4763	-8.9216
18	2.3678	0.4447	-6.4242	-9.2523
19	-2.0214	0.6685		-9.7327

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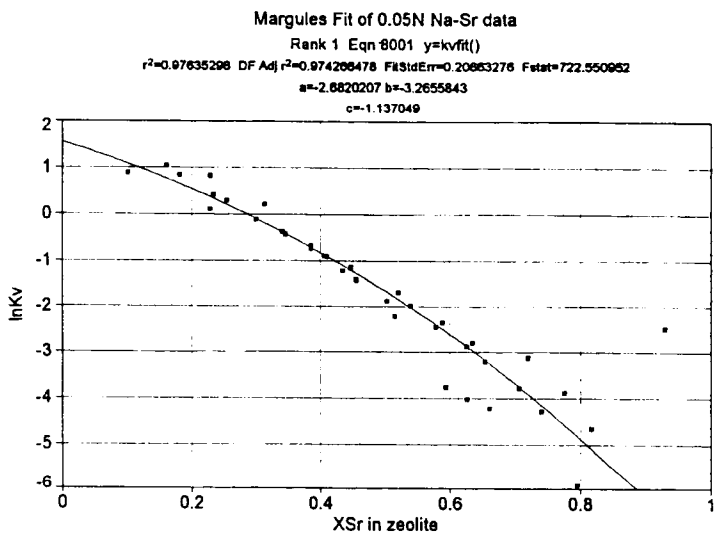
August 10, 1998

The commercial software TABLECURVE2D, Version 2.0, was used to fit the experimental data ($\overline{X}_i$ versus ln $K_{v(i,j)}$) and derive values of the equilibrium constant, $K_{(i,j)}$, and the Margules parameters W_i and W_j. In the case of the Na^+/Sr^{2+} system, only the 0.05 N data were used to derive the parameters.

The following is the result of the Tablecurve fit to the 0.05 N Na^+/Sr^{2+} data:

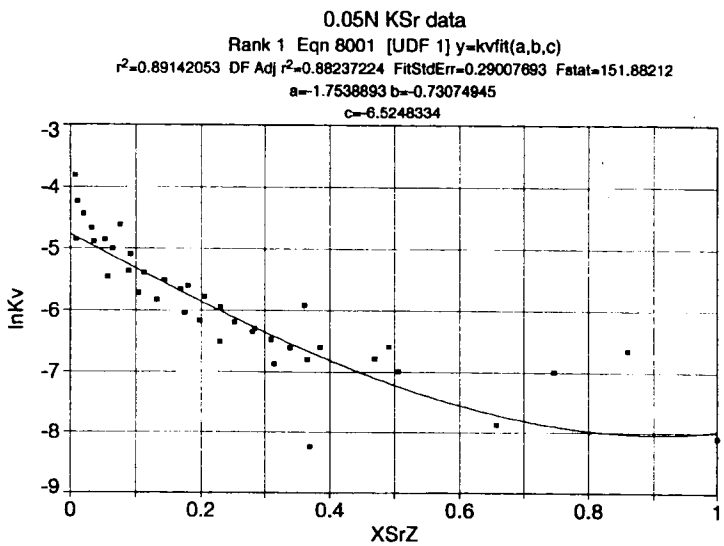


Rank 1 Eqn 8001 y=kvfit()

r^2 Coef Det	DF Adj r^2	Fit Std Err	F-value
0.9763529796	0.9742664778	0.2066327601	722.55095236

Parm	Value	Std Error	t-value	95% Confidence Limits	
a	-2.68202071	0.089659292	-29.9134721	-2.86401565	-2.50002578
b	-3.26558433	0.206553045	-15.8099065	-3.68485607	-2.84631259
c	-1.13704903	0.064290966	-17.6859847	-1.26755006	-1.00654800

The following is the result of the Tablecurve fit to the 0.05 N K^+/Sr^{2+} data:



Rank 1 Eqn 8001 [UDF 1] y=kvfit(a,b,c)

r^2 Coef Det	DF Adj r^2	Fit Std Err	F-value
0.8914205314	0.8823722424	0.2900769292	151.88211956

Parm	Value	Std Error	t-value	95% Confidence Limits	
a	-1.75388927	0.113087746	-15.5091010	-1.98299331	-1.52478523
b	-0.73074945	0.093022847	-7.85559113	-0.91920409	-0.54229482
c	-6.52483341	0.058539937	-111.459523	-6.64342925	-6.40623757

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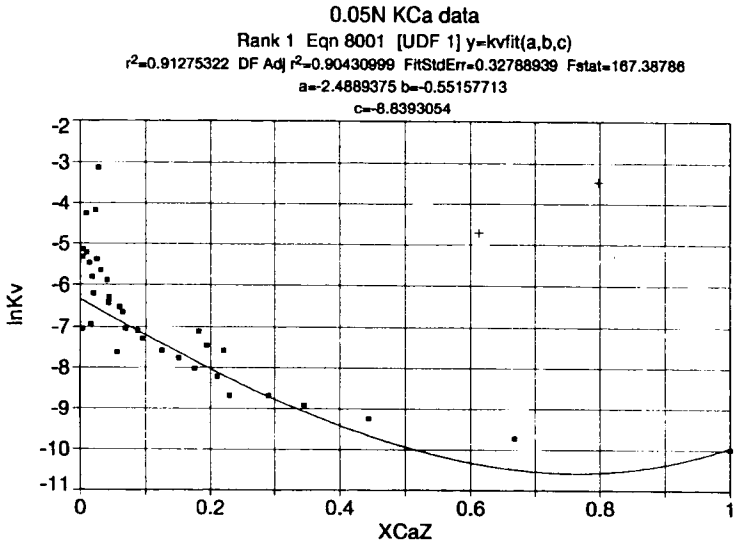
The following is the result of the Tablecurve fit to the 0.05 N K^+/Ca^{2+} data:



Rank 1 Eqn 8001 [UDF 1] y=kvfit(a,b,c)

r^2 Coef Det	DF Adj r^2	Fit Std Err	F-value
0.9127532220	0.9043099854	0.3278893908	167.38786102

Parm	Value	Std Error	t-value	95% Confidence Limits	
a	-2.48893746	0.162011156	-15.3627536	-2.81891624	-2.15895868
b	-0.55157713	0.077134714	-7.15082878	-0.70868248	-0.39447178
c	-8.83930537	0.067447089	-131.055403	-8.97667929	-8.70193144

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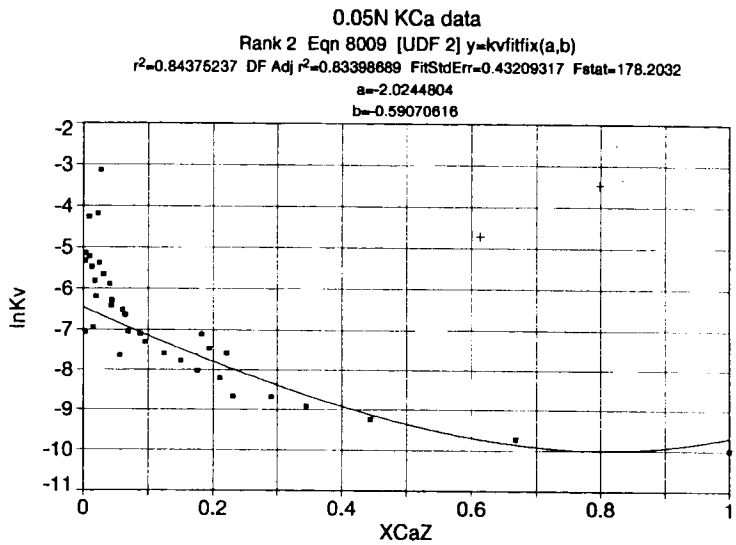
An alternative fit to the 0.05 N K^+/Ca^{2+} data is presented below. In this case, only the two Margules parameters were fit to the data. The ln $K_{v(Ca,K)}$:value was fixed at -8.50, which was determined by an integration method that is described in Pabalan (1994).



Rank 2 Eqn 8009 [UDF 2] y=kvfitfix(a,b)

r^2 Coef Det	DF Adj r^2	Fit Std Err	F-value
0.8437523694	0.8339868925	0.4320931738	178.20320278

Parm	Value	Std Error	t-value	95% Confidence Limits	
a	-2.02448039	0.175439730	-11.5394637	-2.38137964	-1.66758114
b	-0.59070616	0.101130142	-5.84104944	-0.79643648	-0.38497584

The following table lists the model parameters derived from this study and also the parameters for the Na^+/K^+ and Na^+/Ca^{2+} binary systems taken from Pabalan (1994).

Table 18. Values of Margules parameters, equilibrium constants, and Gibbs free energies of ion exchange derived from isotherm data. Values for the Na^+/K^+ and Na^+/Ca^{2+} binary systems are based on experiments at 0.005, 0.05, and 0.5 N solutions reported by Pabalan (1994).

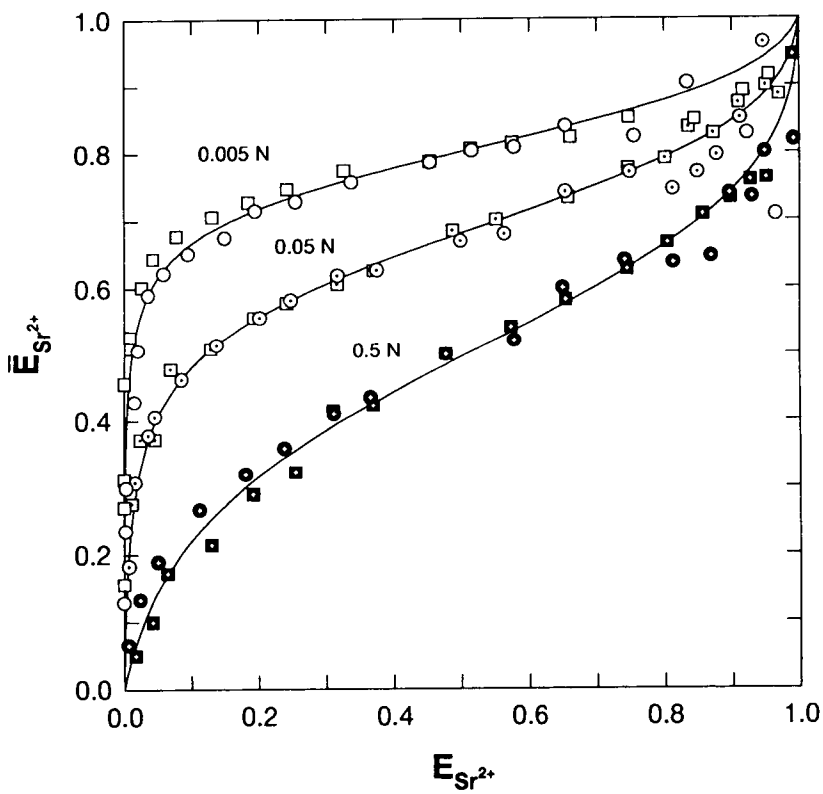
Cations (A,B)	W_A	W_B	ln $K_{(A,B)}$	$\Delta G^o_{(A,B)}$ (J/mol)
K^+,Na^+	-0.98887	-1.4116	3.22±0.03	-7,980±80
Ca^{2+},Na^+	-2.6729	-1.2246	- 1.65±0.08	4,090±200
Sr^{2+},Na^+	-2.6820	-3.2656	-1.14±0.07	2,830±180
Ca^{2+},K^+	-2.0245	-0.59071	-8.50±0.18	21,070±450
Sr^{2+},K^+	-1.7539	-0.73075	-6.52±0.10	16,160±250

August 13, 1998

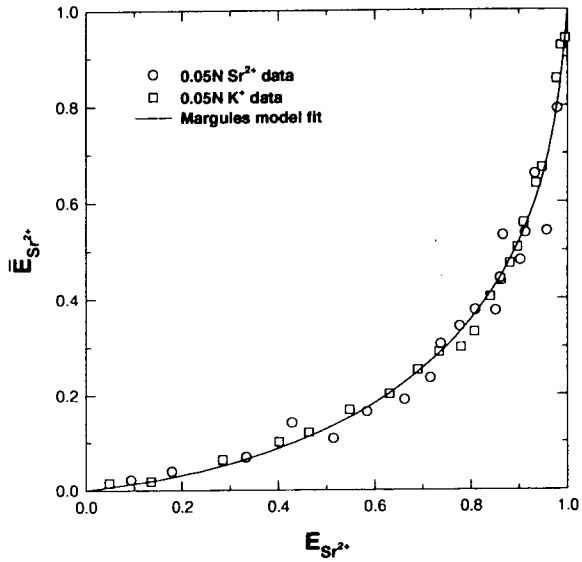
The following figures compares the experimental data on ion exchange with values calculated using the thermodynamic model:

Na^+/Sr^{2+} Ion Exchange

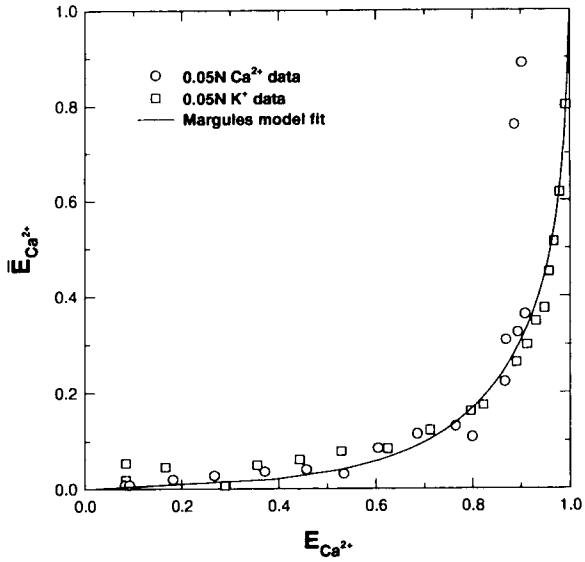
Circles and squares were calculated from Sr^{2+} and Na^+ analytical data, respectively. The curves were calculated using a Margules solid solution model with parameters derived by fitting only the 0.05 N isotherm data.



K^+/Sr^{2+} Ion Exchange



K^+/Ca^{2+} Ion Exchange



August 17, 1998

SOLUTION COMPOSITIONS CALCULATED FROM ZEOLITE ANALYSIS

An interesting application of the ion exchange model is the calculation of groundwater composition based on analytical data on the coexisting zeolite phase. For example, it is difficult to obtain samples of groundwater from hydrologically unsaturated rock units, such as those surrounding the proposed nuclear waste geologic repository at Yucca Mountain, Nevada. Some efforts have been made to extract aqueous solutions by high-pressure triaxial compression of rock samples taken from the vadose zone of Yucca Mountain, but there are large variabilities in the chemical composition of solutions derived using this technique. Aqueous samples have also been extracted from unsaturated soils and sands using ultracentrifugation techniques. It is uncertain whether compositions of water extracted from rock pores by ultracentrifugation or by high-pressure squeezing methods accurately represent the compositions of *in situ* water. Water extracted in these manners may have compositions different from those of *in situ* water due to several possible processes: (i) dilution of pore solutions by water desorbed from hydrated minerals like zeolites and clays, (ii) dissolution reactions due to increased mineral solubility and/or higher carbon dioxide concentration at higher pressures, (iii) membrane filtration by clays and zeolites, and (iv) ion exchange with the zeolites and clays.

The thermodynamic model for ion exchange equilibria discussed in a previous section may help reduce uncertainties associated with sampling and analysis of groundwater in unsaturated stratigraphic horizons by constraining the water cation chemistry. Data from analysis of solid phase (or zeolite) composition, such as those derived by electron microprobe techniques, combined with estimates of the total normality of the aqueous phase, can be used to calculate major cation concentrations in the groundwater. In the following section, the ability of the model to calculate the cationic composition of the aqueous phase based on the chemical composition of the zeolite is evaluated.

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The following section was taken from a manuscript being prepared by R. Pabalan and F.P. Bertetti:

5.1 Equations for Calculating Solution Composition from Zeolite Data

The ratio of the aqueous activities of two cations, A^{z_A+} and B^{z_B+}, participating in an ion exchange reaction such as that represented by Eq. (1) can be written as

$$(a_B)^{z_A}/(a_A)^{z_B} = [(M_B)^{z_A}(\gamma_B)^{z_A}]/[(M_A)^{z_B}(\gamma_A)^{z_B}] = K_{v(A,B)}(\overline{X}_B)^{z_A}/(\overline{X}_A)^{z_B} \tag{12}$$

Substituting $K_{v(A,B)}$ from Eq. (11) and writing the zeolite composition in terms of $\overline{X}_A$ only, the aqueous activity ratio can be represented in terms of $K_{(A,B)}$, W_A, and W_B:

$$\begin{aligned}(a_B)^{z_A}/(a_A)^{z_B} = \{(1-\overline{X}_A)^{z_A}/(\overline{X}_A)^{z_B}\} \exp\{&\ln K_{(A,B)} + z_A(\overline{X}_A)^2[W_B + 2(1-\overline{X}_A)(W_A - W_B)] \\ &- z_B(1-\overline{X}_A)^2[W_A + 2\overline{X}_A(W_B - W_A)]\}\end{aligned} \tag{13}$$

Since the total normality of a binary aqueous solution, TN, can be calculated from

$$TN = z_A M_A + z_B M_B \tag{14}$$

the ratio of the molarities of A^{z_A+} and B^{z_B+} can be written in terms of the molarity of either A^{z_A+} only or B^{z_B+} only. Thus,

$$\begin{aligned}(M_B)^{z_A} / (M_A)^{z_B} &= [(TN - z_A M_A)/z_B]^{z_A}/(M_A)^{z_B} \\ &= [(a_B)^{z_A}/(a_A)^{z_B}][(\gamma_A)^{z_B}/(\gamma_B)^{z_A}]\end{aligned} \tag{15}$$

For binary ion exchange reactions involving monovalent cations ($z_A = z_B = 1$), one can derive from Eq. (15) expressions for M_A and M_B that are fairly simple:

$$M_A = TN/(1 + k);\ M_B = TN - M_A \tag{16}$$

where

$$k = [(a_B)^{z_A}/(a_A)^{z_B}][(\gamma_A)^{z_B}/(\gamma_B)^{z_A}] \tag{17}$$

For exchange reactions where $z_A = 2$ and $z_B = 1$, the solution compositions can be solved using the quadratic formula

$$M_A = (-b \pm\sqrt{b^2-4ac})/2a;\ M_B = TN - 2M_A \tag{18}$$

where

$$a = 1;\ b = [-4TN - k]/4;\ and\ c = (TN/2)^2 \tag{19}$$

Using Eqs. (13) to (19), together with the equilibrium constants and Margules parameters derived from the ion exchange experiments, values of M_A and M_B can be calculated if the value of *TN* is known or can be estimated by independent means. A value of *TN* is required as input into Eqs. (16), (18), and (19) and also in calculating the aqueous activity coefficient ratios, $(\gamma_A)^{z_B}/(\gamma_B)^{z_A}$. For a specific value of *TN*, a range of values corresponding to the activity coefficient ratios for solutions of almost pure $A^{z_A\cdot}$ to almost pure $B^{z_B\cdot}$ can be calculated. The aqueous activity coefficient ratios do not change very much for a particular *TN*. For example, for $NaCl/CaCl_2$ solutions at *TN*=0.5 N, $(\gamma_{Na^+})^2/(\gamma_{Ca^{2+}})$ changes by only ~6 %, from 1.953 to 2.056, over a range of $M_{Na^+}/M_{Ca^{2+}}$ ratio from 0.498/0.001 to 0.002/0.249. The variation in activity coefficient ratios is smaller at lower total normalities or for solutions of homovalent cations (e.g., Na^+/K^+). For instance, for $NaCl/CaCl_2$ solutions at *TN*=0.05 N, $(\gamma_{Na^+})^2/(\gamma_{Ca^{2+}})$ changes by only ~0.3 %, from 1.496 to 1.501, over a range of $M_{Na^+}/M_{Ca^{2+}}$ from 0.0498/0.0001 to

0.0002/0.0249. Likewise, for NaCl/KCl solutions at TN=0.5 N, $\gamma_{Na^+}/\gamma_{K^+}$ changes by less than 3 %, from 1.066 to 1.039, over a range of M_{Na^+}/M_{K^+} from 0.499/0.001 to 0.001/0.499. Thus, although aqueous activity coefficient ratios are required to calculate solution compositions from zeolite data, for a given solution normality an activity coefficient ratio for a solution of median composition (e.g., equal normalities of A^{z_A+} and B^{z_B+}) can be used without resulting in a large error in predicted solution composition.

Groundwaters are typically dilute. For example, ionic strengths of Yucca Mountain saturated zone groundwaters calculated by Turner[41] based on the comprehensive water chemistry data of Perfect et al.[42] average about 0.0081±0.0004 M. Ionic strengths of porewaters from the hydrologically unsaturated zone of Yucca Mountain calculated from the data of Yang et al.[43] also average about 0.008±0.004 M. For these and other dilute groundwaters, it may be sufficient to use an activity coefficient ratio equal to one and still get reasonable predictions of solution compositions.

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August 18, 1998

Measured versus Predicted Solution Compositions in Binary Systems

Data from binary ion exchange experiments were used to evaluate model predictions of solution composition. For this study, clinoptilolite powders that were equilibrated with Na^+/K^+ and Na^+/Ca^{2+} solutions in experiments described by Pabalan (1994) were recovered using standard filtration methods. To avoid altering the clinoptilolite compositions during the filtration step, the zeolites were contacted only with the solutions with which they equilibrated. This is particularly important for the Na^+/Ca^{2+} system where, due to the concentration-valency effect, the zeolite composition may change significantly if the solid was contacted with deionized water. Table 19 presents a summary of the chemical compositions of clinoptilolite powders that were equilibrated with aqueous NaCl-KCl, NaCl-$CaCl_2$, $NaNO_3$-KNO_3, and $NaNO_3$-$Ca(NO_3)_2$ mixtures at a total normality of 0.05 or 0.5 N. The zeolite compositions were determined by ICP analysis, and were originally reported in previous scientific notebooks. Because of the very small amounts of zeolite powder used in the experiments, no duplicate samples could be analyzed. For example, only about 0.1 g or less of the clinoptilolite powders from the 0.05 N experiments were available for ICP analysis, instead of the minimum 0.2 to 0.5 g typically used.

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Table 19. Chemical composition of clinoptilolites equilibrated with Na^+/K^+ and Na^+/Ca^{2+} solutions

Aqueous Mixtures	wt% SiO_2	wt% TiO_2	wt% Al_2O_3	wt% Fe_2O_3	wt% MgO	wt% Na_2O	wt% K_2O	wt% CaO	Total wt%
0.5 N Na/K/Cl	67.81	0.06	11.17	0.36	0.17	1.91	7.52	0.00	89.00
	66.95	0.06	10.98	0.36	0.17	1.23	8.55	0.00	88.30
	65.82	0.06	10.75	0.35	0.16	0.55	9.29	0.01	86.99
	67.80	0.06	10.91	0.34	0.17	0.81	9.34	0.00	89.44
0.05 N Na/K/Cl	67.48	0.06	10.63	0.35	0.17	2.35	6.20	0.01	87.25
	67.58	0.04	10.55	0.25	0.25	0.55	8.43	0.00	87.65
	67.48	0.06	10.66	0.35	0.17	0.56	9.29	0.01	88.58
	67.34	0.06	10.58	0.35	0.17	0.32	9.64	0.00	88.46
0.05 N Na/K/NO_3	68.00	0.06	10.78	0.35	0.17	4.83	2.66	0.00	86.85
	68.00	0.06	10.77	0.38	0.18	2.24	6.71	0.00	88.34
	67.30	0.06	10.79	0.35	0.17	1.52	7.59	0.00	87.78
	66.76	0.06	10.49	0.35	0.17	0.78	8.70	0.01	87.32
	65.65	0.06	10.46	0.34	0.16	0.46	8.85	0.01	85.99
	67.00	0.06	10.72	0.40	0.18	0.17	9.60	0.00	88.13
0.05 N Na/Ca/Cl	68.46	0.06	11.25	0.36	0.18	5.00	0.61	1.32	87.24
	67.02	0.06	10.95	0.4	0.19	4.43	0.62	1.79	85.46
	66.13	0.06	10.57	0.36	0.18	3.79	0.61	2.14	83.84
	67.17	0.06	10.73	0.36	0.19	3.03	0.63	3.10	85.27
	67.32	0.06	10.74	0.36	0.18	2.47	0.63	3.60	85.36
0.05 N Na/Ca/Cl	67.62	0.06	11.10	0.36	0.18	3.57	0.63	2.56	86.08
	67.54	0.05	11.00	0.36	0.20	2.55	0.58	3.52	85.80
	68.03	0.06	11.08	0.36	0.19	2.12	0.61	3.91	86.36
	68.62	0.06	11.33	0.36	0.19	1.72	0.62	4.36	87.26
	67.41	0.06	11.05	0.35	0.20	1.39	0.55	4.51	85.52
0.05 N Na/Ca/NO_3	69.09	0.06	11.30	0.36	0.19	5.10	0.62	1.21	87.93
	66.08	0.06	10.89	0.35	0.18	3.28	0.60	2.66	84.10
	65.74	0.06	10.86	0.38	0.18	2.55	0.62	3.46	83.85
	66.17	0.06	10.98	0.37	0.19	1.90	0.60	4.13	84.40
	65.44	0.06	10.78	0.35	0.19	1.02	0.55	4.92	83.31

Table 20 compares the concentrations of Na^+ and K^+ predicted from the zeolite composition versus those in actual experimental solutions measured using ISEs. Table 21 compares predicted and measured Na^+ and Ca^{2+} solution concentrations. The predicted molarities were calculated using Eqs. (13) to (19) [of the preceding section taken from Pabalan and Bertetti (in preparation)] and values of ln K, W_A, and W_B listed in Table 18. Values of $\overline{X}_K$ listed in Table 20 were normalized to the molar amounts of Na and K only, whereas $\overline{X}_{Ca}$ values in Table 21 were normalized to the molar amounts of Na and Ca only. These calculations assumed that the small amounts of Ca^{2+} and Mg^{2+} present in the zeolite did not participate in the exchange process for the Na^+/K^+ system, and K^+ and Mg^{2+} did not participate in the exchange for the Na^+/Ca^{2+} mixture. This assumption is justified by the zeolite compositions given in Table 19, which show that, within analytical uncertainty, the weight percent of MgO and CaO in the zeolites used in the Na^+/K^+ ion exchange experiments remained equal to the weight percent of MgO and CaO in the original Na-clinoptilolite (Table 1, column-3). Likewise, the weight percent of K_2O and MgO of the zeolites from the Na^+/Ca^{2+} experiments remained equal to those of the Na-clinoptilolite.

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Table 20. Measured K^+ and Na^+ solution concentrations versus values predicted from measured clinoptilolite Na and K content. Also tabulated are cationic mole fractions of K^+ in the zeolite, $\overline{X}_K$, and predicted solution activity ratios of Na^+ and K^+. Calculated K^+ and Na^+ concentrations in parentheses were derived using aqueous activity coefficient ratios equal to 1.0.

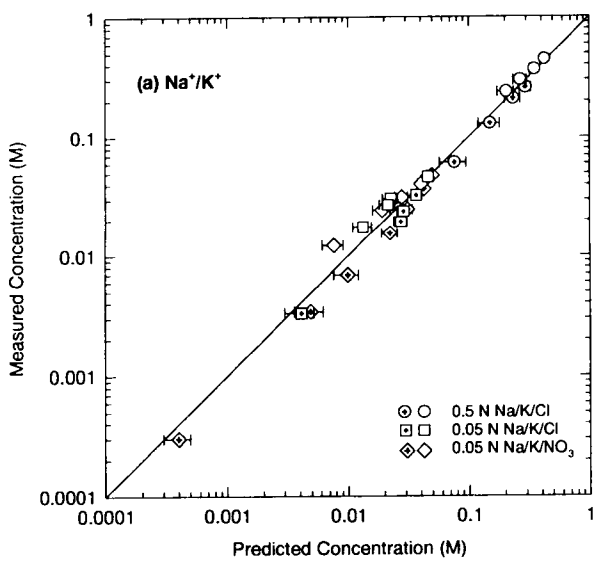
Aqueous Mixtures	wt% Na_2O	wt% K_2O	$\overline{X}_K$	a_{Na}/a_K	Calc. K^+ conc. (M)	Meas. K^+ conc. (M)	Calc. Na^+ conc. (M)	Meas. Na^+ conc. (M)
Na/K/Cl 0.5 N	1.91	7.52	0.721	5.906	0.076±0.019 (0.072)	0.061±0.002	0.424±0.019 (0.428)	0.444±0.009
	1.23	8.55	0.821	2.463	0.150±0.030 (0.144)	0.130±0.004	0.350±0.030 (0.356)	0.366±0.007
	0.55	9.29	0.917	0.7338	0.295±0.032 (0.288)	0.258±0.008	0.205±0.032 (0.212)	0.238±0.005
	0.81	9.34	0.884	1.207	0.233±0.034 (0.227)	0.209±0.006	0.267±0.034 (0.273)	0.298±0.006
Na/K/Cl 0.05 N	2.35	6.20	0.634	11.30	0.0041±0.0011 (0.0041)	0.0033±0.0001	0.0459±0.0011 (0.0459)	0.0465±0.0009
	0.55	8.43	0.910	0.8303	0.0274±0.0033 (0.0273)	0.0194±0.0006	0.0226±0.0033 (0.0227)	0.0306±0.0006
	0.56	9.29	0.916	0.7507	0.0287±0.0032 (0.0286)	0.0239±0.0007	0.0213±0.0032 (0.0214)	0.0271±0.0005
	0.32	9.64	0.952	0.3646	0.0367±0.0024 (0.0366)	0.0327±0.0010	0.0133±0.0024 (0.0134)	0.0174±0.0003
Na/K/NO_3 0.05 N	4.83	2.66	0.266	125.1	0.0004±0.0001	0.0003±0.00001	0.0496±0.0001	0.0476±0.0010
	2.24	6.71	0.663	9.181	0.0050±0.0013	0.0034±0.0001	0.0451±0.0013	0.0457±0.0009
	1.52	7.59	0.767	4.063	0.0100±0.0023	0.0069±0.0002	0.0401±0.0023	0.0404±0.0008
	0.78	8.70	0.880	1.262	0.0223±0.0033	0.0154±0.0005	0.0278±0.0033	0.0314±0.0006
	0.46	8.85	0.927	0.6237	0.0310±0.0031	0.0248±0.0007	0.0191 ±0.0031	0.0243±0.0005
	0.17	9.60	0.974	0.1799	0.0425±0.0015	0.0368±0.0011	0.0076 ±0.0015	0.0121±0.0002

Table 21. Measured Ca^{2+} and Na^{+} solution concentrations versus values predicted from measured clinoptilolite Na and Ca content. Also tabulated are cationic mole fractions of Ca^{2+} in the zeolite, $\overline{X}_{Ca}$, and predicted solution activity ratios of Na^{+} and Ca^{2+}. Calculated Ca^{2+} and Na^{+} concentrations in parentheses were derived using aqueous activity coefficient ratios equal to 1.0.

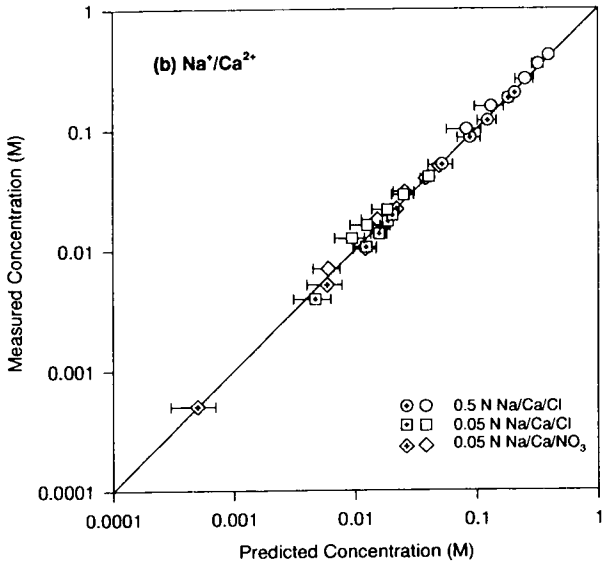
Aqueous Mixtures	wt% Na_2O	wt% CaO	$\overline{X}_{Ca}$	$(a_{Na})^2/(a_{Ca})$	Calc. Ca^{2+} conc. (M)	Meas. Ca^{2+} conc. (M)	Calc. Na^{+} conc. (M)	Meas. Na^{+} conc. (M)
Na/Ca/Cl 0.5 N	5.0	1.32	0.127	5.868	0.052±0.012 (0.032)	0.051±0.002	0.395±0.025 (0.435)	0.409±0.008
	4.43	1.79	0.183	2.314	0.089±0.019 (0.061)	0.085±0.003	0.323±0.037 (0.377)	0.345±0.007
	3.79	2.14	0.238	1.005	0.124±0.022 (0.095)	0.118±0.005	0.252±0.043 (0.309)	0.260±0.005
	3.03	3.1	0.361	0.1885	0.184±0.018 (0.162)	0.180±0.007	0.133±0.036 (0.175)	0.155±0.003
	2.47	3.6	0.446	0.06527	0.208±0.013 (0.194)	0.199±0.008	0.083±0.026 (0.112)	0.100±0.002
Na/Ca/Cl 0.05 N	3.57	2.56	0.284	0.5259	0.0047±0.0016 (0.0035)	0.0039±0.0002	0.0406±0.0031 (0.0430)	0.0406±0.0008
	2.55	3.52	0.433	0.07686	0.0124±0.0026 (0.0107)	0.0105±0.0004	0.0252±0.0052 (0.0286)	0.0285±0.0006
	2.12	3.91	0.505	0.03232	0.0158±0.0023 (0.0143)	0.0136±0.0005	0.0184±0.0046 (0.0215)	0.0214±0.0004
	1.72	4.36	0.583	0.01291	0.0187±0.0018 (0.0175)	0.0173±0.0007	0.0126±0.0035 (0.0150)	0.0159±0.0003
	1.39	4.51	0.642	0.00658	0.0203±0.0013 (0.0194)	0.0194±0.0008	0.0094±0.0026 (0.0113)	0.0124±0.0002
Na/Ca/NO_3 0.05 N	5.1	1.21	0.116	7.251	0.0005±0.0002	0.0005±0.00002	0.0490±0.0003	0.0496±0.0010
	3.28	2.66	0.309	0.3714	0.0059±0.0019	0.0051±0.0002	0.0382±0.0037	0.0392±0.0008
	2.55	3.46	0.429	0.0809	0.0122±0.0026	0.0101±0.0004	0.0257±0.0051	0.0303±0.0006
	1.9	4.13	0.546	0.01999	0.0174±0.0020	0.0159±0.0006	0.0153±0.0040	0.0177±0.0004
	1.02	4.92	0.727	0.00243	0.0220±0.0008	0.0217±0.0009	0.0060±0.0015	0.0069±0.0001

Aqueous activity coefficients were calculated using the Pitzer equations and the parameters listed in Table 12. Values of $\gamma_{Na^+} / \gamma_{K^+}$ equal to 1.05 and 1.007 were used for 0.5 and 0.05 N NaCl/KCl solutions, respectively, and values of $(\gamma_{Na^+})^2 / (\gamma_{Ca^{2+}})$ equal to 1.98 and 1.50 were used for 0.5 and 0.05 N NaCl/$CaCl_2$ solutions, respectively. For $NaNO_3/KNO_3$ and $NaNO_3/Ca(NO_3)_2$ mixtures at 0.05 N, activity coefficient ratios of 1.019 and 1.49, respectively, were used.

The uncertainties in predicted Na^+, K^+, and Ca^{2+} solution concentrations were propagated assuming a ±10 % error in the measured weight percent of Na_2O, K_2O, and CaO, but neglecting regression errors for ln K, W_A, and W_B, and errors due to the use of a single value of activity coefficient ratio at a given solution normality. The results listed in Tables 20 and 21 and plotted in the figures below show that the predicted solution compositions agree very well with measured values, mostly within analytical uncertainty. This agreement demonstrates that it is possible to predict with confidence the cationic composition of an aqueous solution based on chemical analysis of zeolites with which it equilibrated, at least for simple two-cation systems for which the solution normality is known.



Comparison of measured Na^+ and K^+ concentrations in the aqueous phase with values calculated based on the composition of the coexisting zeolite phase. Open symbols are values for Na^+ concentrations; .symbols with cross-hair are data for K^+ concentrations.



Comparison of measured Na^+ and Ca^{2+} concentrations in the aqueous phase with values calculated based on the composition of the coexisting zeolite phase. Open symbols are values for Na^+ concentrations; symbols with cross-hair are data for Ca^{2+} concentrations.

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Entries into Scientific Notebook No. 278 for the period July 1, 1998, to September 30, 1998, have been made by

RT Pabalan 10/27/98

Roberto T. Pabalan / Date

No original text entered into this Scientific Notebook has been removed. RTP 10/27/98

Scientific Notebook #278

RADIONUCLIDE TRANSPORT

Project No. 20-1402-871

Scientific Notebook #278

RADIONUCLIDE TRANSPORT

Project No. 20-1402-871

The entries in this electronic scientific notebook #278 document activities conducted during the Period October 1, 1998, through December 31, 1998, under the Radionuclide Transport Key Technical Issue (Project Number 20-1402-871).

11/3/98

The following entries document the installation testing of The Geochemist's Workbench (GWB), a commercially available set of software tools for conducting geochemical calculations. The GWB was developed by Craig Bethke at the University of Illinois at Urbana-Champaign. The CNWRA copy of GWB was purchased from Rockware (Golden, Colorado; www.rockware.com) and installed on a Windows NT platform.

Below is a description of the GWB taken from the user's guide:

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot. Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

A series of calculations were done to verify correct installation of GWB. The calculations follow the tutorial discussions in the user's guide. For the module Rxn, the following were taken from Chapter 2 of the user's guide:

Chapter 2: Using Rxn

About Rxn

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

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Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

The following was copied from the workstation screen after the interactive Rxn run:

```
--Rxn chemical reaction tool, release 3.0--
 Rxn (c) 1991-98 Craig M. Bethke & Board of Trustees, Univ. of Illinois.
 All rights reserved.
Reading thermodynamic data from: d:\gwb\gtdata\thermo.dat
 Read data for  646 aqueous species,
            624 minerals,
             10 gases.

Rxn > react Analcime
```

```
Rxn > go

    Analcime  + 4*H+  = 3*H2O  + Na+  + Al+++  + 2*SiO2(aq)
Rxn > swap Quartz for SiO2(aq)
Rxn > swap Albite for Al+++
Rxn > go
    Analcime  + Quartz  = H2O  + Albite
Rxn > T=250
Rxn > go
    Analcime  + Quartz  = H2O  + Albite
    Log K at 250 C =    0.3039
Rxn > T=?
    Temperature unset
Rxn > long
Rxn > go
    Analcime  + Quartz  = H2O  + Albite
    Log K's:
          0 C:   0.1982      150 C:   0.2202
         25 C:   0.1834      200 C:   0.2591
         60 C:   0.1794      250 C:   0.3039
        100 C:   0.1909      300 C:   0.3553
    Polynomial fit:
     log K = .1981 - .0008043*T + 9.708e-6*T^2
                 - 2.719e-8*T^3 + 3.197e-11*T^4
    Equilibrium equation:
     log K = log a[H2O]
Rxn > a H2O = 1
    Activity of H2O  =  10^0
Rxn > go
    Analcime  + Quartz  = H2O  + Albite
    Log K's:
          0 C:   0.1982      150 C:   0.2202
         25 C:   0.1834      200 C:   0.2591
```

60 C:	0.1794	250 C:	0.3039
100 C:	0.1909	300 C:	0.3553

Polynomial fit:

log K = .1981 - .0008043*T + 9.708e-6*T^2
- 2.719e-8*T^3 + 3.197e-11*T^4

Assumptions implicit in equilibrium equation:

activity of H2O = 10^0

Equilibrium equation:

log K = 0

Reaction is not in equilibrium between 0 and 300 C

Products favored over this temperature range

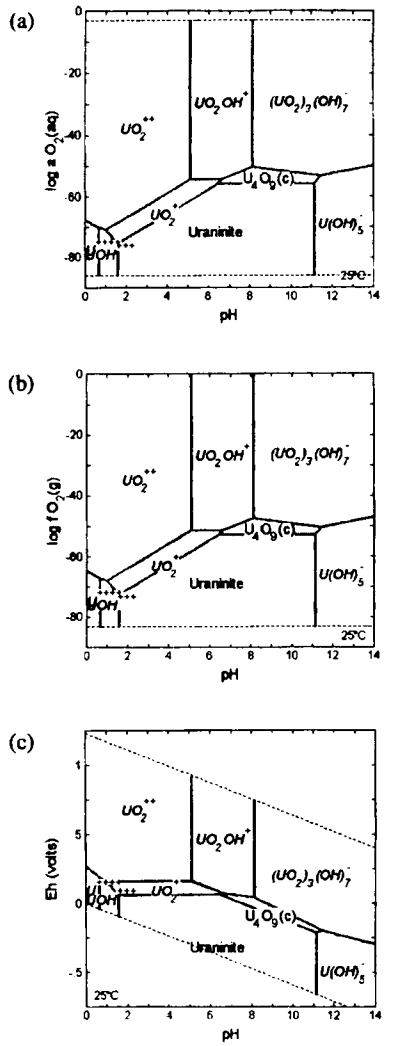
For the module Act2, the following were taken from Chapter 3 of the user's guide:

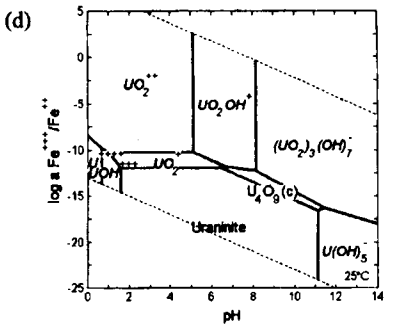
Chapter 3: Using Act2

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

Figure 3.1 Redox-*pH* diagrams for uranium drawn at 25°C and a species activity of 10^{-10}. Diagrams are plotted against the redox variables (a) activity of dissolved oxygen, (b) fugacity of oxygen gas, (c) Eh, and (d) the activity ratio of Fe^{+++} to Fe^{++}. Dashed lines show stability limits of water at 1 atm pressure.





The following were copied from the workstation screen after the interactive Act2 run:

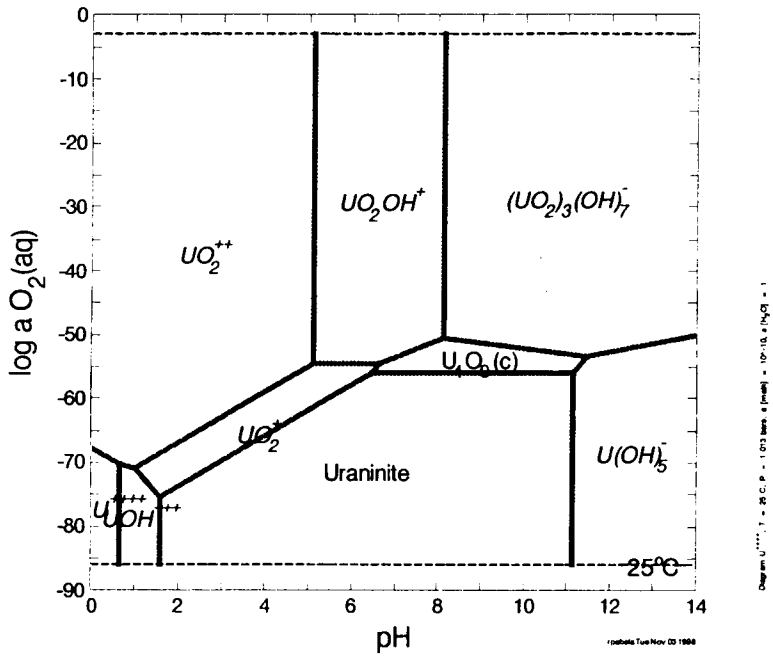
```
--Act2 activity-activity diagram generator, release 3.0--
 Act2 (c) 1989-98 Craig M. Bethke & Board of Trustees, Univ. of Illinois.
 All rights reserved.

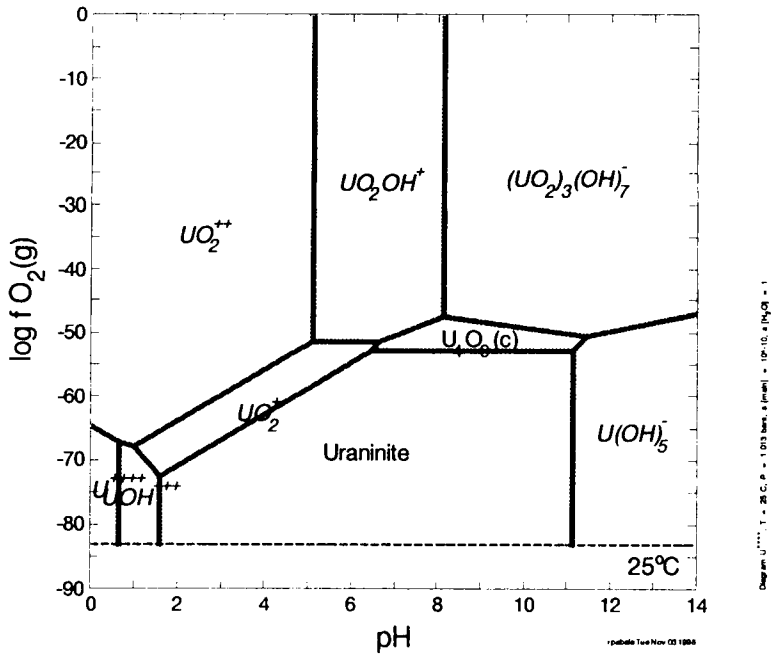
Reading thermodynamic data from: d:\gwb\gtdata\thermo.dat
Read data for 1280 aqueous species, minerals, and gases.
 Act2> diagram U++++ on O2(aq) vs pH
 Act2> log a U++++ = -10
    Activity of U++++ = 10^-10
 Act2> x from 0 to 14; y from -90 to 0
 Act2> go
 Calculating diagram for U++++
  Loaded 25 species and minerals:
     U++++        U+++        UO2+        UO2++
     (UO2)2(OH)2++  (UO2)3(OH)4++  (UO2)3(OH)5+  (UO2)3(OH)7-
     (UO2)4(OH)7+  U(OH)2++     U(OH)3+     U(OH)4
     U(OH)5-     U6(OH)15(9+)  UO2OH+     UOH+++
     Gummite     Schoepite     U(c,alph)     U3O8(c,alph)
     U4O9(c)     UO2(OH)2(c,bet) UO2(am)     UO3(c,gamma)
     Uraninite
>> Click right mouse button on diagram to continue
Act2> swap O2(g) for O2(aq)
Act2> go
Calculating diagram for U++++
 Loaded 25 species and minerals:
     U++++        U+++        UO2+        UO2++
     (UO2)2(OH)2++  (UO2)3(OH)4++  (UO2)3(OH)5+  (UO2)3(OH)7-
     (UO2)4(OH)7+  U(OH)2++     U(OH)3+     U(OH)4
     U(OH)5-     U6(OH)15(9+)  UO2OH+     UOH+++
     Gummite     Schoepite     U(c,alph)     U3O8(c,alph)
     U4O9(c)     UO2(OH)2(c,bet) UO2(am)     UO3(c,gamma)
```

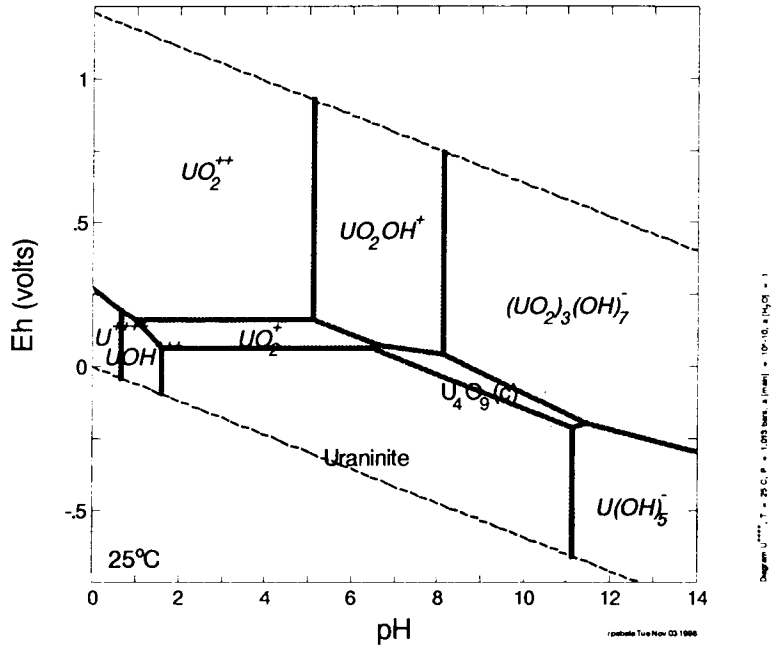
```
    Uraninite
>> Click right mouse button on diagram to continue
Act2> swap e- for O2(aq)
Act2> diagram on Eh
Act2> y from -.75 to 1.25
Act2> go
Calculating diagram for U++++
 Loaded 25 species and minerals:
    U++++        U+++        UO2+        UO2++
    (UO2)2(OH)2++  (UO2)3(OH)4++  (UO2)3(OH)5+  (UO2)3(OH)7-
    (UO2)4(OH)7+  U(OH)2++      U(OH)3+      U(OH)4
    U(OH)5-      U6(OH)15(9+)  UO2OH+       UOH+++
    Gummite      Schoepite     U(c,alph)    U3O8(c,alph)
    U4O9(c)      UO2(OH)2(c,bet) UO2(am)    UO3(c,gamma)
    Uraninite
>> Click right mouse button on diagram to continue
Act2> swap Fe+++/Fe++ for O2(aq)
Act2> y from -25 to 5
Act2> go

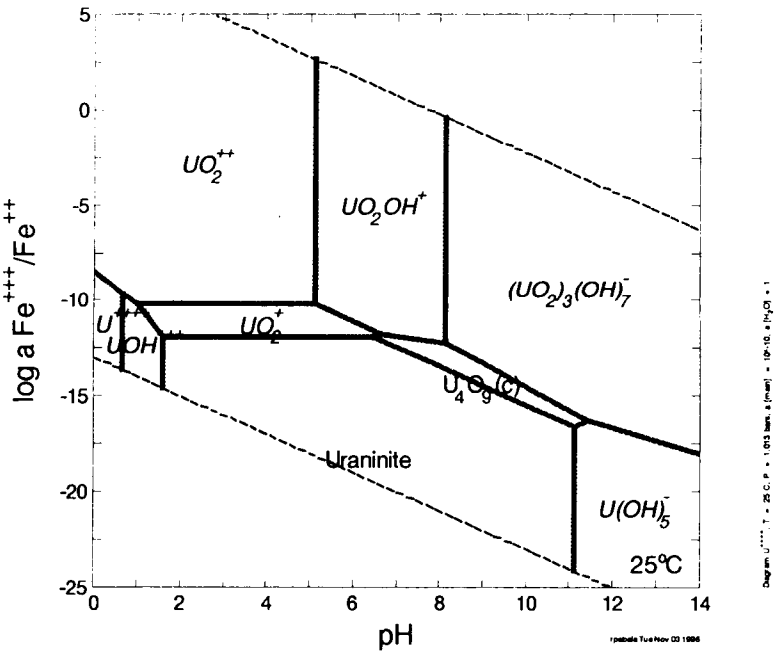
Calculating diagram for U++++
 Loaded 25 species and minerals:
    U++++        U+++        UO2+        UO2++
    (UO2)2(OH)2++  (UO2)3(OH)4++  (UO2)3(OH)5+  (UO2)3(OH)7-
    (UO2)4(OH)7+  U(OH)2++      U(OH)3+      U(OH)4
    U(OH)5-      U6(OH)15(9+)  UO2OH+       UOH+++
    Gummite      Schoepite     U(c,alph)    U3O8(c,alph)
    U4O9(c)      UO2(OH)2(c,bet) UO2(am)    UO3(c,gamma)
    Uraninite
>> Click right mouse button on diagram to continue
```

The calculated figures are shown below:






Eh (volts)
pH
UO_2^{++}
UO_2OH^+
$(UO_2)_3(OH)_7^-$
U^{++}
UOH
UO_2^+
$U_4O_9(c)$
Uraninite
$U(OH)_5^-$
25°C


log a Fe^{+++}/Fe^{++}
pH
UO_2^{++}
UO_2OH^+
$(UO_2)_3(OH)_7^-$
U^{++}
UOH
UO_2^+
$U_4O_9(c)$
Uraninite
$U(OH)_5^-$
25°C

11/4/98

For the Tact module of GWB, the following were taken from Chapter 4 of the user's guide:

About Tact

Figure 4.1 [illegible]

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

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Diagram calculation

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

The following were copied from the workstation screen after the interactive Tact run:

```
--Tact temperature-activity diagram generator, release 3.0--
 Tact (c) 1989-98 Craig M. Bethke & Board of Trustees, Univ. of Illinois.
 All rights reserved.
Reading thermodynamic data from: d:\gwb\gtdata\thermo.dat
Read data for 1280 aqueous species, minerals, and gases.
 Tact> diagram HPO4-- vs pH
 Tact> a HPO4-- = 10^-3
     Activity of HPO4-- = 10^-3
 Tact> x from 0 to 14
 Tact> go
 Loaded 7 species and minerals:
```

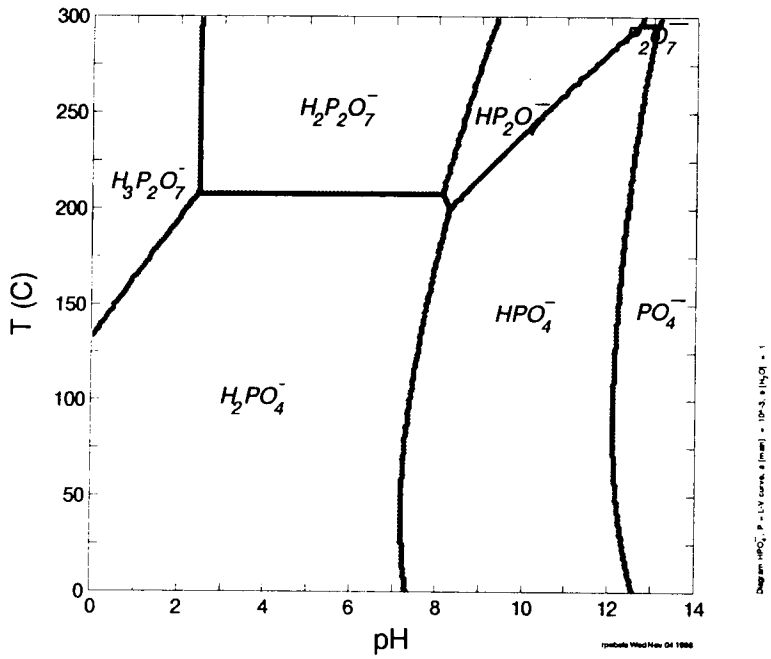
HPO4-- H2P2O7-- H2PO4- H3P2O7-

HP2O7--- P2O7---- PO4---

Calculating diagram for HPO4--

>> Click right mouse button on diagram to continue

Tact>



For comparison with figure 4.2 of the user's guide, another Tact run was done. The following were copied from the workstation screen:

Tact> reset

Tact> swap Kaolinite for Al+++

Tact> swap Ca++/H+^2 for Ca++

Tact> swap K+/H+ for K+

Tact> diagram Kaolinite vs SiO2(aq)

Tact> log ratio Ca++/H+^2 = 10.5

Ratio of Ca++/H+^2 = 10^10.5

Tact> log ratio K+/H+ = 3.5

Ratio of K+/H+ = 10^3.5

Tact> x from -4.5 to -1.5 incr 1/2

Tact> y from 0 to 200

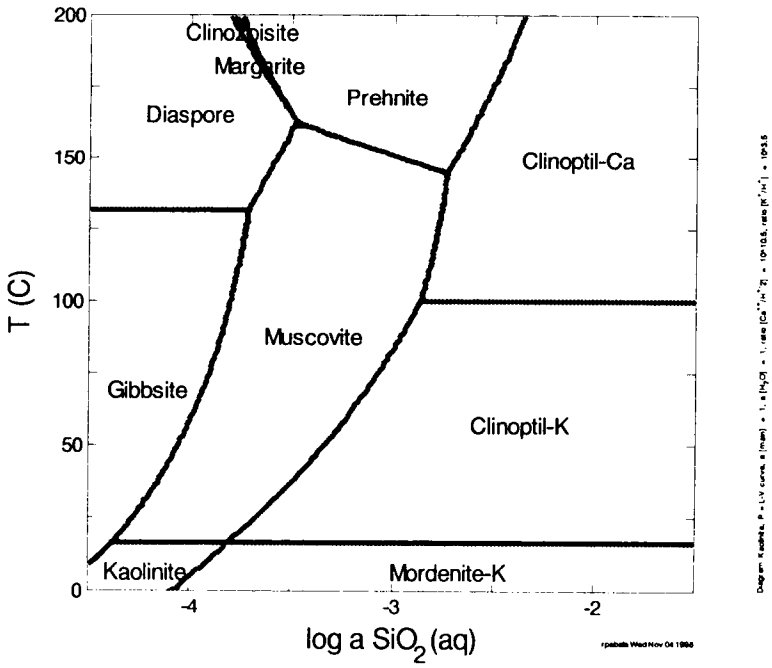
Tact> go

Loaded 33 species and minerals:

Al(OH)3 Andalusite Anorthite Beidellit-Ca
Beidellit-H Beidellit-K Boehmite Ca-Al Pyroxene
Clinoptil-Ca Clinoptil-K Clinozoisite Corundum
Diaspore Gehlenite Gibbsite Grossular
Heulandite K-feldspar Kalsilite Kaolinite
Kyanite Laumontite Lawsonite Margarite
Maximum MicroclineMordenite-K Muscovite Prehnite
Pyrophyllite Sanidine high Sillimanite Wairakite
Zoisite

Calculating diagram for Kaolinite

>> Click right mouse button on diagram to continue



For the React module of GWB, the following were taken from Chapter 5 of the user's guide:

About React

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

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Figure 5.3

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. “The Geochemist’s Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot.” Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

Figure 5.3

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. “The Geochemist’s Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot.” Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

The following were copied from the workstation screen after the interactive React run:

```
--React geochemical reaction model, release 3.0--
 React (c) 1983-98 Craig M. Bethke & Board of Trustees, Univ. of Illinois.
 All rights reserved.

Reading thermodynamic data from: d:\gwb\gtdata\thermo.dat

Read data for 646 aqueous species, 624 minerals, and 10 gases.

React> Na+ = 5 mg/kg
React> K+ = 1 mg/kg
React> Ca++ = 15 mg/kg
React> Mg++ = 3 mg/kg
React> Al+++ = .001 mg/kg
React> SiO2(aq) = 3 mg/kg
React> Cl- = 4 mg/kg
React> SO4-- = 8 mg/kg
React> HCO3- = 50 mg/kg
React> pH = 5
React> react 400 mg of K-feldspar
React> go

Solving for initial system.

 Loaded:  57 aqueous species,
        161 minerals,
          2 gases,
          0 surface species,
         11 elements,
          8 oxides.

N-R converged in  29 its., resmax =   4.32e-012, Xi =  0.0000
```

Charge balance: Cl- molality adjusted from .0001128 to .001047

Following reaction path.

N-R converged in 31 its., resmax = 3.51e-012, Xi = 0.0100

14 supersaturated phases, most = Kaolinite

Swapping Kaolinite in for Al+++

Swapping CO2(aq) in for H+

N-R converged in 11 its., resmax = 3.09e-015, Xi = 0.0100

N-R converged in 9 its., resmax = 1.29e-014, Xi = 0.0200

1 supersaturated phase, Quartz

Swapping Quartz in for SiO2(aq)

N-R converged in 5 its., resmax = 2.44e-013, Xi = 0.0200

N-R converged in 9 its., resmax = 6.83e-015, Xi = 0.0300

N-R converged in 9 its., resmax = 4.39e-015, Xi = 0.0400

N-R converged in 9 its., resmax = 1.18e-015, Xi = 0.0500

N-R converged in 9 its., resmax = 3.74e-015, Xi = 0.0600

N-R converged in 9 its., resmax = 1.95e-015, Xi = 0.0700

N-R converged in 9 its., resmax = 8.14e-016, Xi = 0.0800

N-R converged in 7 its., resmax = 2.54e-013, Xi = 0.0900

N-R converged in 7 its., resmax = 1.76e-013, Xi = 0.1000

N-R converged in 7 its., resmax = 1.2e-013, Xi = 0.1100

N-R converged in 7 its., resmax = 7.89e-014, Xi = 0.1200

N-R converged in 7 its., resmax = 4.85e-014, Xi = 0.1300

N-R converged in 7 its., resmax = 2.46e-014, Xi = 0.1400

N-R converged in 7 its., resmax = 6.18e-015, Xi = 0.1500

N-R converged in 7 its., resmax = 8.79e-015, Xi = 0.1600

N-R converged in 7 its., resmax = 2.08e-014, Xi = 0.1700

N-R converged in 7 its., resmax = 3.09e-014, Xi = 0.1800

N-R converged in 7 its., resmax = 4.21e-014, Xi = 0.1900

N-R converged in 7 its., resmax = 4.88e-014, Xi = 0.2000

N-R converged in 7 its., resmax = 5.55e-014, Xi = 0.2100

N-R converged in 7 its., resmax = 6.17e-014, Xi = 0.2200

```
N-R converged in  7 its., resmax =  6.64e-014, Xi =  0.2300
N-R converged in  7 its., resmax =  7.23e-014, Xi =  0.2400
N-R converged in  7 its., resmax =   7.5e-014, Xi =  0.2500
N-R converged in  7 its., resmax =  8.07e-014, Xi =  0.2600
N-R converged in  7 its., resmax =  8.51e-014, Xi =  0.2700
N-R converged in  7 its., resmax =  8.85e-014, Xi =  0.2800
N-R converged in  7 its., resmax =  9.23e-014, Xi =  0.2900
N-R converged in  7 its., resmax =   9.7e-014, Xi =  0.3000
N-R converged in  7 its., resmax =  1.01e-013, Xi =  0.3100
N-R converged in  7 its., resmax =  1.04e-013, Xi =  0.3200
N-R converged in  7 its., resmax =  1.09e-013, Xi =  0.3300
N-R converged in  7 its., resmax =  1.15e-013, Xi =  0.3400
N-R converged in  7 its., resmax =  1.21e-013, Xi =  0.3500
N-R converged in  7 its., resmax =  1.26e-013, Xi =  0.3600
N-R converged in  7 its., resmax =  1.34e-013, Xi =  0.3700
N-R converged in  7 its., resmax =  1.42e-013, Xi =  0.3800
 1 supersaturated phase, Muscovite
 Swapping Muscovite in for CO2(aq)
N-R converged in  9 its., resmax =  4.76e-015, Xi =  0.3800
N-R converged in  3 its., resmax =  3.64e-013, Xi =  0.3900
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4000
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4100
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4200
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4300
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4400
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4500
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4600
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4700
N-R converged in  3 its., resmax =  2.73e-013, Xi =  0.4800
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.4900
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5000
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5100
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5200
```

```
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5300
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5400
N-R converged in  3 its., resmax =  2.73e-013, Xi =  0.5500
N-R converged in  3 its., resmax =  2.75e-013, Xi =  0.5600
N-R converged in  3 its., resmax =  2.74e-013, Xi =  0.5700
Kaolinite is undersaturated
Swapping CO2(aq) in for Kaolinite
N-R converged in  7 its., resmax =  3.53e-014, Xi =  0.5700
N-R converged in  7 its., resmax =  8.69e-014, Xi =  0.5800
N-R converged in  7 its., resmax =   9.1e-014, Xi =  0.5900
N-R converged in  7 its., resmax =  9.68e-014, Xi =  0.6000
N-R converged in  7 its., resmax =  1.01e-013, Xi =  0.6100
N-R converged in  7 its., resmax =  1.07e-013, Xi =  0.6200
N-R converged in  7 its., resmax =  1.12e-013, Xi =  0.6300
N-R converged in  7 its., resmax =   1.2e-013, Xi =  0.6400
N-R converged in  7 its., resmax =   1.3e-013, Xi =  0.6500
N-R converged in  7 its., resmax =  1.43e-013, Xi =  0.6600
N-R converged in  7 its., resmax =  1.59e-013, Xi =  0.6700
N-R converged in  7 its., resmax =  1.78e-013, Xi =  0.6800
N-R converged in  7 its., resmax =  2.02e-013, Xi =  0.6900
N-R converged in  7 its., resmax =  2.34e-013, Xi =  0.7000
N-R converged in  7 its., resmax =  2.76e-013, Xi =  0.7100
N-R converged in  9 its., resmax =  8.69e-016, Xi =  0.7200
N-R converged in  9 its., resmax =  1.52e-015, Xi =  0.7300
N-R converged in  9 its., resmax =  1.63e-015, Xi =  0.7400
N-R converged in  9 its., resmax =  1.32e-015, Xi =  0.7500
N-R converged in  9 its., resmax =   2.6e-015, Xi =  0.7600
N-R converged in  9 its., resmax =  2.28e-015, Xi =  0.7700
N-R converged in  9 its., resmax =  6.35e-015, Xi =  0.7800
N-R converged in  9 its., resmax =  8.62e-015, Xi =  0.7900
N-R converged in  9 its., resmax =   1.3e-014, Xi =  0.8000
N-R converged in  9 its., resmax =   2.6e-014, Xi =  0.8100
N-R converged in  8 its., resmax =  2.56e-013, Xi =  0.8200
```

3 supersaturated phases, most = Phengite

Swapping Phengite in for CO2(aq)

N-R converged in 7 its., resmax = 1.92e-013, Xi = 0.8200

N-R converged in 7 its., resmax = 4.8e-014, Xi = 0.8300

N-R converged in 7 its., resmax = 5.09e-014, Xi = 0.8400

2 supersaturated phases, most = K-feldspar

Swapping K-feldspar in for Mg++

N-R converged in 7 its., resmax = 1.2e-014, Xi = 0.8400

N-R converged in 3 its., resmax = 1.46e-015, Xi = 0.8500

N-R converged in 3 its., resmax = 3.25e-016, Xi = 0.8600

N-R converged in 3 its., resmax = 3.25e-016, Xi = 0.8700

N-R converged in 3 its., resmax = 1.01e-015, Xi = 0.8800

N-R converged in 3 its., resmax = 3.25e-016, Xi = 0.8900

N-R converged in 3 its., resmax = 1.46e-015, Xi = 0.9000

N-R converged in 3 its., resmax = 8.69e-016, Xi = 0.9100

N-R converged in 3 its., resmax = 1e-015, Xi = 0.9200

N-R converged in 3 its., resmax = 1.46e-015, Xi = 0.9300

N-R converged in 3 its., resmax = 3.25e-016, Xi = 0.9400

N-R converged in 3 its., resmax = 3.25e-016, Xi = 0.9500

N-R converged in 3 its., resmax = 1.46e-015, Xi = 0.9600

N-R converged in 3 its., resmax = 8.69e-016, Xi = 0.9700

N-R converged in 3 its., resmax = 7.48e-016, Xi = 0.9800

N-R converged in 3 its., resmax = 1.01e-015, Xi = 0.9900

N-R converged in 3 its., resmax = 1.16e-015, Xi = 1.0000

Successful completion of reaction path.

The output are in a dataset "React_output.txt" that shows the calculation results in tabular form, and a dataset "React_plot.dat" that passes more complete information to the graphics program Gtplot. The "React_output.txt" file is printed below:

```
Step #      0              Xi = 0.0000
Temperature =  25.0 C      Pressure =  1.013 bars
```

```
pH =  5.000
Ionic strength       =    0.001805
Activity of water    =    0.999963
Solvent mass         =    1.000000 kg
Solution mass        =    1.000109 kg
Solution density     =    1.013    g/cm3
Chlorinity           =    0.001047 molal
Dissolved solids     =         109 mg/kg sol'n
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001437	0.0000	0.0000	0.0000

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9535	-3.0015
CO2(aq)	0.0007839	34.49	1.0000	-3.1058
Ca++	0.0003683	14.76	0.8322	-3.5135
Na+	0.0002174	4.998	0.9541	-3.6831
Mg++	0.0001221	2.968	0.8360	-3.9909
SO4--	7.789e-005	7.481	0.8282	-4.1904
SiO2(aq)	4.993e-005	3.000	1.0005	-4.3014
HCO3-	3.536e-005	2.157	0.9544	-4.4718
K+	2.556e-005	0.9994	0.9535	-4.6131
H+	1.045e-005	0.01053	0.9569	-5.0000
CaSO4	4.130e-006	0.5622	1.0000	-5.3840
CaCl+	1.605e-006	0.1212	0.9541	-5.8151
MgSO4	1.112e-006	0.1338	1.0000	-5.9538
CaHCO3+	1.806e-007	0.01826	0.9548	-6.7633
MgCl+	1.507e-007	0.009007	0.9541	-6.8422
NaSO4-	6.929e-008	0.008248	0.9541	-7.1797
HSO4-	6.653e-008	0.006457	0.9541	-7.1974
MgHCO3+	3.697e-008	0.003154	0.9541	-7.4526
Al+++	1.430e-008	0.0003857	0.6716	-8.0177
AlOH++	1.345e-008	0.0005914	0.8302	-7.9522
KSO4-	1.173e-008	0.001586	0.9541	-7.9509

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.3021	Amrph^silica	-1.5878
Tridymite	-0.4679	Diaspore	-1.7694
Chalcedony	-0.5733	Kaolinite	-2.0675
Cristobalite	-0.8526	Boehmite	-2.6138
Gibbsite	-0.9780		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.02221	-1.653

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg

--

Al+++	3.706e-008	3.706e-008	0.0009999
Ca++	0.0003743	0.0003743	15.00
Cl-	0.001047	0.001047	37.11
H+	0.0007943	0.0007943	0.8005
H2O	55.51	55.51	9.999e+005
HCO3-	0.0008194	0.0008194	49.99
K+	2.558e-005	2.558e-005	0.9999
Mg++	0.0001234	0.0001234	3.000
Na+	0.0002175	0.0002175	4.999
SO4--	8.328e-005	8.328e-005	7.999
SiO2(aq)	4.993e-005	4.993e-005	3.000

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Aluminum	3.706e-008	3.706e-008	0.0009999		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.51	55.51	8.880e+005		
Potassium	2.558e-005	2.558e-005	0.9999		
Silicon	4.993e-005	4.993e-005	1.402		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 1 Xi = 0.0100
Temperature = 25.0 C Pressure = 1.013 bars
pH = 5.131
Ionic strength = 0.001817
Activity of water = 0.999963
Solvent mass = 1.000000 kg
Solution mass = 1.000111 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 111 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001423	1.437e-005	0.004000	0.001565

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	7.136e-006	-5.147	0.001842	0.0007101
(total)			0.001842	0.0007101

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9533	-3.0016
CO2(aq)	0.0007720	33.97	1.0000	-3.1124
Ca++	0.0003683	14.76	0.8317	-3.5138
Na+	0.0002174	4.997	0.9539	-3.6832
Mg++	0.0001221	2.968	0.8356	-3.9912
SiO2(aq)	7.877e-005	4.732	1.0005	-4.1034

SO4--	7.791e-005	7.483	0.8277	-4.1906
HCO3-	4.710e-005	2.874	0.9542	-4.3473
K+	3.993e-005	1.561	0.9533	-4.4195
H+	7.729e-006	0.007790	0.9568	-5.1311
CaSO4	4.126e-006	0.5616	1.0000	-5.3845
CaCl+	1.603e-006	0.1211	0.9539	-5.8154
MgSO4	1.111e-006	0.1337	1.0000	-5.9543
CaHCO3+	2.404e-007	0.02430	0.9546	-6.6392
MgCl+	1.507e-007	0.009002	0.9539	-6.8425
NaSO4-	6.926e-008	0.008245	0.9539	-7.1800
AlOH++	5.041e-008	0.002217	0.8297	-7.3786
MgHCO3+	4.921e-008	0.004198	0.9539	-7.3284
HSO4-	4.919e-008	0.004774	0.9539	-7.3286
Al(OH)2+	4.018e-008	0.002450	0.9539	-7.4165
Al+++	3.966e-008	0.001070	0.6708	-7.5751
KSO4-	1.832e-008	0.002476	0.9539	-7.7575
NaHCO3	1.254e-008	0.001054	1.0000	-7.9015

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Kaolinite	0.0000 sat	Boehmite	-1.7781
Quartz	-0.1041	Pyrophyllite	-1.8375
Gibbsite	-0.1423	Beidellit-Ca	-2.0483
Tridymite	-0.2699	Beidellit-Mg	-2.1087
Chalcedony	-0.3753	Beidellit-H	-2.2014
Cristobalite	-0.6546	Beidellit-K	-2.6560
Diaspore	-0.9337	Muscovite	-2.7091
Amrph^silica	-1.3898	Beidellit-Na	-2.7431

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.02188	-1.660

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	1.441e-005	1.372e-007	0.003702		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	0.0007369	0.0007797	0.7857		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	3.995e-005	3.995e-005	1.562		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	9.304e-005	7.877e-005	4.732		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	1.441e-005	1.372e-007	0.003702		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		

Chlorine	0.001047	0.001047	37.11
Hydrogen	111.0	111.0	1.119e+005
Magnesium	0.0001234	0.0001234	3.000
Oxygen	55.51	55.51	8.880e+005
Potassium	3.995e-005	3.995e-005	1.562
Silicon	9.304e-005	7.877e-005	2.212
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 2 Xi = 0.0200
Temperature = 25.0 C Pressure = 1.013 bars
pH = 5.240
Ionic strength = 0.001829
Activity of water = 0.999963
Solvent mass = 0.999999 kg
Solution mass = 1.000113 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 113 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001408	2.874e-005	0.008000	0.003129

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	1.436e-005	-4.843	0.003706	0.001429
Quartz	7.330e-006	-5.135	0.0004404	0.0001663
(total)			0.004146	0.001595

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9532	-3.0017
CO2(aq)	0.0007595	33.42	1.0000	-3.1195
Ca++	0.0003682	14.76	0.8313	-3.5142
Na+	0.0002174	4.997	0.9538	-3.6833
Mg++	0.0001221	2.968	0.8352	-3.9915
SiO2(aq)	0.0001001	6.015	1.0005	-3.9993
SO4--	7.792e-005	7.484	0.8272	-4.1908
HCO3-	5.952e-005	3.631	0.9541	-4.2457
K+	5.429e-005	2.123	0.9532	-4.2861
H+	6.019e-006	0.006066	0.9566	-5.2397
CaSO4	4.121e-006	0.5610	1.0000	-5.3850
CaCl+	1.602e-006	0.1210	0.9538	-5.8158
MgSO4	1.110e-006	0.1336	1.0000	-5.9547
CaHCO3+	3.036e-007	0.03069	0.9545	-6.5379
MgCl+	1.506e-007	0.008996	0.9538	-6.8428
NaSO4-	6.923e-008	0.008241	0.9538	-7.1802
MgHCO3+	6.215e-008	0.005302	0.9538	-7.2271
HSO4-	3.829e-008	0.003716	0.9538	-7.4375
KSO4-	2.490e-008	0.003365	0.9538	-7.6243
Al(OH)2+	2.462e-008	0.001501	0.9538	-7.6293
AlOH++	2.406e-008	0.001058	0.8292	-7.7000
NaHCO3	1.585e-008	0.001331	1.0000	-7.8000
Al+++	1.475e-008	0.0003978	0.6700	-8.0053

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Kaolinite	0.0000	sat	Pyrophyllite	-1.6293
Quartz	0.0000	sat	Beidellit-Ca	-1.8729
Tridymite	-0.1658		Boehmite	-1.8822
Gibbsite	-0.2464		Beidellit-Mg	-1.9333
Chalcedony	-0.2712		Beidellit-H	-2.0618
Cristobalite	-0.5505		Beidellit-K	-2.4366
Diaspore	-1.0378		Muscovite	-2.4670
Amrph^silica	-1.2857		Beidellit-Na	-2.5677

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.02153	-1.667

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	2.878e-005	6.829e-008	0.001842		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	0.0006794	0.0007655	0.7715		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	5.432e-005	5.432e-005	2.124		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.0001362	0.0001001	6.015		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	2.878e-005	6.829e-008	0.001842		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.51	55.51	8.880e+005		
Potassium	5.432e-005	5.432e-005	2.124		
Silicon	0.0001362	0.0001001	2.811		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 10 Xi = 0.1000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 5.762
Ionic strength = 0.001938
Activity of water = 0.999963
Solvent mass = 0.999996 kg
Solution mass = 1.000116 kg

Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 120 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001293	0.0001437	0.04000	0.01565

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	7.187e-005	-4.143	0.01855	0.007152
Quartz	0.0002372	-3.625	0.01425	0.005382
(total)			0.03281	0.01253

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9519	-3.0022
CO2(aq)	0.0006489	28.56	1.0000	-3.1878
Ca++	0.0003677	14.74	0.8271	-3.5169
Na+	0.0002174	4.997	0.9525	-3.6839
HCO3-	0.0001694	10.34	0.9529	-3.7920
K+	0.0001692	6.615	0.9519	-3.7930
Mg++	0.0001220	2.965	0.8312	-3.9939
SiO2(aq)	0.0001001	6.014	1.0005	-3.9993
SO4--	7.795e-005	7.487	0.8228	-4.1929
CaSO4	4.075e-006	0.5547	1.0000	-5.3899
H+	1.811e-006	0.001825	0.9555	-5.7618
CaCl+	1.592e-006	0.1202	0.9525	-5.8192
MgSO4	1.098e-006	0.1322	1.0000	-5.9593
CaHCO3+	8.588e-007	0.08681	0.9533	-6.0869
MgHCO3+	1.759e-007	0.01501	0.9525	-6.7758
MgCl+	1.497e-007	0.008946	0.9525	-6.8459
KSO4-	7.723e-008	0.01044	0.9525	-7.1333
NaSO4-	6.889e-008	0.008200	0.9525	-7.1830
NaHCO3	4.499e-008	0.003779	1.0000	-7.3469
HSO4-	1.147e-008	0.001113	0.9525	-7.9617

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.0000 sat	Beidellit-Ca	-1.7011
Kaolinite	0.0000 sat	Beidellit-Mg	-1.7614
Tridymite	-0.1658	Boehmite	-1.8822
Gibbsite	-0.2464	Beidellit-H	-2.0618
Chalcedony	-0.2712	Beidellit-K	-2.1016
Cristobalite	-0.5505	Beidellit-Na	-2.3956
Diaspore	-1.0378	Maximum Microcli	-2.3983
Amrph^silica	-1.2857	K-feldspar	-2.3983
Muscovite	-1.4518	Mordenite-K	-2.8638
Pyrophyllite	-1.6293	Illite	-2.9954

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.01839	-1.735

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Al+++	0.0001438	1.573e-008	0.0004243		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	0.0002195	0.0006507	0.6558		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0001693	0.0001693	6.618		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.0004811	0.0001001	6.015		

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Aluminum	0.0001438	1.573e-008	0.0004243		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.51	55.51	8.880e+005		
Potassium	0.0001693	0.0001693	6.618		
Silicon	0.0004811	0.0001001	2.812		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 20 Xi = 0.2000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.133
Ionic strength = 0.002079
Activity of water = 0.999963
Solvent mass = 0.999992 kg
Solution mass = 1.000120 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 128 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001150	0.0002874	0.08000	0.03129

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	0.0001437	-3.842	0.03710	0.01430
Quartz	0.0005246	-3.280	0.03152	0.01190
(total)			0.06863	0.02621

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.

Cl-	0.001045	37.05	0.9503	-3.0030
CO2(aq)	0.0005063	22.28	1.0000	-3.2956
Ca++	0.0003671	14.71	0.8220	-3.5204
K+	0.0003129	12.23	0.9503	-3.5268
HCO3-	0.0003111	18.98	0.9513	-3.5287
Na+	0.0002173	4.996	0.9510	-3.6847
Mg++	0.0001219	2.962	0.8263	-3.9969
SiO2(aq)	0.0001001	6.014	1.0005	-3.9993
SO4--	7.797e-005	7.488	0.8174	-4.1956
CaSO4	4.017e-006	0.5468	1.0000	-5.3961
CaCl+	1.579e-006	0.1193	0.9510	-5.8233
CaHCO3+	1.564e-006	0.1581	0.9518	-5.8271
MgSO4	1.084e-006	0.1304	1.0000	-5.9651
H+	7.718e-007	0.0007778	0.9542	-6.1329
MgHCO3+	3.208e-007	0.02737	0.9510	-6.5156
MgCl+	1.487e-007	0.008883	0.9510	-6.8496
KSO4-	1.419e-007	0.01917	0.9510	-6.8699
NaHCO3	8.233e-008	0.006916	1.0000	-7.0844
NaSO4-	6.844e-008	0.008146	0.9510	-7.1865
CO3--	2.224e-008	0.001335	0.8186	-7.7398
H3SiO4-	2.221e-008	0.002112	0.9510	-7.6753
OH-	1.472e-008	0.0002504	0.9507	-7.8540

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Quartz	0.0000	sat	K-feldspar	-1.7611
Kaolinite	0.0000	sat	Maximum Microcli	-1.7611
Tridymite	-0.1658		Boehmite	-1.8822
Gibbsite	-0.2464		Beidellit-K	-1.8913
Chalcedony	-0.2712		Beidellit-H	-2.0618
Cristobalite	-0.5505		Mordenite-K	-2.2266
Muscovite	-0.8146		Beidellit-Na	-2.2734
Diaspore	-1.0378		Illite	-2.4283
Amrph^silica	-1.2857		Calcite	-2.6293
Beidellit-Ca	-1.5792		Aragonite	-2.7942
Pyrophyllite	-1.6293		Sanidine high	-2.9603
Beidellit-Mg	-1.6395			

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.01435	-1.843

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0002875	1.226e-008	0.0003309		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.0003554	0.0005070	0.5109		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0003130	0.0003130	12.24		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		

SiO2(aq)	0.0009122	0.0001001	6.015

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Aluminum	0.0002875	1.226e-008	0.0003309		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.51	55.51	8.880e+005		
Potassium	0.0003130	0.0003130	12.24		
Silicon	0.0009122	0.0001001	2.812		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 30 Xi = 0.3000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.440
Ionic strength = 0.002221
Activity of water = 0.999963
Solvent mass = 0.999989 kg
Solution mass = 1.000124 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 136 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.001006	0.0004311	0.1200	0.04694

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	0.0002156	-3.666	0.05565	0.02145
Quartz	0.0008120	-3.090	0.04879	0.01842
(total)			0.1044	0.03988

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9488	-3.0037
K+	0.0004565	17.85	0.9488	-3.3634
HCO3-	0.0004534	27.66	0.9498	-3.3659
Ca++	0.0003664	14.68	0.8171	-3.5237
CO2(aq)	0.0003631	15.98	1.0000	-3.4400
Na+	0.0002173	4.995	0.9495	-3.6855
Mg++	0.0001217	2.959	0.8216	-3.9999
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.489	0.8123	-4.1983
CaSO4	3.961e-006	0.5392	1.0000	-5.4022
CaHCO3+	2.262e-006	0.2287	0.9503	-5.6676
CaCl+	1.567e-006	0.1184	0.9495	-5.8274
MgSO4	1.070e-006	0.1287	1.0000	-5.9707
MgHCO3+	4.644e-007	0.03962	0.9495	-6.3556

H+	3.809e-007	0.0003839	0.9529	-6.4401
KSO4-	2.057e-007	0.02780	0.9495	-6.7092
MgCl+	1.477e-007	0.008823	0.9495	-6.8532
NaHCO3	1.196e-007	0.01004	1.0000	-6.9223
NaSO4-	6.800e-008	0.008094	0.9495	-7.1900
CO3--	6.607e-008	0.003964	0.8135	-7.2697
H3SiO4-	4.513e-008	0.004292	0.9495	-7.3680
OH-	2.992e-008	0.0005088	0.9491	-7.5467
CaCO3	2.645e-008	0.002647	1.0000	-7.5775
KCl	1.110e-008	0.0008274	1.0000	-7.9547
Al(OH)4-	1.047e-008	0.0009943	0.9495	-8.0027

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Kaolinite	0.0000	sat	Beidellit-Mg	-1.5386
Quartz	0.0000	sat	Pyrophyllite	-1.6293
Tridymite	-0.1658		Beidellit-K	-1.7360
Gibbsite	-0.2464		Mordenite-K	-1.7559
Chalcedony	-0.2712		Boehmite	-1.8822
Muscovite	-0.3440		Illite	-1.9931
Cristobalite	-0.5505		Beidellit-H	-2.0618
Diaspore	-1.0378		Calcite	-2.1625
Amrph^silica	-1.2857		Beidellit-Na	-2.1723
K-feldspar	-1.2905		Aragonite	-2.3274
Maximum Microcli	-1.2905		Sanidine high	-2.4897
Beidellit-Ca	-1.4784			

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.01029	-1.988

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0004312	1.565e-008	0.0004222		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.0009302	0.0003633	0.3661		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0004567	0.0004567	17.85		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.001343	0.0001001	6.017		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.0004312	1.565e-008	0.0004222		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		

Magnesium	0.0001234	0.0001234	3.000
Oxygen	55.51	55.51	8.880e+005
Potassium	0.0004567	0.0004567	17.85
Silicon	0.001343	0.0001001	2.812
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 38 Xi = 0.3800
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.690
Ionic strength = 0.002330
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000128 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 142 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0008910	0.0005461	0.1520	0.05946

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	0.0002664	-3.574	0.06877	0.02651
Muscovite	4.450e-006	-5.352	0.001773	0.0006262
Quartz	0.001042	-2.982	0.06261	0.02364
(total)			0.1331	0.05078

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9476	-3.0042
K+	0.0005670	22.16	0.9476	-3.2698
HCO3-	0.0005628	34.33	0.9487	-3.2725
Ca++	0.0003659	14.66	0.8134	-3.5263
CO2(aq)	0.0002529	11.13	1.0000	-3.5970
Na+	0.0002173	4.994	0.9484	-3.6860
Mg++	0.0001216	2.956	0.8182	-4.0021
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.490	0.8084	-4.2004
CaSO4	3.920e-006	0.5335	1.0000	-5.4068
CaHCO3+	2.791e-006	0.2822	0.9493	-5.5768
CaCl+	1.558e-006	0.1177	0.9484	-5.8305
MgSO4	1.059e-006	0.1275	1.0000	-5.9750
MgHCO3+	5.735e-007	0.04892	0.9484	-6.2645
KSO4-	2.543e-007	0.03437	0.9484	-6.6177
H+	2.143e-007	0.0002159	0.9519	-6.6905
NaHCO3	1.481e-007	0.01244	1.0000	-6.8295
MgCl+	1.469e-007	0.008778	0.9484	-6.8560
CO3--	1.465e-007	0.008788	0.8097	-6.9259
H3SiO4-	8.042e-008	0.007647	0.9484	-7.1177
NaSO4-	6.767e-008	0.008055	0.9484	-7.1926
CaCO3	5.803e-008	0.005808	1.0000	-7.2363
OH-	5.332e-008	0.0009066	0.9480	-7.2963
Al(OH)4-	1.865e-008	0.001772	0.9484	-7.7523

KCl	1.375e-008	0.001025	1.0000	-7.8616

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Quartz	0.0000	sat	Beidellit-Mg	-1.4563
Kaolinite	0.0000	sat	Beidellit-K	-1.6225
Muscovite	0.0000	sat	Pyrophyllite	-1.6293
Tridymite	-0.1658		Illite	-1.6620
Gibbsite	-0.2464		Calcite	-1.8213
Chalcedony	-0.2712		Boehmite	-1.8822
Cristobalite	-0.5505		Aragonite	-1.9862
K-feldspar	-0.9465		Beidellit-H	-2.0618
Maximum Microcli	-0.9465		Beidellit-Na	-2.0899
Diaspore	-1.0378		Sanidine high	-2.1457
Amrph^silica	-1.2857		Clinoptil-K	-2.8140
Beidellit-Ca	-1.3962		Monohydrocalcite	-2.8152
Mordenite-K	-1.4120			

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.007168	-2.145

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0005461	2.308e-008	0.0006227		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.001390	0.0002527	0.2547		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0005717	0.0005672	22.18		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.001688	0.0001002	6.019		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.0005461	2.308e-008	0.0006227		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.52	55.51	8.880e+005		
Potassium	0.0005717	0.0005672	22.18		
Silicon	0.001688	0.0001002	2.813		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

```
Step #    40                Xi = 0.4000
Temperature =  25.0 C       Pressure =  1.013 bars
pH =  6.690
Ionic strength       =      0.002330
Activity of water    =      0.999963
Solvent mass         =      0.999986 kg
Solution mass        =      1.000128 kg
Solution density     =      1.013    g/cm3
Chlorinity           =      0.001047 molal
Dissolved solids     =          142 mg/kg sol'n
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Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0008623	0.0005749	0.1600	0.06258

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	0.0002376	-3.624	0.06135	0.02365
Muscovite	3.319e-005	-4.479	0.01322	0.004671
Quartz	0.001099	-2.959	0.06606	0.02494
(total)			0.1406	0.05327

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9476	-3.0042
K+	0.0005670	22.16	0.9476	-3.2698
HCO3-	0.0005628	34.33	0.9487	-3.2725
Ca++	0.0003659	14.66	0.8134	-3.5263
CO2(aq)	0.0002529	11.13	1.0000	-3.5970
Na+	0.0002173	4.994	0.9484	-3.6860
Mg++	0.0001216	2.956	0.8182	-4.0021
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.490	0.8084	-4.2004
CaSO4	3.920e-006	0.5335	1.0000	-5.4068
CaHCO3+	2.791e-006	0.2822	0.9493	-5.5768
CaCl+	1.558e-006	0.1177	0.9484	-5.8305
MgSO4	1.059e-006	0.1275	1.0000	-5.9750
MgHCO3+	5.735e-007	0.04892	0.9484	-6.2645
KSO4-	2.543e-007	0.03437	0.9484	-6.6177
H+	2.143e-007	0.0002159	0.9519	-6.6905
NaHCO3	1.481e-007	0.01244	1.0000	-6.8295
MgCl+	1.469e-007	0.008778	0.9484	-6.8560
CO3--	1.465e-007	0.008788	0.8097	-6.9259
H3SiO4-	8.042e-008	0.007647	0.9484	-7.1177
NaSO4-	6.767e-008	0.008055	0.9484	-7.1926
CaCO3	5.803e-008	0.005808	1.0000	-7.2363
OH-	5.332e-008	0.0009066	0.9480	-7.2963
Al(OH)4-	1.865e-008	0.001772	0.9484	-7.7523
KCl	1.375e-008	0.001025	1.0000	-7.8616

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.0000 sat	Beidellit-Mg	-1.4563
Kaolinite	0.0000 sat	Beidellit-K	-1.6225
Muscovite	0.0000 sat	Pyrophyllite	-1.6293

Tridymite	-0.1658	Illite	-1.6620
Gibbsite	-0.2464	Calcite	-1.8213
Chalcedony	-0.2712	Boehmite	-1.8822
Cristobalite	-0.5505	Aragonite	-1.9862
K-feldspar	-0.9465	Beidellit-H	-2.0618
Maximum Microcli	-0.9465	Beidellit-Na	-2.0899
Diaspore	-1.0378	Sanidine high	-2.1457
Amrph^silica	-1.2857	Clinoptil-K	-2.8140
Beidellit-Ca	-1.3962	Monohydrocalcite	-2.8152
Mordenite-K	-1.4120		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.007168	-2.145

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0005749	2.308e-008	0.0006227		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.001505	0.0002527	0.2547		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0006004	0.0005672	22.18		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.001774	0.0001002	6.019		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.0005749	2.308e-008	0.0006227		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.52	55.51	8.880e+005		
Potassium	0.0006004	0.0005672	22.18		
Silicon	0.001774	0.0001002	2.813		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 50 Xi = 0.5000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.690
Ionic strength = 0.002330
Activity of water = 0.999963
Solvent mass = 0.999989 kg
Solution mass = 1.000131 kg
Solution density = 1.013 g/cm3

Chlorinity = 0.001047 molal
Dissolved solids = 142 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0007186	0.0007186	0.2000	0.07823

Minerals in system	moles	log moles	grams	volume (cm3)
Kaolinite	9.393e-005	-4.027	0.02425	0.009348
Muscovite	0.0001769	-3.752	0.07046	0.02489
Quartz	0.001387	-2.858	0.08333	0.03147
(total)			0.1780	0.06571

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9476	-3.0042
K+	0.0005670	22.16	0.9476	-3.2698
HCO3-	0.0005628	34.33	0.9487	-3.2725
Ca++	0.0003659	14.66	0.8134	-3.5263
CO2(aq)	0.0002529	11.13	1.0000	-3.5970
Na+	0.0002173	4.994	0.9484	-3.6860
Mg++	0.0001216	2.956	0.8182	-4.0021
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.490	0.8084	-4.2004
CaSO4	3.920e-006	0.5335	1.0000	-5.4068
CaHCO3+	2.791e-006	0.2822	0.9493	-5.5768
CaCl+	1.558e-006	0.1177	0.9484	-5.8305
MgSO4	1.059e-006	0.1275	1.0000	-5.9750
MgHCO3+	5.735e-007	0.04892	0.9484	-6.2645
KSO4-	2.543e-007	0.03436	0.9484	-6.6177
H+	2.143e-007	0.0002159	0.9519	-6.6905
NaHCO3	1.481e-007	0.01244	1.0000	-6.8295
MgCl+	1.469e-007	0.008778	0.9484	-6.8560
CO3--	1.465e-007	0.008788	0.8097	-6.9259
H3SiO4-	8.042e-008	0.007647	0.9484	-7.1177
NaSO4-	6.767e-008	0.008055	0.9484	-7.1926
CaCO3	5.803e-008	0.005808	1.0000	-7.2363
OH-	5.332e-008	0.0009066	0.9480	-7.2963
Al(OH)4-	1.865e-008	0.001772	0.9484	-7.7523
KCl	1.375e-008	0.001025	1.0000	-7.8616

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Quartz	0.0000	sat	Beidellit-Mg	-1.4563
Kaolinite	0.0000	sat	Beidellit-K	-1.6225
Muscovite	0.0000	sat	Pyrophyllite	-1.6293
Tridymite	-0.1658		Illite	-1.6620
Gibbsite	-0.2464		Calcite	-1.8213
Chalcedony	-0.2712		Boehmite	-1.8822
Cristobalite	-0.5505		Aragonite	-1.9862
K-feldspar	-0.9465		Beidellit-H	-2.0618
Maximum Microcli	-0.9465		Beidellit-Na	-2.0899
Diaspore	-1.0378		Sanidine high	-2.1457
Amrph^silica	-1.2857		Clinoptil-K	-2.8140
Beidellit-Ca	-1.3962		Monohydrocalcite	-2.8152

```
  Mordenite-K        -1.4120
   (only minerals with log Q/K > -3 listed)

 Gases                  fugacity      log fug.
-----------------------------------------------
  Steam                   0.03131       -1.504
  CO2(g)                 0.007168       -2.145

                                      In fluid                    Sorbed
 Original basis  total moles     moles        mg/kg        moles        mg/kg
-----------------------------------------------------------------------------
--
  Al+++            0.0007186   2.308e-008   0.0006227
  Ca++             0.0003743    0.0003743       15.00
  Cl-               0.001047     0.001047       37.11
  H+               -0.002080    0.0002527      0.2547
  H2O                  55.51        55.51  9.999e+005
  HCO3-            0.0008194    0.0008194       49.99
  K+               0.0007441    0.0005672       22.18
  Mg++             0.0001234    0.0001234       3.000
  Na+              0.0002175    0.0002175       4.999
  SO4--           8.328e-005   8.328e-005       7.999
  SiO2(aq)          0.002206    0.0001002       6.019

 Elemental composition                In fluid                    Sorbed
                 total moles     moles        mg/kg        moles        mg/kg
-----------------------------------------------------------------------------
--
  Aluminum         0.0007186   2.308e-008   0.0006227
  Calcium          0.0003743    0.0003743       15.00
  Carbon           0.0008194    0.0008194       9.841
  Chlorine          0.001047     0.001047       37.11
  Hydrogen             111.0        111.0  1.119e+005
  Magnesium        0.0001234    0.0001234       3.000
  Oxygen               55.52        55.51  8.880e+005
  Potassium        0.0007441    0.0005672       22.18
  Silicon           0.002206    0.0001002       2.813
  Sodium           0.0002175    0.0002175       4.999
  Sulfur          8.328e-005   8.328e-005       2.670


        Step #    57              Xi = 0.5700
        Temperature =  25.0 C     Pressure =  1.013 bars
        pH =  6.702
        Ionic strength      =     0.002335
        Activity of water   =     0.999963
        Solvent mass        =     0.999990 kg
        Solution mass       =     1.000133 kg
        Solution density    =     1.013    g/cm3
        Chlorinity          =     0.001047 molal
        Dissolved solids    =          142 mg/kg sol'n

                          moles        moles         grams         cm3
 Reactants              remaining     reacted       reacted       reacted
-----------------------------------------------------------------------------
  K-feldspar            0.0006180     0.0008192        0.2280       0.08918

 Minerals in system     moles      log moles      grams        volume (cm3)
```

Muscovite	0.0002731	-3.564	0.1088	0.03842
Quartz	0.001588	-2.799	0.09542	0.03603
(total)			0.2042	0.07445

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9476	-3.0042
K+	0.0005714	22.34	0.9476	-3.2664
HCO3-	0.0005672	34.60	0.9487	-3.2692
Ca++	0.0003659	14.66	0.8133	-3.5264
CO2(aq)	0.0002485	10.94	1.0000	-3.6046
Na+	0.0002173	4.994	0.9483	-3.6860
Mg++	0.0001216	2.956	0.8180	-4.0022
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.490	0.8083	-4.2005
CaSO4	3.918e-006	0.5333	1.0000	-5.4070
CaHCO3+	2.812e-006	0.2843	0.9492	-5.5736
CaCl+	1.558e-006	0.1176	0.9483	-5.8306
MgSO4	1.059e-006	0.1274	1.0000	-5.9751
MgHCO3+	5.779e-007	0.04930	0.9483	-6.2612
KSO4-	2.562e-007	0.03463	0.9483	-6.6144
H+	2.089e-007	0.0002105	0.9518	-6.7015
CO3--	1.514e-007	0.009086	0.8095	-6.9115
NaHCO3	1.492e-007	0.01253	1.0000	-6.8262
MgCl+	1.469e-007	0.008776	0.9483	-6.8561
H3SiO4-	8.249e-008	0.007845	0.9483	-7.1066
NaSO4-	6.766e-008	0.008054	0.9483	-7.1927
CaCO3	5.997e-008	0.006002	1.0000	-7.2220
OH-	5.469e-008	0.0009300	0.9480	-7.2853
Al(OH)4-	1.892e-008	0.001797	0.9483	-7.7461
KCl	1.386e-008	0.001033	1.0000	-7.8582
MgCO3	1.008e-008	0.0008500	1.0000	-7.9964

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Muscovite	0.0000 sat	Beidellit-Mg	-1.4639
Quartz	0.0000 sat	Beidellit-K	-1.6289
Kaolinite	-0.0096	Pyrophyllite	-1.6389
Tridymite	-0.1658	Illite	-1.6589
Gibbsite	-0.2512	Calcite	-1.8070
Chalcedony	-0.2712	Boehmite	-1.8870
Cristobalite	-0.5505	Aragonite	-1.9719
K-feldspar	-0.9369	Beidellit-H	-2.0730
Maximum Microcli	-0.9369	Beidellit-Na	-2.0974
Diaspore	-1.0426	Sanidine high	-2.1361
Amrph^silica	-1.2857	Clinoptil-K	-2.7948
Mordenite-K	-1.4024	Monohydrocalcite	-2.8010
Beidellit-Ca	-1.4038		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.007043	-2.152

	In fluid	Sorbed

Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0008192	2.328e-008	0.0006281		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.002482	0.0002483	0.2502		
H2O	55.51	55.51	9.999e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.0008447	0.0005717	22.35		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.002507	0.0001002	6.019		

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Aluminum	0.0008192	2.328e-008	0.0006281		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.52	55.51	8.880e+005		
Potassium	0.0008447	0.0005717	22.35		
Silicon	0.002507	0.0001002	2.813		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 60 Xi = 0.6000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 6.776
Ionic strength = 0.002363
Activity of water = 0.999963
Solvent mass = 0.999990 kg
Solution mass = 1.000134 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 144 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0005749	0.0008623	0.2400	0.09388

Minerals in system	moles	log moles	grams	volume (cm3)
Muscovite	0.0002874	-3.541	0.1145	0.04044
Quartz	0.001674	-2.776	0.1006	0.03799
(total)			0.2151	0.07843

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9473	-3.0043

K+	0.0006001	23.46	0.9473	-3.2453
HCO3-	0.0005956	36.34	0.9484	-3.2481
Ca++	0.0003658	14.66	0.8123	-3.5271
CO2(aq)	0.0002199	9.676	1.0000	-3.6578
Na+	0.0002173	4.994	0.9480	-3.6862
Mg++	0.0001216	2.955	0.8171	-4.0027
SiO2(aq)	0.0001001	6.014	1.0006	-3.9993
SO4--	7.798e-005	7.490	0.8073	-4.2010
CaSO4	3.907e-006	0.5318	1.0000	-5.4081
CaHCO3+	2.949e-006	0.2981	0.9489	-5.5531
CaCl+	1.555e-006	0.1174	0.9480	-5.8314
MgSO4	1.056e-006	0.1271	1.0000	-5.9762
MgHCO3+	6.060e-007	0.05170	0.9480	-6.2407
KSO4-	2.688e-007	0.03632	0.9480	-6.5937
CO3--	1.888e-007	0.01133	0.8086	-6.8162
H+	1.761e-007	0.0001775	0.9516	-6.7758
NaHCO3	1.566e-007	0.01315	1.0000	-6.8053
MgCl+	1.467e-007	0.008764	0.9480	-6.8568
H3SiO4-	9.790e-008	0.009310	0.9480	-7.0324
CaCO3	7.458e-008	0.007464	1.0000	-7.1274
NaSO4-	6.758e-008	0.008044	0.9480	-7.1934
OH-	6.491e-008	0.001104	0.9477	-7.2111
Al(OH)4-	2.087e-008	0.001982	0.9480	-7.7037
KCl	1.455e-008	0.001084	1.0000	-7.8372
MgCO3	1.254e-008	0.001057	1.0000	-7.9016

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Muscovite	0.0000 sat	Illite	-1.6379
Quartz	0.0000 sat	Beidellit-K	-1.6716
Kaolinite	-0.0732	Pyrophyllite	-1.7025
Tridymite	-0.1658	Calcite	-1.7124
Chalcedony	-0.2712	Aragonite	-1.8773
Gibbsite	-0.2830	Boehmite	-1.9188
Cristobalite	-0.5505	Sanidine high	-2.0725
Maximum Microcli	-0.8733	Beidellit-Na	-2.1471
K-feldspar	-0.8733	Beidellit-H	-2.1471
Diaspore	-1.0744	Clinoptil-K	-2.6675
Amrph^silica	-1.2857	Monohydrocalcite	-2.7063
Mordenite-K	-1.3388	Magnesite	-2.9115
Beidellit-Ca	-1.4535	Dolomite-ord	-2.9951
Beidellit-Mg	-1.5136	Dolomite	-2.9951

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.006232	-2.205

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.0008623	2.479e-008	0.0006688		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.002655	0.0002195	0.2212		
H2O	55.51	55.51	9.999e+005		

HCO3-	0.0008194	0.0008194	49.99
K+	0.0008879	0.0006004	23.47
Mg++	0.0001234	0.0001234	3.000
Na+	0.0002175	0.0002175	4.999
SO4--	8.328e-005	8.328e-005	7.999
SiO2(aq)	0.002637	0.0001002	6.020

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.0008623	2.479e-008	0.0006688		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.52	55.51	8.880e+005		
Potassium	0.0008879	0.0006004	23.47		
Silicon	0.002637	0.0001002	2.814		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 70 Xi = 0.7000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.085
Ionic strength = 0.002458
Activity of water = 0.999963
Solvent mass = 0.999988 kg
Solution mass = 1.000137 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 149 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0004311	0.001006	0.2800	0.1095

Minerals in system	moles	log moles	grams	volume (cm3)
Muscovite	0.0003353	-3.475	0.1336	0.04718
Quartz	0.001962	-2.707	0.1179	0.04451
(total)			0.2514	0.09169

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9463	-3.0048
K+	0.0006959	27.21	0.9463	-3.1814
HCO3-	0.0006898	42.08	0.9475	-3.1847
Ca++	0.0003653	14.64	0.8093	-3.5293
Na+	0.0002172	4.993	0.9471	-3.6867
CO2(aq)	0.0001247	5.488	1.0000	-3.9040
Mg++	0.0001215	2.953	0.8142	-4.0046
SiO2(aq)	0.0001001	6.013	1.0006	-3.9993
SO4--	7.799e-005	7.490	0.8041	-4.2027

CaSO4	3.872e-006	0.5270	1.0000	-5.4121
CaHCO3+	3.398e-006	0.3434	0.9480	-5.4920
CaCl+	1.547e-006	0.1168	0.9471	-5.8341
MgSO4	1.048e-006	0.1261	1.0000	-5.9798
MgHCO3+	6.988e-007	0.05962	0.9471	-6.1792
CO3--	4.475e-007	0.02685	0.8054	-6.4432
KSO4-	3.105e-007	0.04195	0.9471	-6.5316
H3SiO4-	1.999e-007	0.01901	0.9471	-6.7228
NaHCO3	1.810e-007	0.01520	1.0000	-6.7424
CaCO3	1.751e-007	0.01753	1.0000	-6.7566
MgCl+	1.460e-007	0.008726	0.9471	-6.8591
OH-	1.325e-007	0.002254	0.9467	-6.9015
H+	8.641e-008	8.708e-005	0.9508	-7.0854
NaSO4-	6.731e-008	0.008011	0.9471	-7.1956
Al(OH)4-	3.199e-008	0.003039	0.9471	-7.5186
MgCO3	2.947e-008	0.002485	1.0000	-7.5306
KCl	1.683e-008	0.001255	1.0000	-7.7738

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.0000 sat	Beidellit-Ca	-1.6417
Muscovite	0.0000 sat	Beidellit-Mg	-1.7018
Tridymite	-0.1658	Sanidine high	-1.8235
Chalcedony	-0.2712	Beidellit-K	-1.8384
Kaolinite	-0.3222	Pyrophyllite	-1.9515
Gibbsite	-0.4075	Boehmite	-2.0433
Cristobalite	-0.5505	Clinoptil-K	-2.1696
Maximum Microcli	-0.6243	Dolomite-ord	-2.2533
K-feldspar	-0.6243	Dolomite	-2.2533
Mordenite-K	-1.0898	Phengite	-2.3312
Diaspore	-1.1989	Beidellit-Na	-2.3351
Amrph^silica	-1.2857	Monohydrocalcite	-2.3355
Calcite	-1.3416	Beidellit-H	-2.4372
Aragonite	-1.5065	Magnesite	-2.5405
Illite	-1.5458		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.003535	-2.452

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001006	3.467e-008	0.0009354		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.003230	0.0001237	0.1246		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001032	0.0006962	27.22		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.003068	0.0001003	6.026		

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Aluminum	0.001006	3.467e-008	0.0009354		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001234	3.000		
Oxygen	55.52	55.51	8.880e+005		
Potassium	0.001032	0.0006962	27.22		
Silicon	0.003068	0.0001003	2.816		
Sodium	0.0002175	0.0002175	4.999		
Sulfur	8.328e-005	8.328e-005	2.670		

Step # 80 Xi = 0.8000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.720
Ionic strength = 0.002552
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000141 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 155 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0002874	0.001150	0.3200	0.1252

Minerals in system	moles	log moles	grams	volume (cm3)
Muscovite	0.0003832	-3.417	0.1526	0.05392
Quartz	0.002248	-2.648	0.1351	0.05101
(total)			0.2877	0.1049

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9454	-3.0052
K+	0.0007917	30.95	0.9454	-3.1258
HCO3-	0.0007788	47.51	0.9466	-3.1324
Ca++	0.0003642	14.60	0.8063	-3.5321
Na+	0.0002172	4.993	0.9462	-3.6871
Mg++	0.0001213	2.948	0.8115	-4.0068
SiO2(aq)	0.0001001	6.013	1.0007	-3.9993
SO4--	7.799e-005	7.491	0.8010	-4.2043
CO2(aq)	3.265e-005	1.437	1.0000	-4.4861
CaSO4	3.832e-006	0.5216	1.0000	-5.4165
CaHCO3+	3.811e-006	0.3853	0.9472	-5.4425
CO3--	2.183e-006	0.1310	0.8023	-5.7566
CaCl+	1.537e-006	0.1161	0.9462	-5.8373
MgSO4	1.038e-006	0.1250	1.0000	-5.9837
H3SiO4-	8.621e-007	0.08198	0.9462	-6.0884
CaCO3	8.456e-007	0.08463	1.0000	-6.0728

MgHCO3+	7.850e-007	0.06697	0.9462	-6.1291
OH-	5.716e-007	0.009720	0.9458	-6.2671
KSO4-	3.519e-007	0.04755	0.9462	-6.4777
NaHCO3	2.039e-007	0.01713	1.0000	-6.6905
MgCl+	1.453e-007	0.008682	0.9462	-6.8617
MgCO3	1.425e-007	0.01201	1.0000	-6.8461
Al(OH)4-	8.125e-008	0.007718	0.9462	-7.1142
NaSO4-	6.704e-008	0.007980	0.9462	-7.1977
H+	2.007e-008	2.023e-005	0.9500	-7.7197
KCl	1.911e-008	0.001425	1.0000	-7.7186

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.0000 sat	Illite	-1.3442
Muscovite	0.0000 sat	Sanidine high	-1.3636
K-feldspar	-0.1644	Diaspore	-1.4289
Maximum Microcli	-0.1644	Monohydrocalcite	-1.6517
Tridymite	-0.1658	Magnesite	-1.8560
Chalcedony	-0.2712	Beidellit-Ca	-1.9687
Cristobalite	-0.5505	Beidellit-Mg	-2.0286
Phengite	-0.6048	Beidellit-K	-2.1465
Mordenite-K	-0.6298	Boehmite	-2.2733
Gibbsite	-0.6375	Pyrophyllite	-2.4114
Calcite	-0.6578	Dolomite-dis	-2.4295
Kaolinite	-0.7821	Beidellit-Na	-2.6617
Aragonite	-0.8227	Saponite-Ca	-2.8197
Dolomite-ord	-0.8851	Saponite-Mg	-2.8797
Dolomite	-0.8851	Beidellit-H	-2.9730
Clinoptil-K	-1.2497	Saponite-K	-2.9977
Amrph^silica	-1.2857		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.0009254	-3.034

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001150	8.272e-008	0.002231		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.003804	2.772e-005	0.02793		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001175	0.0007921	30.96		
Mg++	0.0001234	0.0001234	3.000		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.003499	0.0001010	6.066		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.001150	8.272e-008	0.002231		

Calcium	0.0003743	0.0003743	15.00
Carbon	0.0008194	0.0008194	9.841
Chlorine	0.001047	0.001047	37.11
Hydrogen	111.0	111.0	1.119e+005
Magnesium	0.0001234	0.0001234	3.000
Oxygen	55.52	55.51	8.880e+005
Potassium	0.001175	0.0007921	30.96
Silicon	0.003499	0.0001010	2.835
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 82 Xi = 0.8200
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.946
Ionic strength = 0.002567
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000142 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 156 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0002587	0.001178	0.3280	0.1283

Minerals in system	moles	log moles	grams	volume (cm3)
Muscovite	0.0003924	-3.406	0.1563	0.05522
Phengite	1.094e-006	-5.961	0.0004340	0.0001719
Quartz	0.002302	-2.638	0.1383	0.05223
(total)			0.2951	0.1076

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9452	-3.0053
K+	0.0008101	31.67	0.9452	-3.1159
HCO3-	0.0007895	48.17	0.9465	-3.1265
Ca++	0.0003636	14.57	0.8059	-3.5331
Na+	0.0002172	4.993	0.9461	-3.6872
Mg++	0.0001201	2.919	0.8110	-4.0114
SiO2(aq)	0.0001001	6.013	1.0007	-3.9993
SO4--	7.801e-005	7.492	0.8005	-4.2045
CO2(aq)	1.967e-005	0.8655	1.0000	-4.7062
CaHCO3+	3.855e-006	0.3897	0.9470	-5.4376
CaSO4	3.822e-006	0.5202	1.0000	-5.4177
CO3--	3.725e-006	0.2235	0.8019	-5.5247
CaCl+	1.534e-006	0.1158	0.9461	-5.8384
H3SiO4-	1.451e-006	0.1380	0.9461	-5.8624
CaCO3	1.439e-006	0.1440	1.0000	-5.8419
MgSO4	1.027e-006	0.1236	1.0000	-5.9884
OH-	9.619e-007	0.01636	0.9456	-6.0411
MgHCO3+	7.876e-007	0.06719	0.9461	-6.1278
KSO4-	3.599e-007	0.04863	0.9461	-6.4679
MgCO3	2.406e-007	0.02028	1.0000	-6.6188

NaHCO3	2.067e-007	0.01736	1.0000	-6.6847
MgCl+	1.438e-007	0.008592	0.9461	-6.8663
Al(OH)4-	1.141e-007	0.01084	0.9461	-6.9668
NaSO4-	6.701e-008	0.007977	0.9461	-7.1979
KCl	1.955e-008	0.001458	1.0000	-7.7088
MgOH+	1.471e-008	0.0006076	0.9461	-7.8565
H+	1.193e-008	1.202e-005	0.9499	-7.9457

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Quartz	0.0000	sat	Amrph^silica	-1.2857
Muscovite	0.0000	sat	Monohydrocalcite	-1.4209
Phengite	0.0000	sat	Saponite-Ca	-1.4288
K-feldspar	-0.0071		Saponite-Mg	-1.4893
Maximum Microcli	-0.0071		Diaspore	-1.5075
Tridymite	-0.1658		Saponite-K	-1.6033
Chalcedony	-0.2712		Magnesite	-1.6287
Dolomite	-0.4268		Talc	-1.9199
Dolomite-ord	-0.4268		Dolomite-dis	-1.9712
Calcite	-0.4269		Beidellit-Ca	-2.0775
Mordenite-K	-0.4726		Saponite-Na	-2.1218
Cristobalite	-0.5505		Beidellit-Mg	-2.1380
Aragonite	-0.5918		Beidellit-K	-2.2519
Gibbsite	-0.7161		Boehmite	-2.3519
Clinoptil-K	-0.9351		Saponite-H	-2.4970
Kaolinite	-0.9394		Phlogopite	-2.5069
Sanidine high	-1.2063		Pyrophyllite	-2.5687
Illite	-1.2716		Beidellit-Na	-2.7704

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.0005574	-3.254

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001178	1.153e-007	0.003111		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.003919	1.136e-005	0.01145		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001204	0.0008105	31.68		
Mg++	0.0001234	0.0001223	2.973		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.003585	0.0001016	6.101		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.001178	1.153e-007	0.003111		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		

Chlorine	0.001047	0.001047	37.11
Hydrogen	111.0	111.0	1.119e+005
Magnesium	0.0001234	0.0001223	2.973
Oxygen	55.52	55.51	8.880e+005
Potassium	0.001204	0.0008105	31.68
Silicon	0.003585	0.0001016	2.852
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 84 Xi = 0.8400
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.951
Ionic strength = 0.002562
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000142 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 156 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0002299	0.001207	0.3360	0.1314

Minerals in system	moles	log moles	grams	volume (cm3)
K-feldspar	8.725e-006	-5.059	0.002428	0.0009499
Muscovite	0.0003975	-3.401	0.1583	0.05593
Phengite	5.979e-006	-5.223	0.002372	0.0009393
Quartz	0.002327	-2.633	0.1398	0.05280
(total)			0.3030	0.1106

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9453	-3.0053
K+	0.0008202	32.06	0.9453	-3.1105
HCO3-	0.0007897	48.18	0.9465	-3.1264
Ca++	0.0003636	14.57	0.8060	-3.5331
Na+	0.0002172	4.993	0.9461	-3.6872
Mg++	0.0001153	2.802	0.8112	-4.0290
SiO2(aq)	0.0001001	6.013	1.0007	-3.9993
SO4--	7.804e-005	7.495	0.8006	-4.2042
CO2(aq)	1.944e-005	0.8553	1.0000	-4.7113
CaHCO3+	3.856e-006	0.3898	0.9471	-5.4375
CaSO4	3.825e-006	0.5206	1.0000	-5.4174
CO3--	3.771e-006	0.2263	0.8020	-5.5193
CaCl+	1.534e-006	0.1158	0.9461	-5.8383
H3SiO4-	1.469e-006	0.1396	0.9461	-5.8572
CaCO3	1.457e-006	0.1458	1.0000	-5.8365
MgSO4	9.869e-007	0.1188	1.0000	-6.0057
OH-	9.736e-007	0.01656	0.9457	-6.0359
MgHCO3+	7.564e-007	0.06453	0.9461	-6.1453
KSO4-	3.646e-007	0.04927	0.9461	-6.4623
MgCO3	2.339e-007	0.01972	1.0000	-6.6310
NaHCO3	2.067e-007	0.01736	1.0000	-6.6846

MgCl+	1.381e-007	0.008250	0.9461	-6.8839
Al(OH)4-	1.145e-007	0.01088	0.9461	-6.9651
NaSO4-	6.705e-008	0.007981	0.9461	-7.1976
KCl	1.980e-008	0.001476	1.0000	-7.7034
MgOH+	1.430e-008	0.0005905	0.9461	-7.8688
H+	1.179e-008	1.188e-005	0.9499	-7.9510

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Maximum Microcli	0.0000	sat	Amrph^silica	-1.2857
Quartz	0.0000	sat	Monohydrocalcite	-1.4154
Muscovite	0.0000	sat	Saponite-Ca	-1.4495
K-feldspar	0.0000	sat	Diaspore	-1.5111
Phengite	0.0000	sat	Saponite-Mg	-1.5129
Tridymite	-0.1658		Saponite-K	-1.6222
Chalcedony	-0.2712		Magnesite	-1.6409
Calcite	-0.4215		Talc	-1.9413
Dolomite	-0.4336		Dolomite-dis	-1.9780
Dolomite-ord	-0.4336		Beidellit-Ca	-2.0841
Mordenite-K	-0.4654		Saponite-Na	-2.1425
Cristobalite	-0.5505		Beidellit-Mg	-2.1475
Aragonite	-0.5864		Beidellit-K	-2.2567
Gibbsite	-0.7197		Boehmite	-2.3554
Clinoptil-K	-0.9209		Saponite-H	-2.5195
Kaolinite	-0.9465		Phlogopite	-2.5211
Sanidine high	-1.1992		Pyrophyllite	-2.5758
Illite	-1.2752		Beidellit-Na	-2.7770

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.0005509	-3.259

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001207	1.157e-007	0.003122		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.004034	1.104e-005	0.01113		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001233	0.0008206	32.08		
Mg++	0.0001234	0.0001175	2.854		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.003672	0.0001016	6.102		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.001207	1.157e-007	0.003122		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		

Hydrogen	111.0	111.0	1.119e+005
Magnesium	0.0001234	0.0001175	2.854
Oxygen	55.52	55.51	8.880e+005
Potassium	0.001233	0.0008206	32.08
Silicon	0.003672	0.0001016	2.852
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 90 Xi = 0.9000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.951
Ionic strength = 0.002562
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000142 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 156 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	0.0001437	0.001293	0.3600	0.1408

Minerals in system	moles	log moles	grams	volume (cm3)
K-feldspar	9.495e-005	-4.022	0.02643	0.01034
Muscovite	0.0003975	-3.401	0.1583	0.05593
Phengite	5.979e-006	-5.223	0.002372	0.0009393
Quartz	0.002327	-2.633	0.1398	0.05280
(total)			0.3270	0.1200

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9453	-3.0053
K+	0.0008202	32.06	0.9453	-3.1105
HCO3-	0.0007897	48.18	0.9465	-3.1264
Ca++	0.0003636	14.57	0.8060	-3.5331
Na+	0.0002172	4.993	0.9461	-3.6872
Mg++	0.0001153	2.802	0.8112	-4.0290
SiO2(aq)	0.0001001	6.013	1.0007	-3.9993
SO4--	7.804e-005	7.495	0.8006	-4.2042
CO2(aq)	1.944e-005	0.8553	1.0000	-4.7113
CaHCO3+	3.856e-006	0.3898	0.9471	-5.4375
CaSO4	3.825e-006	0.5206	1.0000	-5.4174
CO3--	3.771e-006	0.2263	0.8020	-5.5193
CaCl+	1.534e-006	0.1158	0.9461	-5.8383
H3SiO4-	1.469e-006	0.1396	0.9461	-5.8572
CaCO3	1.457e-006	0.1458	1.0000	-5.8365
MgSO4	9.869e-007	0.1188	1.0000	-6.0057
OH-	9.736e-007	0.01656	0.9457	-6.0359
MgHCO3+	7.564e-007	0.06453	0.9461	-6.1453
KSO4-	3.646e-007	0.04927	0.9461	-6.4623
MgCO3	2.339e-007	0.01972	1.0000	-6.6310
NaHCO3	2.067e-007	0.01736	1.0000	-6.6846
MgCl+	1.381e-007	0.008250	0.9461	-6.8839

Al(OH)4-	1.145e-007	0.01088	0.9461	-6.9651
NaSO4-	6.705e-008	0.007981	0.9461	-7.1976
KCl	1.980e-008	0.001476	1.0000	-7.7034
MgOH+	1.430e-008	0.0005905	0.9461	-7.8688
H+	1.179e-008	1.188e-005	0.9499	-7.9510

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Maximum Microcli	0.0000	sat	Amrph^silica	-1.2857
Quartz	0.0000	sat	Monohydrocalcite	-1.4154
Muscovite	0.0000	sat	Saponite-Ca	-1.4495
K-feldspar	0.0000	sat	Diaspore	-1.5111
Phengite	0.0000	sat	Saponite-Mg	-1.5129
Tridymite	-0.1658		Saponite-K	-1.6222
Chalcedony	-0.2712		Magnesite	-1.6409
Calcite	-0.4215		Talc	-1.9413
Dolomite	-0.4336		Dolomite-dis	-1.9780
Dolomite-ord	-0.4336		Beidellit-Ca	-2.0841
Mordenite-K	-0.4654		Saponite-Na	-2.1425
Cristobalite	-0.5505		Beidellit-Mg	-2.1475
Aragonite	-0.5864		Beidellit-K	-2.2567
Gibbsite	-0.7197		Boehmite	-2.3554
Clinoptil-K	-0.9209		Saponite-H	-2.5195
Kaolinite	-0.9465		Phlogopite	-2.5211
Sanidine high	-1.1992		Pyrophyllite	-2.5758
Illite	-1.2752		Beidellit-Na	-2.7770

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.0005509	-3.259

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001293	1.157e-007	0.003122		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.004379	1.104e-005	0.01113		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001319	0.0008206	32.08		
Mg++	0.0001234	0.0001175	2.854		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.003930	0.0001016	6.102		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.001293	1.157e-007	0.003122		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		

Magnesium	0.0001234	0.0001175	2.854
Oxygen	55.52	55.51	8.880e+005
Potassium	0.001319	0.0008206	32.08
Silicon	0.003930	0.0001016	2.852
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Step # 100 Xi = 1.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.951
Ionic strength = 0.002562
Activity of water = 0.999963
Solvent mass = 0.999986 kg
Solution mass = 1.000142 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001047 molal
Dissolved solids = 156 mg/kg sol'n

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
K-feldspar	3.037e-018	0.001437	0.4000	0.1565

Minerals in system	moles	log moles	grams	volume (cm3)
K-feldspar	0.0002387	-3.622	0.06643	0.02598
Muscovite	0.0003975	-3.401	0.1583	0.05593
Phengite	5.979e-006	-5.223	0.002372	0.0009393
Quartz	0.002327	-2.633	0.1398	0.05280
(total)			0.3670	0.1357

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.001045	37.05	0.9453	-3.0053
K+	0.0008202	32.06	0.9453	-3.1105
HCO3-	0.0007897	48.18	0.9465	-3.1264
Ca++	0.0003636	14.57	0.8060	-3.5331
Na+	0.0002172	4.993	0.9461	-3.6872
Mg++	0.0001153	2.802	0.8112	-4.0290
SiO2(aq)	0.0001001	6.013	1.0007	-3.9993
SO4--	7.804e-005	7.495	0.8006	-4.2042
CO2(aq)	1.944e-005	0.8553	1.0000	-4.7113
CaHCO3+	3.856e-006	0.3898	0.9471	-5.4375
CaSO4	3.825e-006	0.5206	1.0000	-5.4174
CO3--	3.771e-006	0.2263	0.8020	-5.5193
CaCl+	1.534e-006	0.1158	0.9461	-5.8383
H3SiO4-	1.469e-006	0.1396	0.9461	-5.8572
CaCO3	1.457e-006	0.1458	1.0000	-5.8365
MgSO4	9.869e-007	0.1188	1.0000	-6.0057
OH-	9.736e-007	0.01656	0.9457	-6.0359
MgHCO3+	7.564e-007	0.06453	0.9461	-6.1453
KSO4-	3.646e-007	0.04927	0.9461	-6.4623
MgCO3	2.339e-007	0.01972	1.0000	-6.6310
NaHCO3	2.067e-007	0.01736	1.0000	-6.6846
MgCl+	1.381e-007	0.008250	0.9461	-6.8839
Al(OH)4-	1.145e-007	0.01088	0.9461	-6.9651

NaSO4-	6.705e-008	0.007981	0.9461	-7.1976
KCl	1.980e-008	0.001476	1.0000	-7.7034
MgOH+	1.430e-008	0.0005905	0.9461	-7.8688
H+	1.179e-008	1.188e-005	0.9499	-7.9510

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K			log Q/K
Maximum Microcli	0.0000	sat	Amrph^silica	-1.2857
Quartz	0.0000	sat	Monohydrocalcite	-1.4154
Muscovite	0.0000	sat	Saponite-Ca	-1.4495
K-feldspar	0.0000	sat	Diaspore	-1.5111
Phengite	0.0000	sat	Saponite-Mg	-1.5129
Tridymite	-0.1658		Saponite-K	-1.6222
Chalcedony	-0.2712		Magnesite	-1.6409
Calcite	-0.4215		Talc	-1.9413
Dolomite	-0.4336		Dolomite-dis	-1.9780
Dolomite-ord	-0.4336		Beidellit-Ca	-2.0841
Mordenite-K	-0.4654		Saponite-Na	-2.1425
Cristobalite	-0.5505		Beidellit-Mg	-2.1475
Aragonite	-0.5864		Beidellit-K	-2.2567
Gibbsite	-0.7197		Boehmite	-2.3554
Clinoptil-K	-0.9209		Saponite-H	-2.5195
Kaolinite	-0.9465		Phlogopite	-2.5211
Sanidine high	-1.1992		Pyrophyllite	-2.5758
Illite	-1.2752		Beidellit-Na	-2.7770

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
Steam	0.03131	-1.504
CO2(g)	0.0005509	-3.259

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Al+++	0.001437	1.157e-007	0.003122		
Ca++	0.0003743	0.0003743	15.00		
Cl-	0.001047	0.001047	37.11		
H+	-0.004954	1.104e-005	0.01113		
H2O	55.51	55.51	9.998e+005		
HCO3-	0.0008194	0.0008194	49.99		
K+	0.001463	0.0008206	32.08		
Mg++	0.0001234	0.0001175	2.854		
Na+	0.0002175	0.0002175	4.999		
SO4--	8.328e-005	8.328e-005	7.999		
SiO2(aq)	0.004361	0.0001016	6.102		

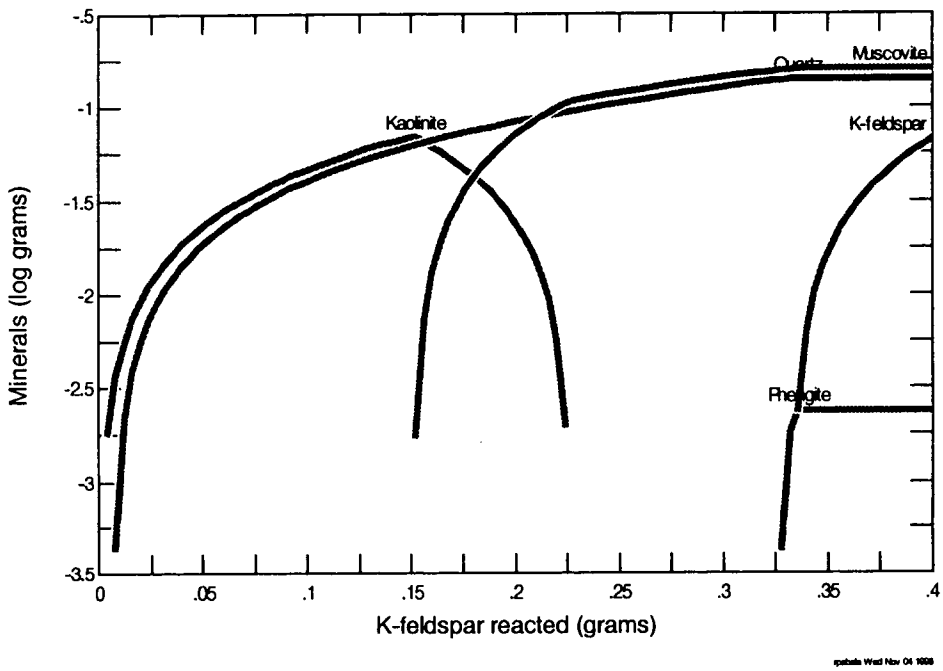
		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Aluminum	0.001437	1.157e-007	0.003122		
Calcium	0.0003743	0.0003743	15.00		
Carbon	0.0008194	0.0008194	9.841		
Chlorine	0.001047	0.001047	37.11		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001234	0.0001175	2.854		

Oxygen	55.52	55.51	8.880e+005
Potassium	0.001463	0.0008206	32.08
Silicon	0.004361	0.0001016	2.852
Sodium	0.0002175	0.0002175	4.999
Sulfur	8.328e-005	8.328e-005	2.670

Following typing the following command:

React> gtplot

The module Gtplot plotted the results of the React calculations (compare with figure 5.3 of the user's guide):



Thus, based on the calculations documented in this notebook, the Geochemist's Workbench software appears to be installed properly on a Windows NT workstation.

11/5/98

The database provided with the GWB software are not up-to-date. The latest version of the database is available from a Lawrence Livermore National Laboratory (LLNL) computer. The following information was copied from the GWB user's guide and includes instructions on how to download a recent version of the GWB database:

Thermodynamic datasets

Information potentially subject to copyright protection was redacted from this location. The redacted material is from the following reference:

Bethke, C.M. "The Geochemist's Workbench: A Users Guide to Rxn, Act2, Tact, React, and Gtplot." Urbana, Illinois: University of Illinois, Hydrogeology Program. 1992.

Per the instructions discussed above, a recent GWB database was download from the LLNL site. The following message (italicized here) was copied from the ftp site:

Index of /users/johnson/gwb/v2.3

*****

James W. Johnson (jwjohnson@llnl.gov) ... November 27, 1996

*****

Available in this directory:

GEMBOCHS thermodynamic datafile suite for GWB, version 2.3.

IMPORTANT NOTE: The number of secondary aqueous species contained in the "composite" datafile exceeds the maximum limit (1251) that can be read into GWB_v2.3 programs. In order to facilitate use of this database with GWB_v2.3, an abridged version of the composite datafile is provided, as described below. It is anticipated that maximum number-of-species limits will be eliminated in future releases of GWB.

**com*full ... the complete composite database; NOTE: THIS FILE CANNOT BE USED DIRECTLY WITH ANY OF THE GWB_V2.3 CODE MODULES ("ARRAY OVERFLOW" WILL OCCUR). IN ORDER TO USE THIS FILE, THE BLOCK OF [SECONDARY] AQUEOUS SPECIES MUST BE EDITED (REDUCED IN SIZE) TO ACHIEVE <= 1251 [SECONDARY] AQUEOUS SPECIES.*

**com*230 ... abridged version of the composite database; NOTE: THIS FILE CAN BE USED DIRECTLY WITH ALL CODE MODULES OF GWB_V2.3. In this database, secondary aqueous organic species and associated data provided by 95sho/kor and 90sho/hel (complete references available in *.full) have been eliminated.*

The complete SUPCRT96, NEA/CODATA, Pitzer, and Harvie-Moller-Weare (1984) databases can be used directly with all modules of GWB_v2.3.

In the following list of files contained in this directory, "V8" and "R6" refer to the corresponding version of EQ3/6 and the release number of the datafiles, respectively.

thermo.com.V8.R6.full ... complete "composite" database
thermo.com.V8.R6.230 ... abridged "composite" database
thermo.sup.V8.R6 ... SUPCRT96 database
thermo.nea.V8.R6 ... NEA/CODATA database
thermo.pit.V8.R6 ... Pitzer database
thermo.hmw.V8.R6 ... Harvie-Moller-Weare (1984) database

****

This summary is also available in the file README.gwb.v2.3

****

Please read the file README.gwb.v2.3
it was last modified on Thu Dec 5 17:11:53 1996 - 698 days ago

Name	Last modified	Size
Parent directory		
.message	06-Dec-96 00:00	2K
README.gwb.v2.3	06-Dec-96 00:00	2K
thermo.com.V8.R6.230	03-Sep-98 22:30	1.4M
thermo.com.V8.R6.full	03-Sep-98 22:29	1.6M
thermo.hmw.V8.R6	27-Nov-96 00:00	42K
thermo.nea.V8.R6	04-Dec-96 00:00	234K
thermo.pit.V8.R6	27-Nov-96 00:00	351K
thermo.sup.V8.R6	27-Nov-96 00:00	601K

8 files

A copy of each of the thermo.* files was downloaded.

For the purposes of installation verification, the React module was run using the thermo.com.V8.R6.full database (a copy was renamed thermo.dat, which is the database that GWB accesses by default).

Test Case 1:

The speciation of U(6+) was calculated for the following conditions: U concentration = 1.0E-5 molal, 0.1 m NaNO3, carbonate absent, f O2(g) = 0.2 atm, pH from 2 to 10. The following input commands were copied from the workstation screen:

React> UO2++ = 1.e-5 molal
React> swap NO3- for NH3(aq)
React> swap O2(g) for O2(aq)
React> f O2(g) = .1
React> Na+ = .1
-- No unit specified
React> Na+ = .1 molal
React> NO3- = .1 molal
React> balance on NO3-
React> noprecip
React> pH = 2
React> slide pH to 10
React> go

The following was the output copied from the screen:

Solving for initial system.

Loaded: 40 aqueous species,
35 minerals,
12 gases,
0 surface species,
5 elements,

2 oxides.

N-R converged in 16 its., resmax = 3.79e-013, Xi = 0.0000
Charge balance: NO3- molality adjusted from .1 to .1123

Removing O2(g) from basis vector
Swapping N2(aq) in for O2(g)

Following reaction path.

N-R converged in 14 its., resmax = 6.51e-013, Xi = 0.0100
Charge balance: NO3- molality adjusted from .1122 to .1102
N-R converged in 14 its., resmax = 3.32e-013, Xi = 0.0200
Charge balance: NO3- molality adjusted from .1102 to .1085
N-R converged in 13 its., resmax = 3.36e-013, Xi = 0.0300
Charge balance: NO3- molality adjusted from .1085 to .107
N-R converged in 13 its., resmax = 1.7e-013, Xi = 0.0400
Charge balance: NO3- molality adjusted from .107 to .1059
N-R converged in 11 its., resmax = 4.37e-011, Xi = 0.0500
Charge balance: NO3- molality adjusted from .1059 to .1049
N-R converged in 11 its., resmax = 2.5e-011, Xi = 0.0600
Charge balance: NO3- molality adjusted from .1049 to .1041
N-R converged in 11 its., resmax = 1.42e-011, Xi = 0.0700
Charge balance: NO3- molality adjusted from .1041 to .1034
N-R converged in 11 its., resmax = 7.96e-012, Xi = 0.0800
Charge balance: NO3- molality adjusted from .1034 to .1028
N-R converged in 11 its., resmax = 4.45e-012, Xi = 0.0900
Charge balance: NO3- molality adjusted from .1028 to .1023
N-R converged in 11 its., resmax = 2.46e-012, Xi = 0.1000
Charge balance: NO3- molality adjusted from .1024 to .102
N-R converged in 11 its., resmax = 1.35e-012, Xi = 0.1100
Charge balance: NO3- molality adjusted from .102 to .1016
N-R converged in 11 its., resmax = 7.4e-013, Xi = 0.1200

Charge balance: NO3- molality adjusted from .1016 to .1014

N-R converged in 11 its., resmax = 4.02e-013, Xi = 0.1300

Charge balance: NO3- molality adjusted from .1014 to .1011

N-R converged in 11 its., resmax = 2.17e-013, Xi = 0.1400

Charge balance: NO3- molality adjusted from .1011 to .101

N-R converged in 10 its., resmax = 4.19e-013, Xi = 0.1500

Charge balance: NO3- molality adjusted from .101 to .1008

N-R converged in 10 its., resmax = 2.44e-013, Xi = 0.1600

Charge balance: NO3- molality adjusted from .1008 to .1007

N-R converged in 9 its., resmax = 9.76e-013, Xi = 0.1700

Charge balance: NO3- molality adjusted from .1007 to .1006

N-R converged in 9 its., resmax = 5.7e-013, Xi = 0.1800

Charge balance: NO3- molality adjusted from .1006 to .1005

N-R converged in 9 its., resmax = 3.31e-013, Xi = 0.1900

Charge balance: NO3- molality adjusted from .1005 to .1004

N-R converged in 9 its., resmax = 1.92e-013, Xi = 0.2000

Charge balance: NO3- molality adjusted from .1004 to .1003

N-R converged in 8 its., resmax = 4.82e-011, Xi = 0.2100

Charge balance: NO3- molality adjusted from .1003 to .1003

N-R converged in 8 its., resmax = 3e-011, Xi = 0.2200

Charge balance: NO3- molality adjusted from .1003 to .1002

N-R converged in 8 its., resmax = 1.86e-011, Xi = 0.2300

Charge balance: NO3- molality adjusted from .1002 to .1002

N-R converged in 8 its., resmax = 1.15e-011, Xi = 0.2400

Charge balance: NO3- molality adjusted from .1002 to .1002

N-R converged in 8 its., resmax = 7.09e-012, Xi = 0.2500

Charge balance: NO3- molality adjusted from .1002 to .1001

N-R converged in 8 its., resmax = 4.38e-012, Xi = 0.2600

Charge balance: NO3- molality adjusted from .1001 to .1001

N-R converged in 8 its., resmax = 2.92e-012, Xi = 0.2700

Charge balance: NO3- molality adjusted from .1001 to .1001

N-R converged in 8 its., resmax = 2.58e-012, Xi = 0.2800

Charge balance: NO3- molality adjusted from .1001 to .1001

N-R converged in 8 its., resmax = 2.29e-012, Xi = 0.2900

Charge balance: NO3- molality adjusted from .1001 to .1001

N-R converged in 8 its., resmax = 2.07e-012, Xi = 0.3000

Charge balance: NO3- molality adjusted from .1001 to .1001

N-R converged in 8 its., resmax = 1.88e-012, Xi = 0.3100

N-R converged in 8 its., resmax = 1.74e-012, Xi = 0.3200

N-R converged in 8 its., resmax = 1.62e-012, Xi = 0.3300

N-R converged in 8 its., resmax = 1.48e-012, Xi = 0.3400

N-R converged in 8 its., resmax = 1.26e-012, Xi = 0.3500

N-R converged in 8 its., resmax = 7.7e-013, Xi = 0.3600

N-R converged in 9 its., resmax = 4.24e-013, Xi = 0.3700

N-R converged in 9 its., resmax = 4.27e-012, Xi = 0.3800

N-R converged in 9 its., resmax = 7.93e-012, Xi = 0.3900

N-R converged in 9 its., resmax = 1.4e-011, Xi = 0.4000

N-R converged in 9 its., resmax = 2.28e-011, Xi = 0.4100

N-R converged in 11 its., resmax = 3.07e-012, Xi = 0.4200

N-R converged in 11 its., resmax = 6.17e-012, Xi = 0.4300

2 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 1.09e-011, Xi = 0.4400

2 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 1.72e-011, Xi = 0.4500

2 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 2.45e-011, Xi = 0.4600

3 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 3.2e-011, Xi = 0.4700

5 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 3.89e-011, Xi = 0.4800

5 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 4.48e-011, Xi = 0.4900

5 supersaturated phases, most = Schoepite

N-R converged in 11 its., resmax = 4.92e-011, Xi = 0.5000

7 supersaturated phases, most = Schoepite

N-R converged in 12 its., resmax = 2.19e-013, Xi = 0.5100

7 supersaturated phases, most = Schoepite

N-R converged in 12 its., resmax = 2.22e-013, Xi = 0.5200

7 supersaturated phases, most = Schoepite

N-R converged in 12 its., resmax = 2.25e-013, Xi = 0.5300

7 supersaturated phases, most = Schoepite

Swapping UO2(OH)2(aq) in for UO2++

N-R converged in 9 its., resmax = 1.78e-014, Xi = 0.5400

7 supersaturated phases, most = Schoepite

N-R converged in 8 its., resmax = 4.91e-015, Xi = 0.5500

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 3.33e-011, Xi = 0.5600

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 1.9e-011, Xi = 0.5700

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 1.05e-011, Xi = 0.5800

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 5.5e-012, Xi = 0.5900

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 2.73e-012, Xi = 0.6000

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 1.26e-012, Xi = 0.6100

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 5.28e-013, Xi = 0.6200

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 1.93e-013, Xi = 0.6300

7 supersaturated phases, most = Schoepite

N-R converged in 7 its., resmax = 5.78e-014, Xi = 0.6400

7 supersaturated phases, most = Schoepite

N-R converged in 6 its., resmax = 1.2e-011, Xi = 0.6500

8 supersaturated phases, most = Schoepite

N-R converged in 6 its., resmax = 1.98e-012, Xi = 0.6600

8 supersaturated phases, most = Schoepite

N-R converged in 6 its., resmax = 7.62e-015, Xi = 0.6700

8 supersaturated phases, most = Na2U2O7

N-R converged in 6 its., resmax = 3.77e-013, Xi = 0.6800

8 supersaturated phases, most = Na2U2O7

N-R converged in 6 its., resmax = 5.97e-012, Xi = 0.6900

8 supersaturated phases, most = Na2U2O7

N-R converged in 6 its., resmax = 2.52e-011, Xi = 0.7000

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 5.96e-014, Xi = 0.7100

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 1.6e-013, Xi = 0.7200

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 3.81e-013, Xi = 0.7300

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 8.41e-013, Xi = 0.7400

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 1.75e-012, Xi = 0.7500

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 3.5e-012, Xi = 0.7600

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 6.74e-012, Xi = 0.7700

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 1.25e-011, Xi = 0.7800

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 2.23e-011, Xi = 0.7900

8 supersaturated phases, most = Na2U2O7

N-R converged in 7 its., resmax = 3.84e-011, Xi = 0.8000

8 supersaturated phases, most = Na2U2O7

N-R converged in 8 its., resmax = 5.12e-013, Xi = 0.8100

8 supersaturated phases, most = Na2U2O7

N-R converged in 8 its., resmax = 8.34e-013, Xi = 0.8200

8 supersaturated phases, most = Na2U2O7

N-R converged in 8 its., resmax = 1.34e-012, Xi = 0.8300

6 supersaturated phases, most = Na2U2O7

N-R converged in 8 its., resmax = 2.09e-012, Xi = 0.8400

6 supersaturated phases, most = Na2U2O7

N-R converged in 8 its., resmax = 3.2e-012, Xi = 0.8500

4 supersaturated phases, most = Na2U2O7

N-R converged in 9 its., resmax = 6.56e-013, Xi = 0.8600

4 supersaturated phases, most = Na2U2O7

N-R converged in 9 its., resmax = 2.86e-012, Xi = 0.8700

3 supersaturated phases, most = Na2U2O7

N-R converged in 10 its., resmax = 9.74e-013, Xi = 0.8800

3 supersaturated phases, most = Na2U2O7

N-R converged in 10 its., resmax = 1.35e-012, Xi = 0.8900

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 1.82e-012, Xi = 0.9000

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 2.4e-012, Xi = 0.9100

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 3.09e-012, Xi = 0.9200

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 3.9e-012, Xi = 0.9300

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 4.82e-012, Xi = 0.9400

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 5.88e-012, Xi = 0.9500

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 7.08e-012, Xi = 0.9600

Charge balance: NO3- molality adjusted from .09994 to .09993

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 8.45e-012, Xi = 0.9700

Charge balance: NO3- molality adjusted from .09993 to .09991

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 1e-011, Xi = 0.9800

Charge balance: NO3- molality adjusted from .09991 to .0999

1 supersaturated phase, Na2U2O7

N-R converged in 10 its., resmax = 1.18e-011, Xi = 0.9900

Charge balance: NO3- molality adjusted from .0999 to .09988

1 supersaturated phase, Na2U2O7

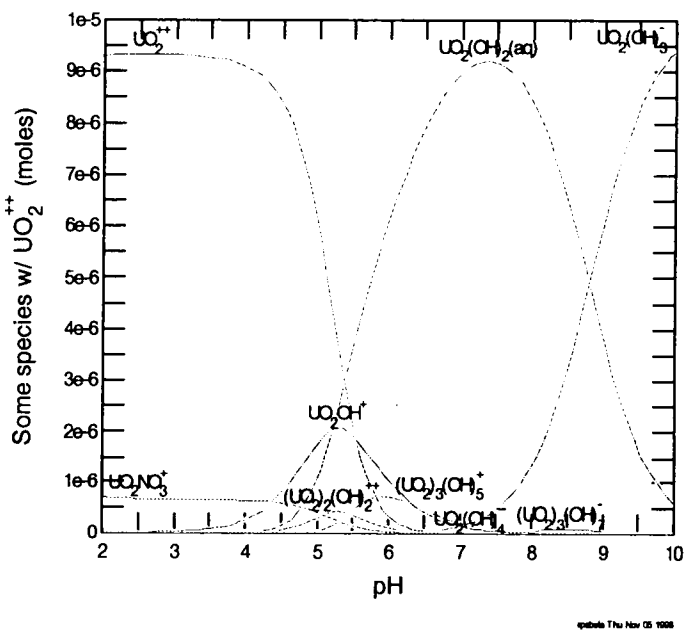
N-R converged in 10 its., resmax = 1.39e-011, Xi = 1.0000

Charge balance: NO3- molality adjusted from .09988 to .09986

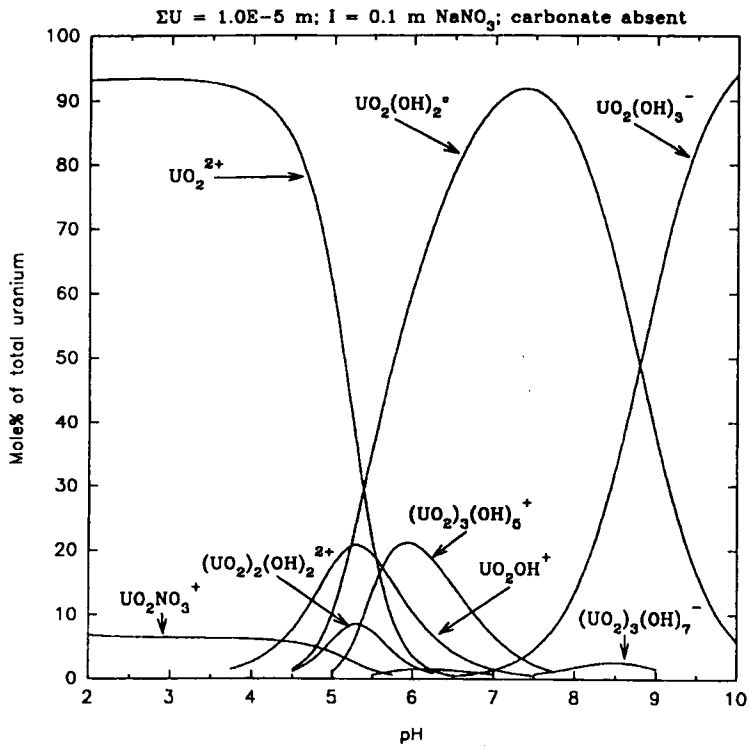
1 supersaturated phase, Na2U2O7

Successful completion of reaction path.

The following is the plot calculated by Gtplot (with some minor species eliminated from the figure for clarity):



For comparison, the following illustrates the U(6+) speciation for the same conditions that was calculated about 8 years ago using EQ3. It is not clear if the same values are in the database used in these EQ3 and GWB calculations. The figures are similar but not exactly the same. The stability field of the $(UO2)3(OH)5^+$ species is smaller for the GWB results compared to the EQ3 result. Thus, the parameter values may be different.



Test Case 2: (CO2 present)

React> UO2++ = 2.1e-7 molal

React> swap NO3- for NH3(aq)

React> swap O2(g) for O2(aq)

React> f O2(g) = .2

React> Na+ = .1 molal

React> NO3- = .1 molal

React> balance on NO3-

React> noprecip

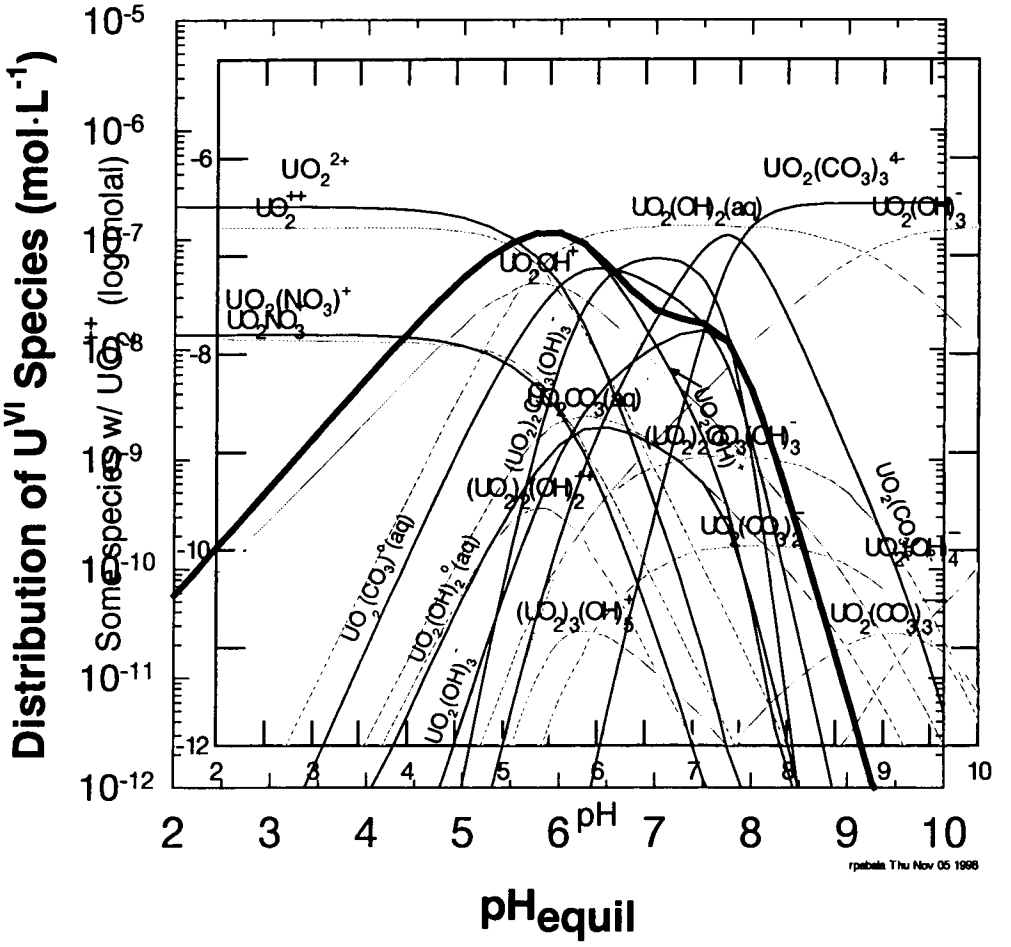
React> swap CO2(g) for HCO3-

React> log f CO2(g) = -3.5

React> pH = 2

React> slide pH to 10

React> go



The following is the resulting Gtplot figure:

The above result is different from the results illustrated in the figure below, which is based on EQ3 calculations published in Pabalan et al. [1998; Figure 2 in Uranium(VI) sorption onto selected mineral surfaces: Key geochemical parameters, Chapter 3 in Jenne, E. (ed.) *Adsorption of Metals by Geomedia*, Academic Press, San Diego, CA: 99-130].

It appears that the U carbonate complexes calculated using GWB do not become predominant, as calculated with EQ3. Need to check the database parameters.

(The rest of this page is left blank).

11/6/98

A comparison of the thermodynamic data for uranyl (UO2++) species in the EQ3 and GWB databases was made. The following values were copied from the EQ3 (data0.com.R2; CII: GEMBOCHS.V2-EQ8-DATA0.COM.R2 THERMODYNAMIC DATABASE; generated by GEMBOCHS.V2-JEWEL.SRC.R3 02-aug-1995 16:45:06) and GWB (dataset of thermodynamic data for gwb programs dataset format: oct94; activity model: debye-huckel; THERMODYNAMIC DATABASE: thermo.com.V8.R6.full; generated by GEMBOCHS.V2-Jewel.src.R6 03-dec-1996 16:55:04) database. Values in italics are from the GWB database.

Note that the 25 C log K values are the same for the two databases. However, the log Ks at other temperatures are different (a value of 500 is listed if no data is available). Need to check this with Jim Johnson at LLNL.

```
+-----------------------------------------------------------------------
UO2++
     sp.type =  basis
*    EQ3/6   =  com, alt, pit, nea
     revised =  28-jun-1993
*    mol.wt. = 270.028 g/mol
*    DHazero =   4.5
     charge  =   2.0
****
     2 element(s):
      2.0000 O              1.0000 U
****
*    gflag = 2 [calculated delG0f(delH0f,S0PrTr) used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 89cox/wag ]
*         delG0f =   -952.551 kj/mol       [reported]
*         delG0f =   -952.551 kj/mol       [calculated]
*         delH0f =  -1019.000 kj/mol       [reported]
*         S0PrTr =    -98.200 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

UO2++
"
     charge=  2.0      ion size=  4.5 A      mole wt.=  270.0277 g
     2 elements in species
      2.0000 O              1.0000 U
*    gflag = 2 [calculated delG0f(delH0f,S0PrTr) used]
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 89cox/wag
*         delG0f =   -952.551 kj/mol
*         delH0f =  -1019.000 kj/mol
*         S0PrTr =    -98.200 j/(mol*K)


+-----------------------------------------------------------------------
"
UO2(CO3)2--
"
```

```
     sp.type =  aqueous
"
*    EQ3/6   =  com, alt, nea
"
     revised =  29-jun-1993
*    mol.wt. = 390.046 g/mol
*    DHazero =   4.0
     charge  =  -2.0
****
     3 element(s):
      2.0000 C              8.0000 O              1.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  UO2(CO3)2--                  -2.0000  H+
     1.0000  UO2++                         2.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
         3.8228    3.7467    3.6456    4.3115
         4.9151    5.3004    5.4545    5.2796
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -2105.044 kj/mol       [reported]
*         delG0f =  -2105.044 kj/mol       [calculated]
*         delH0f =  -2350.960 kj/mol       [reported]
*         S0PrTr =    188.163 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

UO2(CO3)2--
"
     charge= -2.0      ion size=  4.0 A      mole wt.=  390.0461 g
"
     3 species in reaction
 -2.0000 H+                   1.0000 UO2++                2.0000 HCO3-
         4.4957    3.7467    2.8158    1.8343
         0.6657   -0.4826   -1.7152   -3.1632
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 92gre/fug
*         delG0f =  -2105.044 kj/mol
*         delH0f =  -2350.960 kj/mol
*         S0PrTr =    188.163 j/(mol*K)

+-----------------------------------------------------------------------
UO2(CO3)3(5-)
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  29-jun-1993
*    mol.wt. = 450.055 g/mol
*    DHazero =   4.0
     charge  =  -5.0
****
```

```
     3 element(s):
      3.0000 C              11.0000 O              1.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  UO2(CO3)3(5-)                -3.0000  H+
     1.0000  UO2+                          3.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   23.6241  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -2586.994 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      3.561 j/(mol*K) [source: 72kes    ]

UO2(CO3)3(5-)
"
     charge= -5.0      ion size=  4.0 A      mole wt.=  450.0553 g
"
     3 species in reaction
"
 -3.0000 H+                  1.0000 UO2+                3.0000 HCO3-
"
       500.0000   23.6241  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -2586.994 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-------------------------------------------------------------------
UO2(CO3)3----
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  29-jun-1993
*    mol.wt. = 450.055 g/mol
*    DHazero =   4.0
     charge  =  -4.0
****
     3 element(s):
      3.0000 C              11.0000 O              1.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  UO2(CO3)3----                -3.0000  H+
     1.0000  UO2++                         3.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
         9.1716    9.4302    9.6793   10.2268
        10.6880   10.9156   10.8633   10.3670
```

```
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -2659.543 kj/mol       [reported]
*         delG0f =  -2659.543 kj/mol       [calculated]
*         delH0f =  -3083.890 kj/mol       [reported]
*         S0PrTr =     33.852 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

UO2(CO3)3----
"
     charge= -4.0      ion size=  4.0 A      mole wt.=  450.0553 g
"
     3 species in reaction
"
 -3.0000 H+                  1.0000 UO2++                3.0000 HCO3-
"
         9.5017    9.4302    9.2905    9.0025
         8.4209    7.6495    6.6200    5.1589
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 92gre/fug
*         delG0f =  -2659.543 kj/mol
*         delH0f =  -3083.889 kj/mol
*         S0PrTr =     33.852 j/(mol*K)
+-----------------------------------------------------------------------
(UO2)11(CO3)6(OH)12-- (not in GWB)
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  24-aug-1990
*    mol.wt. =3534.448 g/mol
*    DHazero =   4.0
     charge  =  -2.0
****
     4 element(s):
      6.0000 C             12.0000 H             52.0000 O
     11.0000 U
****
     5 species in aqueous dissociation reaction:
    -1.0000  (UO2)11(CO3)6(OH)12--      -18.0000  H+
     6.0000  HCO3-                       11.0000  UO2++
    12.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   25.7347  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f = -16698.980 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
```

```
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]
+-----------------------------------------------------------------
(UO2)2(OH)2++
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  28-jun-1993
*    mol.wt. = 574.070 g/mol
*    DHazero =   4.5
     charge  =   2.0
****
     3 element(s):
      2.0000 H              6.0000 O              2.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)2(OH)2++                -2.0000  H+
     2.0000  H2O                           2.0000  UO2++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
         5.8968    5.6346    5.4302    5.7736
         6.2224    6.6745    7.1193    7.5512
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -2347.302 kj/mol       [reported]
*         delG0f =  -2347.302 kj/mol       [calculated]
*         delH0f =  -2572.065 kj/mol       [reported]
*         S0PrTr =    -38.000 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)2(OH)2++
"
     charge=  2.0      ion size=  4.5 A      mole wt.=  574.0701 g
"
     3 species in reaction
"
 -2.0000 H+                  2.0000 H2O                 2.0000 UO2++
         6.2772    5.6346    4.9999    4.5413
         4.2278    4.1102    4.1173    4.2062
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 92gre/fug
*         delG0f =  -2347.302 kj/mol
*         delH0f =  -2572.064 kj/mol
*         S0PrTr =    -38.000 j/(mol*K)

+-----------------------------------------------------------------
(UO2)2CO3(OH)3-
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  29-jun-1993
*    mol.wt. = 651.087 g/mol
*    DHazero =   4.0
```

```
     charge  =  -1.0
****
     4 element(s):
      1.0000 C              3.0000 H              10.0000 O
      2.0000 U
****
     5 species in aqueous dissociation reaction:
    -1.0000  (UO2)2CO3(OH)3-              -4.0000  H+
     1.0000  HCO3-                         2.0000  UO2++
     3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   11.2229  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -3139.525 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)2CO3(OH)3-
"
     charge= -1.0      ion size=  4.0 A      mole wt.=  651.0866 g
"
     4 species in reaction
"
 -4.0000 H+                  1.0000 HCO3-                2.0000 UO2++
"
  3.0000 H2O
"
       500.0000   11.2229  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -3139.525 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------
(UO2)2OH+++
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  13-aug-1990
*    mol.wt. = 557.063 g/mol
*    DHazero =   5.0
     charge  =   3.0
****
     3 element(s):
      1.0000 H              5.0000 O              2.0000 U
****
     4 species in aqueous dissociation reaction:
```

```
    -1.0000  (UO2)2OH+++                    -1.0000  H+
     1.0000  H2O                             2.0000  UO2++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000    2.7072  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -2126.830 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)2OH+++
~
     charge=  3.0      ion size=  5.0 A      mole wt.=  557.0627 g
~
     3 species in reaction
~
 -1.0000 H+                  1.0000 H2O                  2.0000 UO2++
       500.0000    2.7072  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -2126.830 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------------
(UO2)3(CO3)6(6-)
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  29-jun-1993
*    mol.wt. =1170.138 g/mol
*    DHazero =   4.0
     charge  =  -6.0
****
     3 element(s):
      6.0000 C             24.0000 O              3.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)3(CO3)6(6-)            -6.0000  H+
     3.0000  UO2++                        6.0000  HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        7.1839    8.0601    8.9944   11.2004
       13.2162   14.5337   15.1266   14.7097
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -6333.284 kj/mol       [reported]
```

```
*         delG0f =  -6333.284 kj/mol       [calculated]
*         delH0f =  -7171.080 kj/mol       [reported]
*         S0PrTr =    228.926 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3(CO3)6(6-)
"
     charge= -6.0      ion size=  4.0 A      mole wt.= 1170.1383 g
"
     3 species in reaction
"
 -6.0000 H+                  3.0000 UO2++                6.0000 HCO3-
         8.3431    8.0601    7.3190    5.9681
         3.6805    0.8685   -2.6241   -7.0853
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 92gre/fug
*         delG0f =  -6333.284 kj/mol
*         delH0f =  -7171.079 kj/mol
*         S0PrTr =    228.926 j/(mol*K)

+-----------------------------------------------------------------------
(UO2)3(OH)4++
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  28-jun-1993
*    mol.wt. = 878.112 g/mol
*    DHazero =   4.5
     charge  =   2.0
****
     3 element(s):
      4.0000 H             10.0000 O              3.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)3(OH)4++                -4.0000  H+
     3.0000  UO2++                         4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   11.9290  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -3738.287 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3(OH)4++
"
     charge=  2.0      ion size=  4.5 A      mole wt.=  878.1125 g
"
```

```
     3 species in reaction
"
 -4.0000 H+                    3.0000 UO2++                 4.0000 H2O
"
       500.0000   11.9290  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -3738.287 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------------
(UO2)3(OH)5+
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  28-jun-1993
*    mol.wt. = 895.120 g/mol
*    DHazero =   4.0
     charge  =   1.0
****
     3 element(s):
      5.0000 H              11.0000 O              3.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)3(OH)5+                  -5.0000  H+
     3.0000  UO2++                          5.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        16.3345   15.5862   14.9673   15.6767
        16.6516   17.6662   18.6845   19.6870
*
*    gflag = 1 [reported delG0f used]
*    extrapolation algorithm: 64cri/cob
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -3954.593 kj/mol       [reported]
*         delG0f =  -3954.593 kj/mol       [calculated]
*         delH0f =  -4389.086 kj/mol       [reported]
*         S0PrTr =     83.000 j/(mol*K)    [reported]
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3(OH)5+
"
     charge=  1.0      ion size=  4.0 A      mole wt.=  895.1198 g
"
     3 species in reaction
"
 -5.0000 H+                    3.0000 UO2++                 5.0000 H2O
"
        17.2322   15.5862   13.9178   12.6297
        11.6179   11.0604   10.7863   10.6975
*    gflag = 1 [reported delG0f used]
```

```
*    extrapolation algorithm: 64cri/cob
*    reference-state data source = 92gre/fug
*         delG0f =  -3954.593 kj/mol
*         delH0f =  -4389.086 kj/mol
*         S0PrTr =     83.000 j/(mol*K)

+-----------------------------------------------------------------
(UO2)3(OH)5CO2+
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  16-aug-1990
*    mol.wt. = 939.130 g/mol
*    DHazero =   4.0
     charge  =   1.0
****
     4 element(s):
      1.0000 C              5.0000 H             13.0000 O
      3.0000 U
****
     5 species in aqueous dissociation reaction:
    -1.0000  (UO2)3(OH)5CO2+             -4.0000  H+
     1.0000  HCO3-                        3.0000  UO2++
     4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000    9.6194  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -4338.410 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3(OH)5CO2+

     charge=  1.0      ion size=  4.0 A      mole wt.=  939.1296 g
     4 species in reaction
 -4.0000 H+                  1.0000 HCO3-                3.0000 UO2++
  4.0000 H2O
       500.0000    9.6194  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -4338.410 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------
(UO2)3(OH)7-
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
```

```
     revised =  28-jun-1993
*    mol.wt. = 929.134 g/mol
*    DHazero =   4.0
     charge  =  -1.0
****
     3 element(s):
      7.0000 H              13.0000 O              3.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)3(OH)7-                  -7.0000  H+
     3.0000  UO2++                          7.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   31.0508  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -4340.684 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3(OH)7-
"
     charge= -1.0      ion size=  4.0 A      mole wt.=  929.1345 g
"
     3 species in reaction
"
 -7.0000 H+                   3.0000 UO2++                7.0000 H2O
       500.0000   31.0508  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -4340.684 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------------
(UO2)3O(OH)2(HCO3)+
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  06-jul-1993
*    mol.wt. = 921.114 g/mol
*    DHazero =   4.0
     charge  =   1.0
****
     4 element(s):
      1.0000 C              3.0000 H              12.0000 O
      3.0000 U
****
     5 species in aqueous dissociation reaction:
    -1.0000  (UO2)3O(OH)2(HCO3)+          -4.0000  H+
```

```
     1.0000  HCO3-                          3.0000  H2O
     3.0000  UO2++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000    9.7129  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -4100.695 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]

(UO2)3O(OH)2(HCO3)+
     charge=  1.0      ion size=  4.0 A      mole wt.=  921.1143 g
     4 species in reaction
 -4.0000 H+                  1.0000 HCO3-                3.0000 H2O
  3.0000 UO2++
       500.0000    9.7129  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -4100.695 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A

+-----------------------------------------------------------------------
(UO2)4(OH)7+
     sp.type =  aqueous
*    EQ3/6   =  com, alt, nea
     revised =  28-jun-1993
*    mol.wt. =1199.162 g/mol
*    DHazero =   4.0
     charge  =   1.0
****
     3 element(s):
      7.0000 H             15.0000 O              4.0000 U
****
     4 species in aqueous dissociation reaction:
    -1.0000  (UO2)4(OH)7+                -7.0000  H+
     4.0000  UO2++                        7.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       500.0000   21.9508  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*
*    gflag = 1 [reported delG0f used]
*    ref-state data  [source: 92gre/fug ]
*         delG0f =  -5345.177 kj/mol       [reported]
*         delH0f =      N/A
*         S0PrTr =      N/A
*         Selec  =      0.000 j/(mol*K) [source: 72kes    ]
```

```
(UO2)4(OH)7+
''
     charge=  1.0       ion size=  4.0 A       mole wt.= 1199.1622 g
''
     3 species in reaction
''
 -7.0000 H+                    4.0000 UO2++                    7.0000 H2O
       500.0000   21.9508  500.0000  500.0000
       500.0000  500.0000  500.0000  500.0000
*    gflag = 1 [reported delG0f used]
*    reference-state data source = 92gre/fug
*         delG0f =  -5345.177 kj/mol
*         delH0f =      N/A
*         S0PrTr =      N/A
```

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11/6/98

A copy of the most recent thermodynamic database for EQ3/6 was downloaded from the LLNL ftp site. The file heading is (data0.com.V8.R6 CII: GEMBOCHS.V2-EQ8-data0.com.V8.R6 THERMODYNAMIC DATABASE generated by GEMBOCHS.V2-Jewel.src.R5 03-dec-1996 14:19:25). A comparison of the uranyl species thermodynamic data with values in the older EQ3/6 database [with file heading (data0.com.R2 CII: GEMBOCHS.V2-EQ8-DATA0.COM.R2 THERMODYNAMIC DATABASE generated by GEMBOCHS.V2-JEWEL.SRC.R3 02-aug-1995 16:45:06)] show that the new EQ3/6 data are consistent with the GWB data downloaded yesterday, but is inconsistent with the old EQ3/6 database.

An e-mail was sent to Jim Johnson at LLNL to determine why there is an inconsistency between the new and old EQ3/6 datafiles. Below is a copy of his reply to my e-mail:

```
Hi Bobby,
Thanks for your note.  The elevated-T logK data for charged aqueous uranyl
species are correct in data0.com.V8.R6, and incorrect in data0.com.R2.
Between
the release of version R1 (which was release 25 of the previous naming
convention) and R2 of these datafiles (I believe the R2s were released in Aug
'95), large-scale changes/updates were made to the generating software;
unfortunately, a subtle bug was inadvertently introduced that corrupted
implementation of the Criss-Cobble extrapolation algorithm for certain charged
aqueous species.  This caused the erroneous high-T logK values you note; the
problem has long since been rectified.  However, as an outgrowth of this
experience more stringent pre-release testing of new datafile suites was
implemented, which has thus far prevented subsequent difficulties of this
kind.

A greatly expanded and more extensively documented EQ3/6 datafile suite will
soon be available; I'll send you an email when the new suite is posted on our
ftp site so you can upgrade.

Meantime, please let me know if you encounter any difficulties with the R6
datafiles.  Thanks.

Regards, Jim

On Nov 6,  2:49pm, rpabalan@swri.edu wrote:
> Subject: question on log Ks for uranyl species
>
> Jim:
>
> I was comparing the log Ks for the aqueous uranyl species that are in the
> data0.com.V8.R6 file and in the older data0.com.R2 file.  I noticed that all
the
> information is the same, except the log Ks at temperatures not equal to 25
C.
> Could you please let me know why there are large differences in the log Ks
> between the two files? An example comparison is shown below.
```

```
>
> Thanks.
>
> bobby pabalan
> Southwest Research Institute
> 210-522-5304
>
> data0.com.V8.R6
> CII: GEMBOCHS.V2-EQ8-data0.com.V8.R6
> THERMODYNAMIC DATABASE
> generated by GEMBOCHS.V2-Jewel.src.R5 03-dec-1996 14:19:25
>
> +-----------------------------------------------------------------
> UO2(CO3)2--
>      sp.type =  aqueous
> *    EQ3/6   =  com, alt, nea
>      revised =  29-jun-1993
> *    mol.wt. = 390.046 g/mol
> *    DHazero =   4.0
>      charge  =  -2.0
> ****
>      3 element(s):
>       2.0000 C              8.0000 O              1.0000 U
> ****
>      4 species in aqueous dissociation reaction:
>     -1.0000  UO2(CO3)2--                  -2.0000  H+
>      1.0000  UO2++                         2.0000  HCO3-
> *
> **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
>          4.4957    3.7467    2.8158    1.8343
>          0.6657   -0.4826   -1.7152   -3.1632
> *
> *    gflag = 1 [reported delG0f used]
> *    extrapolation algorithm: 64cri/cob
> *    ref-state data  [source: 92gre/fug ]
> *         delG0f =  -2105.044 kj/mol       [reported]
> *         delG0f =  -2105.044 kj/mol       [calculated]
> *         delH0f =  -2350.960 kj/mol       [reported]
> *         S0PrTr =    188.163 j/(mol*K)    [reported]
> *         Selec  =      0.000 j/(mol*K) [source: 72kes    ]
> +-----------------------------------------------------------------
>
> data0.com.R2
> CII: GEMBOCHS.V2-EQ8-DATA0.COM.R2
> THERMODYNAMIC DATABASE
> generated by GEMBOCHS.V2-JEWEL.SRC.R3 02-aug-1995 16:45:06
> Output package:  eq3
> Data set:        com
>
> +-----------------------------------------------------------------
> UO2(CO3)2--
>      sp.type =  aqueous
> *    EQ3/6   =  com, alt, nea
>      revised =  29-jun-1993
> *    mol.wt. = 390.046 g/mol
> *    DHazero =   4.0
>      charge  =  -2.0
> ****
>      3 element(s):
>       2.0000 C              8.0000 O              1.0000 U
```

```
> ****
>      4 species in aqueous dissociation reaction:
>     -1.0000  UO2(CO3)2--                  -2.0000  H+
>      1.0000  UO2++                         2.0000  HCO3-
> *
> **** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
>          3.8228    3.7467    3.6456    4.3115
>          4.9151    5.3004    5.4545    5.2796
> *
> *    gflag = 1 [reported delG0f used]
> *    extrapolation algorithm: 64cri/cob
> *    ref-state data  [source: 92gre/fug ]
> *         delG0f =  -2105.044 kj/mol       [reported]
> *         delG0f =  -2105.044 kj/mol       [calculated]
> *         delH0f =  -2350.960 kj/mol       [reported]
> *         S0PrTr =    188.163 j/(mol*K)    [reported]
> *         Selec  =      0.000 j/(mol*K) [source: 72kes    ]
> +-----------------------------------------------------------------
>
>
>-- End of excerpt from rpabalan@swri.edu
```


--
James W. Johnson

email: jwjohnson@llnl.gov
phone: 925-423-7352
fax: 925-422-0208

GET Division, L-219
Lawrence Livermore Natl. Lab.
Livermore, CA 94550

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Entries into Scientific Notebook No. 278 for the period October 1, 1998, to December 31, 1998, have been made by

RTPabalan 1/6/99

Roberto T. Pabalan / Date

No original entry into this Scientific Notebook has been removed.

Scientific Notebook #278

RADIONUCLIDE TRANSPORT

Project No. 20-1402-871

Scientific Notebook #278

RADIONUCLIDE TRANSPORT

Project No. 20-1402-871

The entries in this electronic scientific notebook #278 document activities conducted during the Period April 1, 1999, through June 30, 1999, under the Radionuclide Transport Key Technical Issue (Project Number 20-1402-871). **Note that no entries were made during the period January 1, 1999 through March 31, 1999. This lack of entry for that period was communicated to Bruce Mabrito via email.**

04/09/99

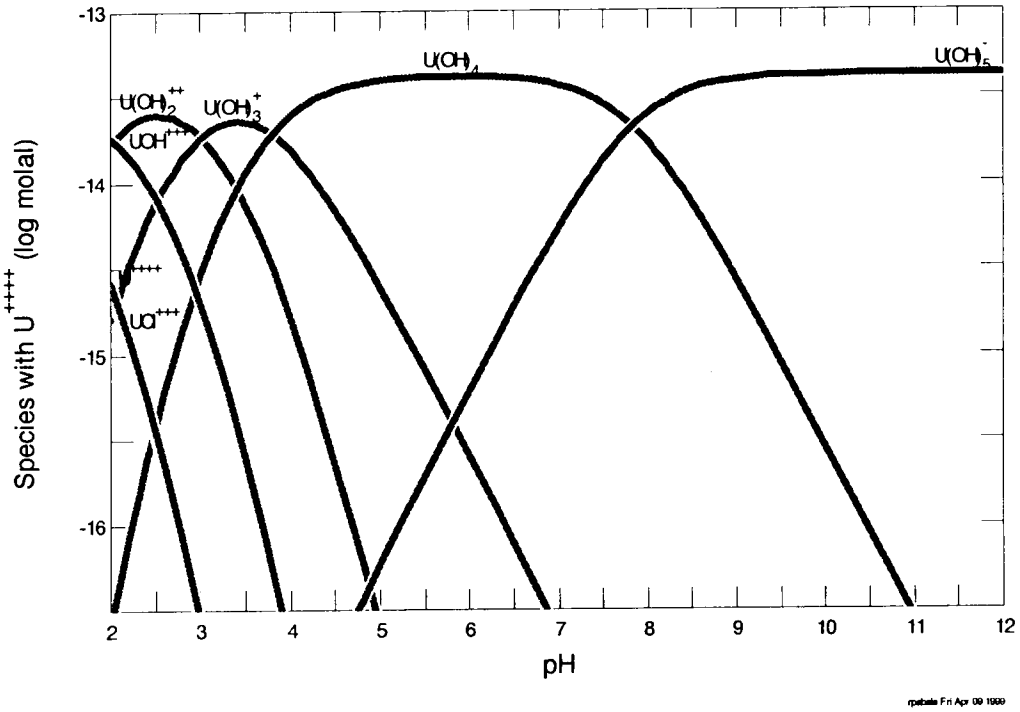
The following entries document the speciation calculations done using The Geochemist's Workbench (GWB), a commercially available set of software tools for conducting geochemical calculations. Installation of GWB was documented in scientific notebook #278 (last quarter of CY 1998). The following calculations were done to allow the author to become familiar with the program, and also to calculate uranium speciation calculations and saturation conditions for the uranium solutions that were used to prepare the EXAFS samples that LLNL investigators analyzed.

1. The following run was done using React to try to duplicate the example given on page 108 of the GWB user's guide. The example is a calculation of the species distribution of U(IV) versus pH by sliding pH from 2 to 12. The database needed for this example is the thermo.dat file that came with the installation diskettes. The newer database downloaded from LLNL has different basis species, including uranium, and gives different results.

The following commands were copied from the React window:

React> log ug/kg U++++ = -5
React> Na+ = .2 molal
React> balance on Cl-
React> pH = 2
React> slide pH to 12
React> go

The following is the resulting Gtplot figure:



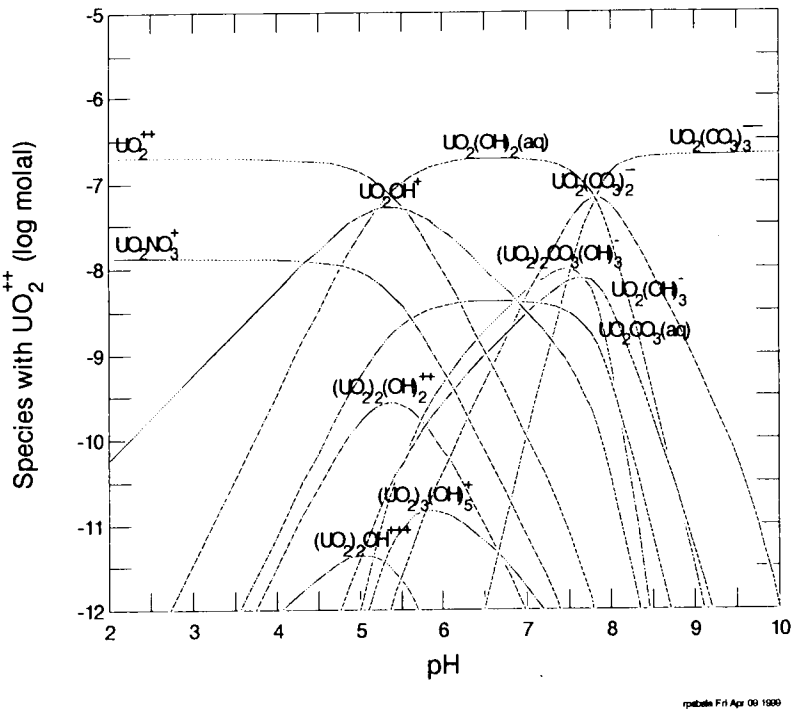
A comparison of the figure with the figure in the user's guide indicate the results are identical.

2. A uranium speciation calculation was done using React for comparison with Figure 1 in Pabalan et al. (1998; Chapter 3 in Adsorption of Metals by Geomedia). The following script, which was used in the calculation, was provided by Lauren Browning:

```
# React script, saved Mon Mar 15 1999 by lbrowning
data = "C:\Program Files\Gwb\Gtdata\thermoEQ6V8.dat" verify
work_dir = D:\
temperature = 25
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
swap NO3- for NH3(aq)
1 kg free H2O
fugacity O2(g) = .199526231
fugacity CO2(g) = .000316227766
total molality NO3- = .1
pH = 2
total molality UO2++ = 2.1e-7
balance on Na+
total molality Na+ = .1
slide pH to 10
fix fugacity of CO2(g)
delxi = .001
```

Note that the database used is the V8.R6 release of thermo.dat.

The following is the resulting Gtplot figure of uranium speciation:



3. The same script as in #2 was used. However, the database revised by Lauren Browning was used. See the following transmittal email from LB:

```
Date:                4/9/99
"
Sender:                Lauren Browning
"
To:               Roberto Pabalan
"
Priority:               Normal
Subject:               Speciation files
              ---------------------------------------------------------------
---------------
              Hi Bobby,

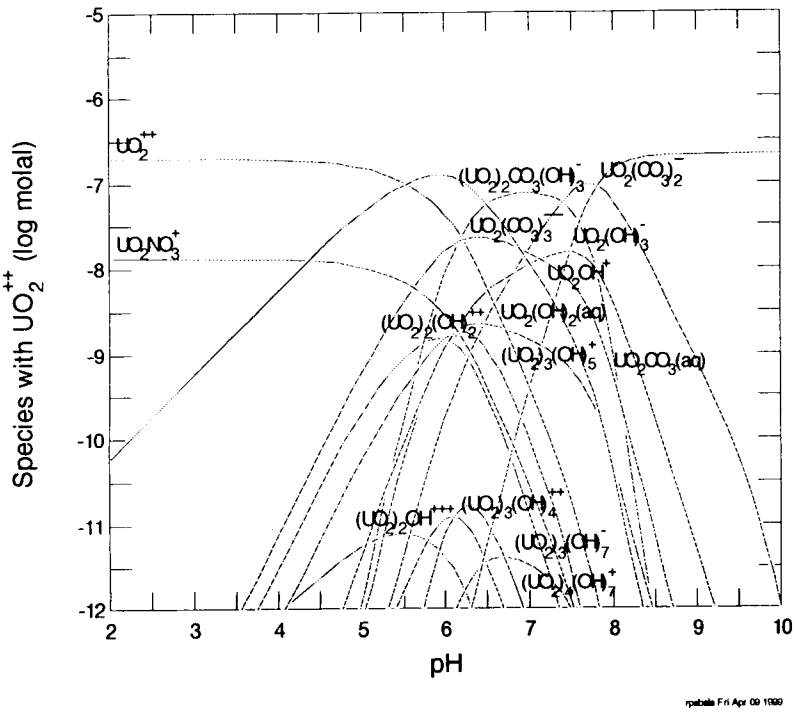
                   Here are the files you requested. If you want to reproduce
the results that I showed you, then you also need the EQ3 format database
that I downloaded and revised. It is enclosed. I noticed that when log K for
UO2CO3 is ~0.2619, the standard EQ3/6 log K value for 60 C, the GWB curves
match yours better. So, make some changes to the database to see this
difference.
```

Let me know if you have any questions.

Lauren

Values for the UO2(OH)2 and UO2CO3 neutral aqueous species in the LB database are different from the V8R6 database. Values of log Ks from the V8R6 database are : UO2(OH)2(aq)—10.3146; UO2CO3(aq) —0.6634. Values of log Ks from LB are: UO2(OH)2(aq) —13.0000; UO2CO3(aq) —0.2619. Note that the value of 0.2619 for UO2CO3(aq) is the 60 C value in the original EQ3 database.

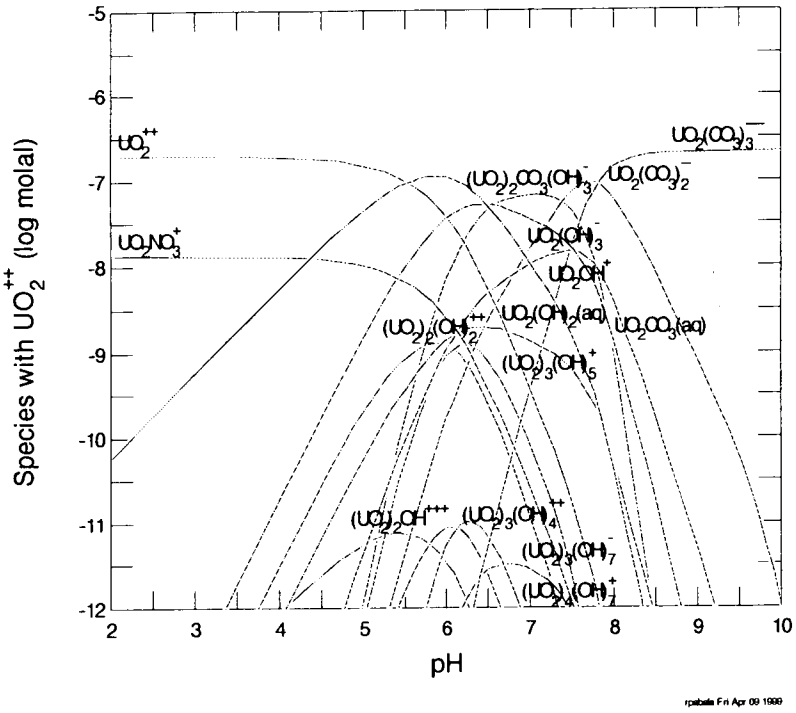
The following is the resulting Gtplot figure of uranium speciation:



Note the differences in the stability field of the neutral hydroxy and neutral carbonate complexes in #2 and #3.

4. The same script as in #2 and #3 was used. In this case, the V8R6 thermo.dat file was modified to change the value of log K for UO2(OH2) to 13.000.

The resulting Gtplot figure is shown below:



Compare the figure in #3, the curve for the UO2CO3(aq) is shifted down.

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April 13, 1999

The following documents additional benchmarking calculations of uranium speciation using GWB.

5. Calculate uranium speciation and mineral saturation for a solution with 2.1E-7 molal UO2(NO3)2, no CO2, 0.1 m NaNO3 background electrolyte, charge balance on NO3-.

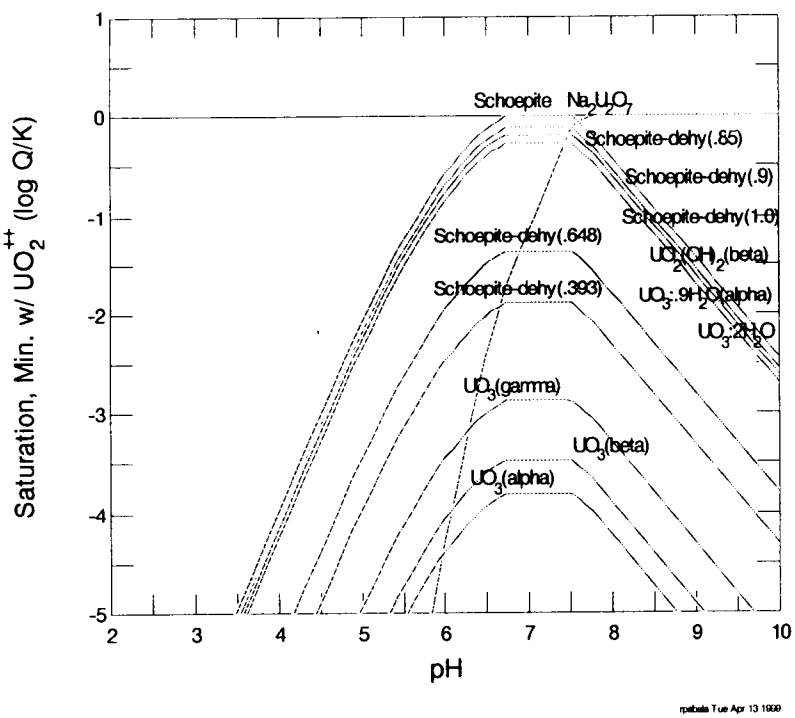
   5a. Using D. Turner log K for UO2(OH)2(aq):

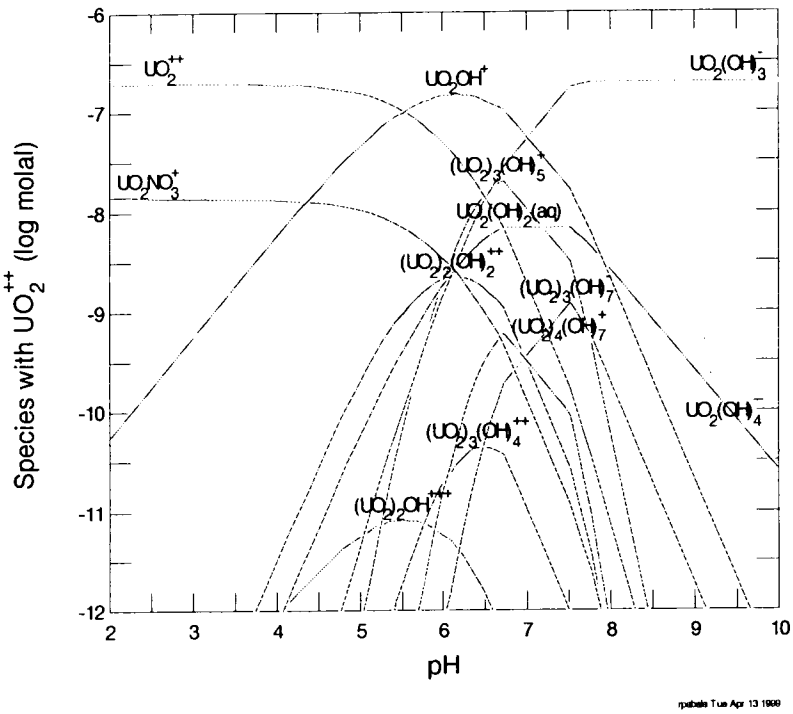
   Temperature is 25 C
   Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
   Working directory: d:\temp\gwb temp
   Options: Debye-Huckel

   Basis is:

H2O	1 kg solvent
O2(g) (swapped for O2(aq))	fugacity = .2
NO3- (swapped for NH3(aq))	total molality = .1 (charge balance)
UO2++	total molality = 2.1e-7
H+	pH = 2
Na+	total molality = .1

   Reactants:
   Slide pH to 10



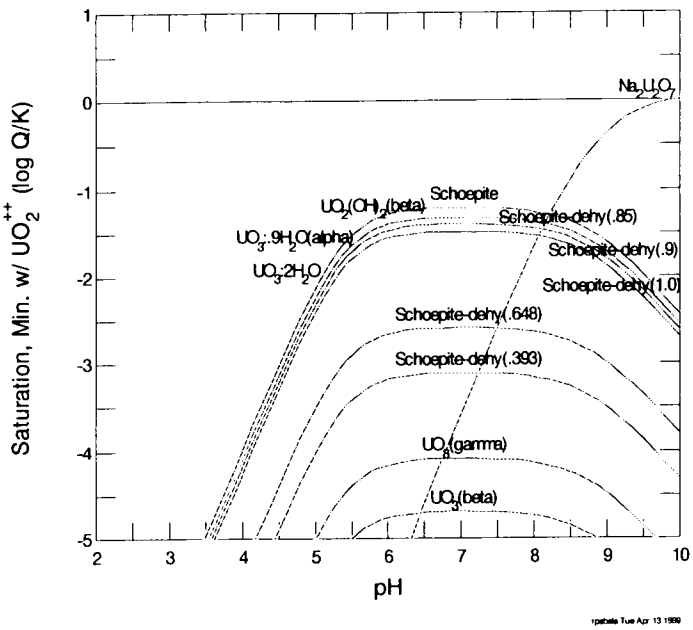


5b. Using LLNL V8.R6 thermo.dat:

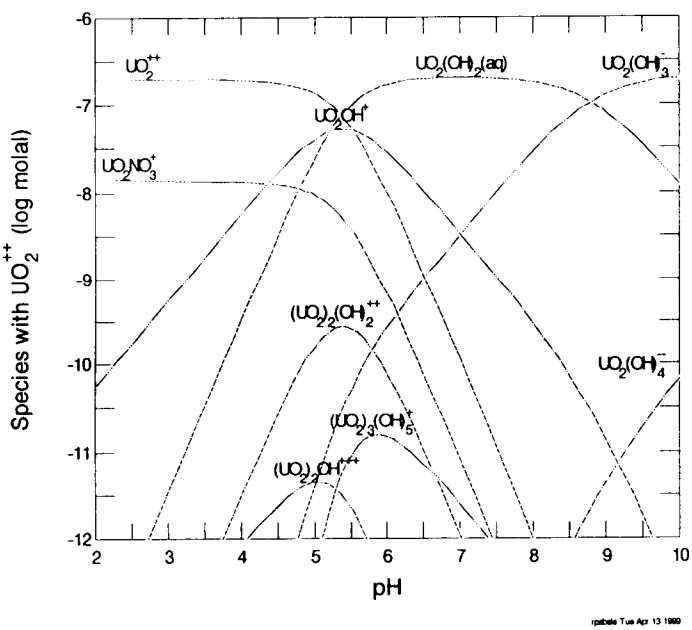
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .1 (charge balance)
UO2++ total molality = 2.1e-7
H+ pH = 2
Na+ total molality = .1

Reactants:
Slide pH to 10



Note that the saturation index is much lower compared to case 5a in which a different log K for the neutral hydroxy species was used.



Note the much bigger stability field for UO2(OH)2(aq) compared to 5a.

6. Calculate uranium speciation and mineral saturation for a solution with 2.1E-7 molal UO2(NO3)2, no CO2. (low concentration of NaNO3 for charge balance constraints)

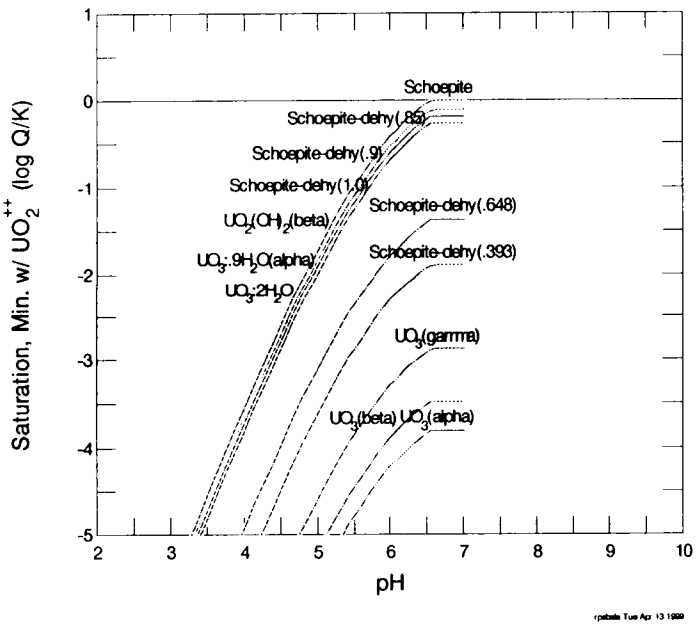
6a. Using D. Turner log K for UO2(OH)2(aq):

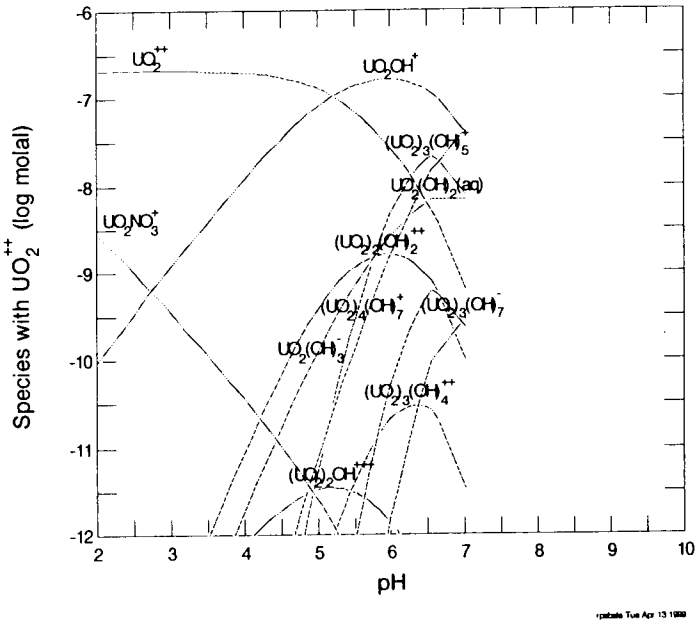
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel

Basis is:

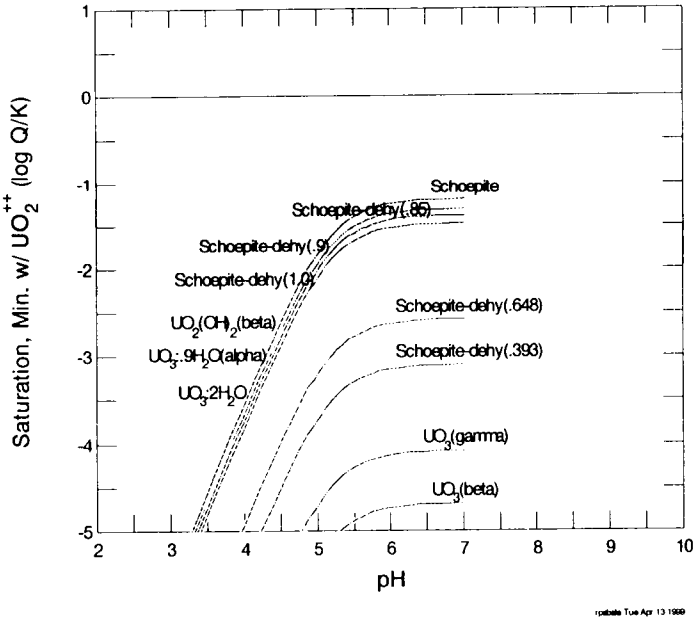
H2O	1 kg solvent
O2(g) (swapped for O2(aq))	fugacity = .2
NO3- (swapped for NH3(aq))	total molality = 4.2e-7 (charge balance)
UO2++	total molality = 2.1e-7
H+	pH = 2
Na+	total molality = 1e-8

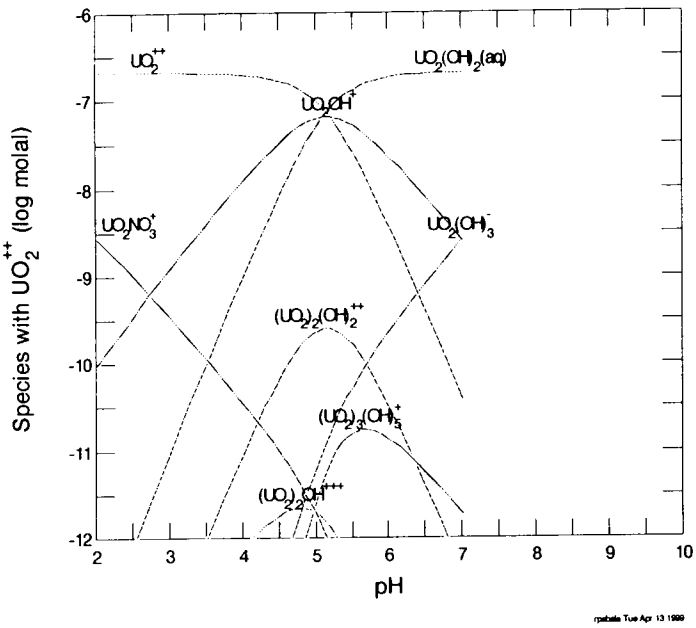
Reactants:
Slide pH to 10





6b. Using V8.R6 thermo.dat:





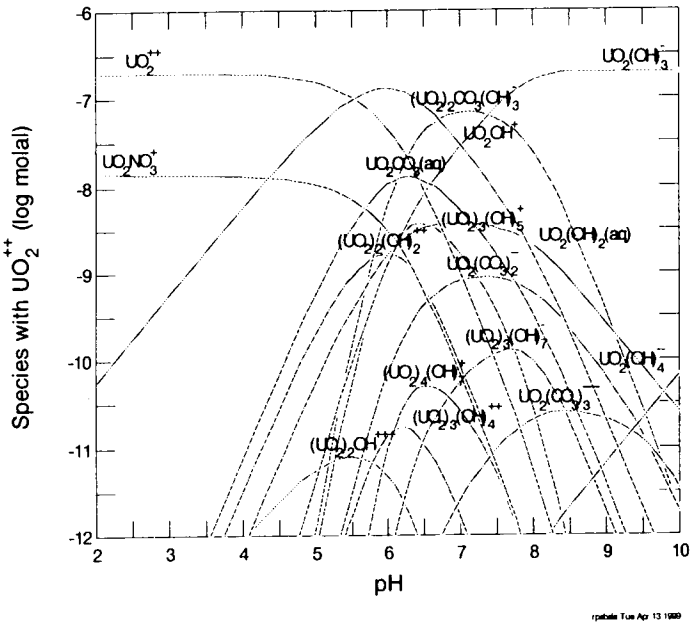
7. Calculate uranium speciation and mineral saturation for a solution with 2.1E-7 molal UO2(NO3)2, log pCO2 = -3.5 atm, 0.1 NaNO3 background electrolyte, charge balance on NO3-

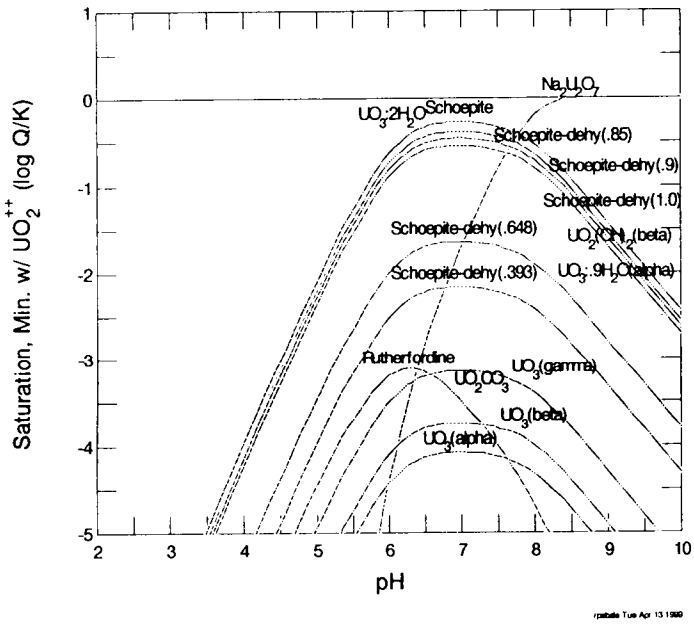
7a. Using D. Turner log K for UO2(OH)2(aq):

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel

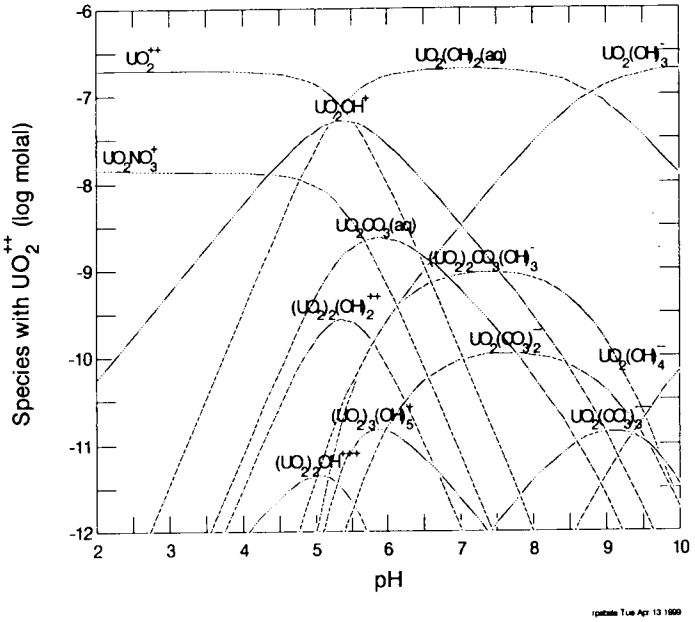
Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .1 (charge balance)
UO2++ total molality = 2.1e-7
H+ pH = 2
Na+ total molality = .1
CO2(g) (swapped for HCO3-) fugacity = .000316227766

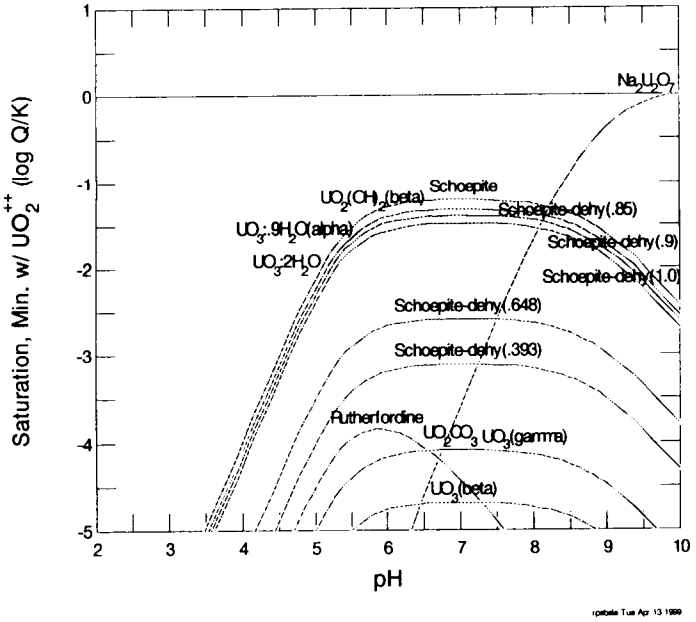
Reactants:
Slide pH to 10


Species with UO_2^{++} (log molal)
pH
UO_2^{++}
$UO_2(OH)_3^-$
$(UO_2)_2CO_3(OH)_3^-$
UO_2OH^+
$UO_2NO_3^+$
$UO_2CO_3(aq)$
$(UO_2)_3(OH)_5^+$
$UO_2(OH)_2(aq)$
$(UO_2)_2(OH)_2^{++}$
$UO_2(CO_3)_2^-$
$(UO_2)_3(OH)_7^-$
$UO_2(OH)_4^-$
$(UO_2)_4(OH)_7^+$
$UO_2(CO_3)_3^-$
$(UO_2)_3(OH)_4^{++}$
$(UO_2)_2OH^{+++}$


Saturation, Min. w/ UO_2^{++} (log Q/K)
pH
$Na_2U_2O_7$
$UO_3 \cdot 2H_2O$ Schoepite
Schoepite-dehy(.85)
Schoepite-dehy(.9)
Schoepite-dehy(1.0)
Schoepite-dehy(.648)
$UO_2(OH)_2$(beta)
Schoepite-dehy(.393)
$UO_3 \cdot .9H_2O$(alpha)
Rutherfordine
UO_2CO_3
UO_3(gamma)
UO_3(beta)
UO_3(alpha)

7a. Using V8.R6 thermo.dat:





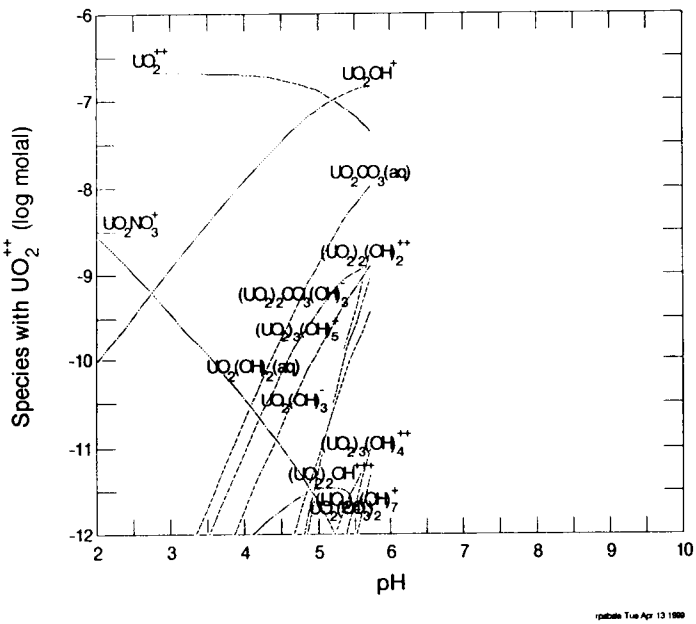
8. Calculate uranium speciation and mineral saturation for a solution with 2.1E-7 molal UO2(NO3)2, log pCO2 = -3.5 atm, low NaNO3 for charge balance constraint

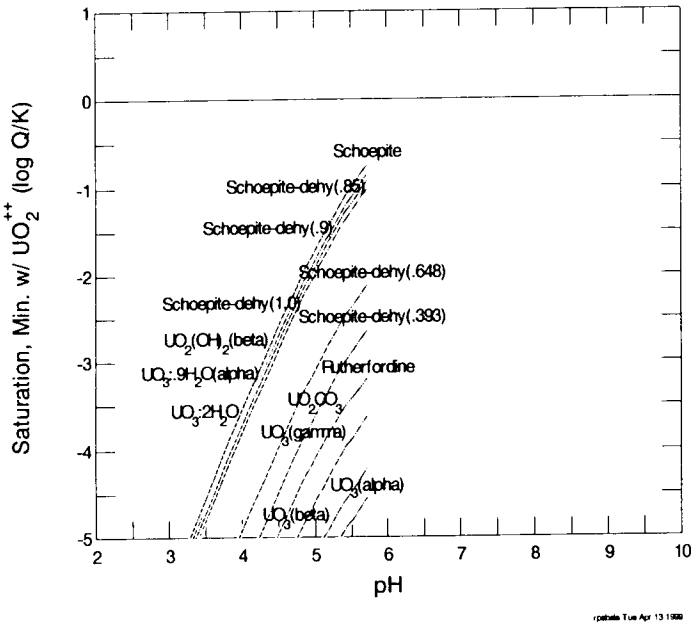
8a. Using D. Turner log K for UO2(OH)2(aq):

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel

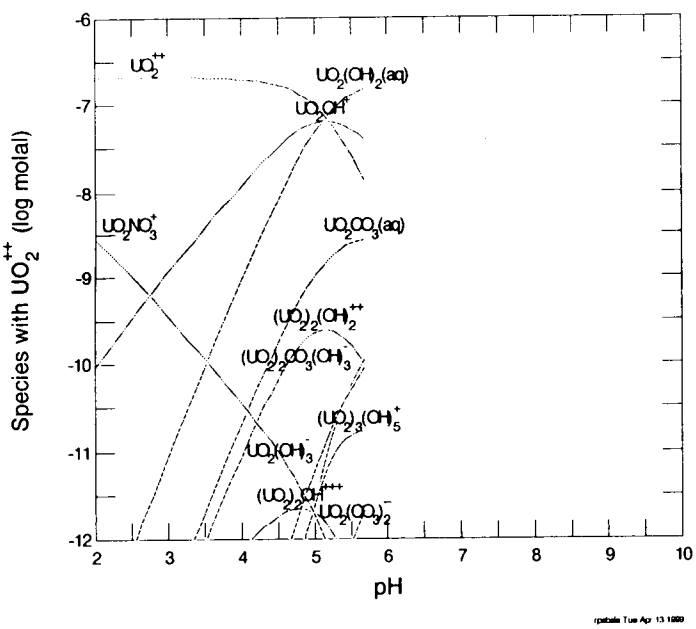
Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 4.2e-7 (charge balance)
UO2++ total molality = 2.1e-7
H+ pH = 2
Na+ total molality = 1e-8
CO2(g) (swapped for HCO3-) fugacity = .000316227766

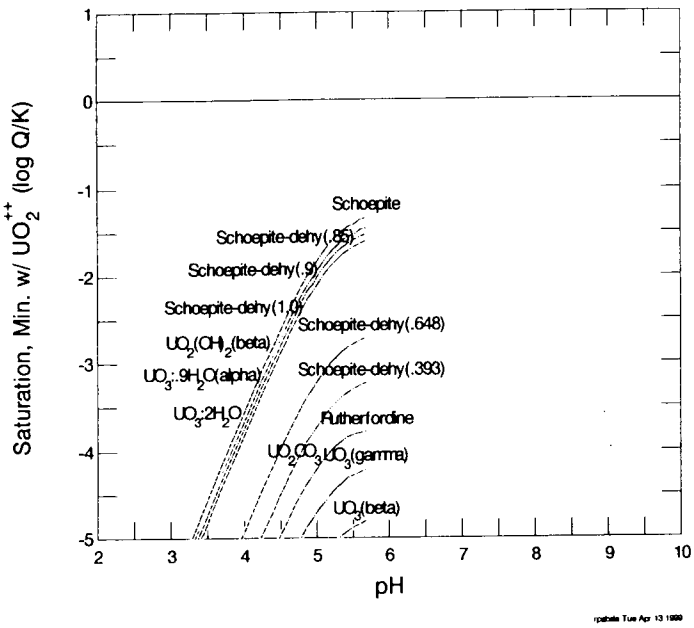
Reactants:
Slide pH to 10





8b. Use V8.R6 thermo.dat:





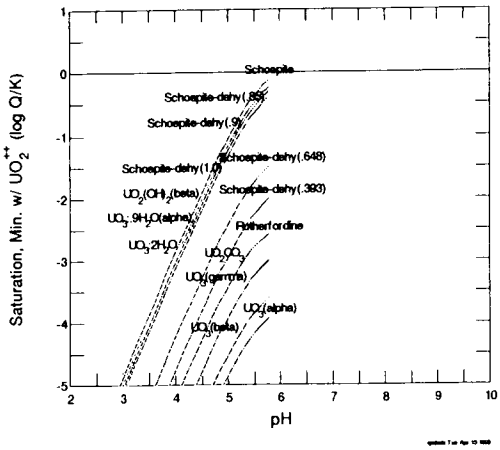
9. Calculate uranium speciation and mineral saturation for a solution with 1.02E-6 molal UO2(NO3)2 (final U concentration in manuscript by Sylwester et al, *in preparation*), log pCO2 = -3.5 atm, low NaNO3 for charge balance constraint

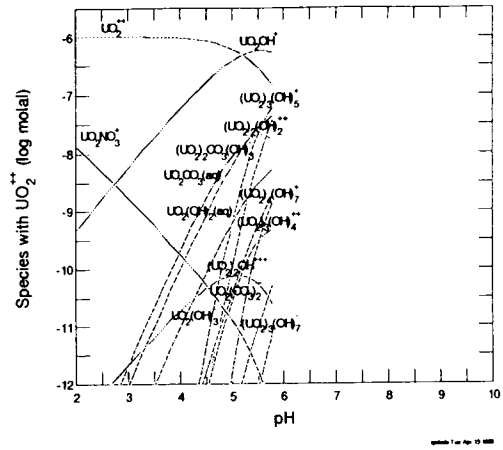
8a. Using D. Turner log K for UO2(OH)2(aq):

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel

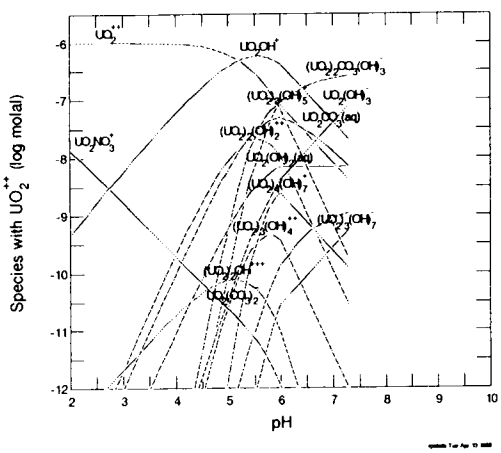
Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 2.04e-6 (charge balance)
UO2++ total molality = 1.02e-6
H+ pH = 2
Na+ total molality = 1e-8
CO2(g) (swapped for HCO3-) fugacity = .000316227766

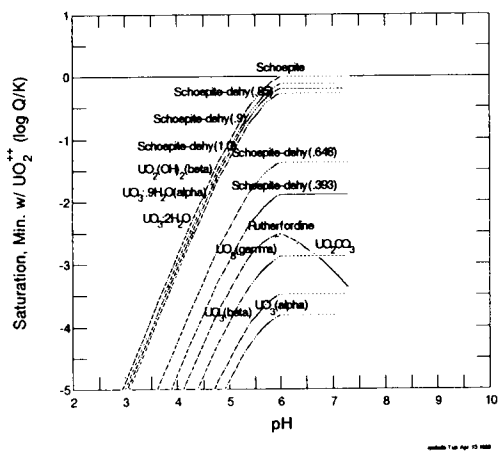
Reactants:
Slide pH to 10



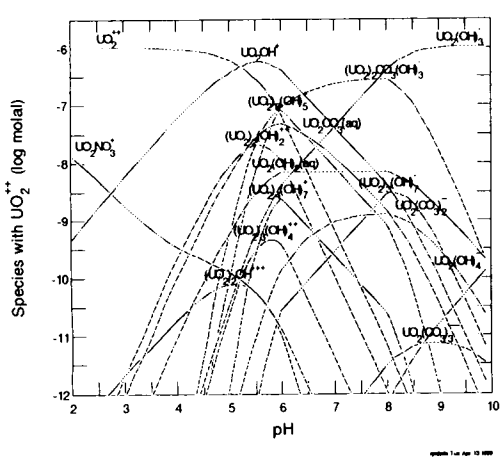


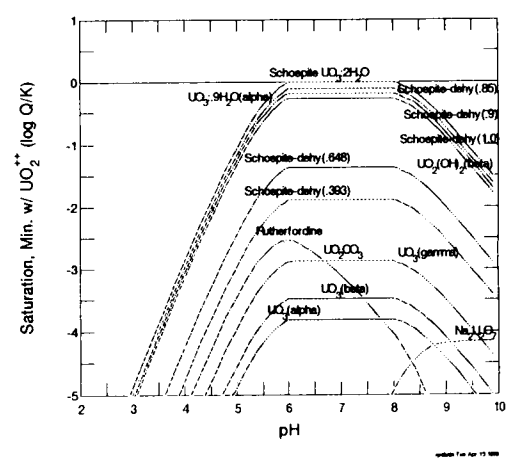
9b. As in 9a, but raise the Na+ and NO3- concentration to 1.e-5 molal:



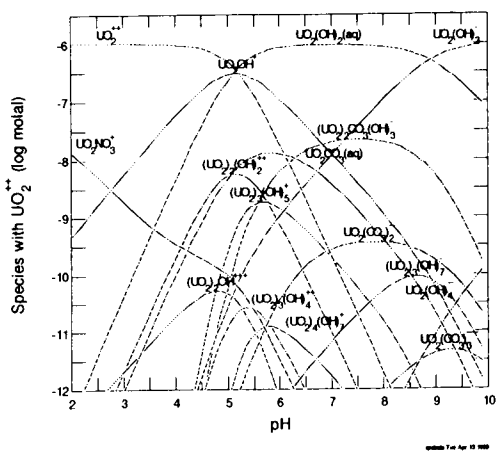


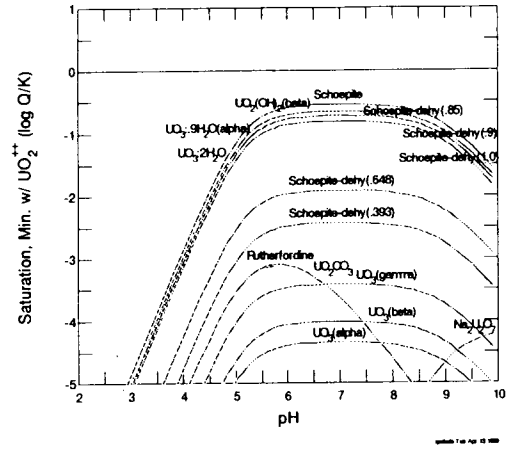
9c. As in 9a and 9b, but NO3- and Na+ = 1.e-4 molal





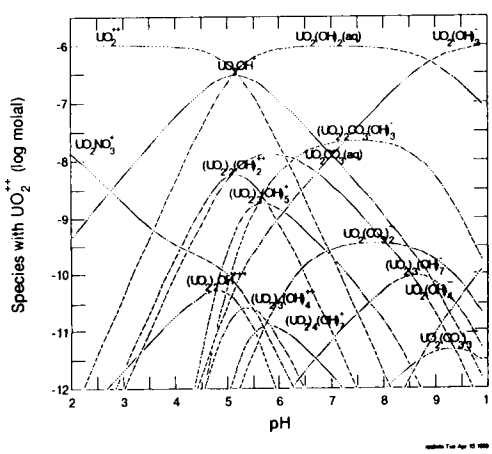
9d. As in 9c, but use V8.R6 thermo.dat:

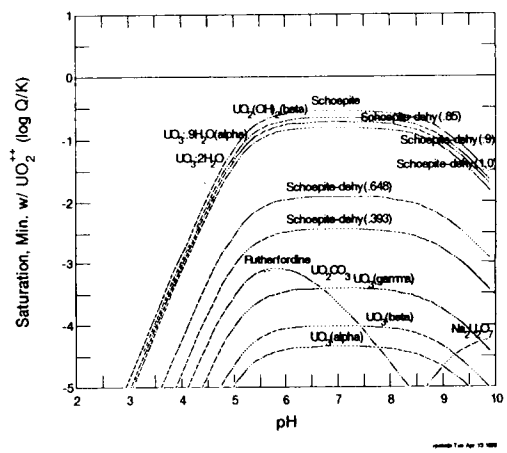




Note that using the V8.R6 thermo.dat, with its higher stability constant for UO2(OH)2(aq), results in undersaturation for the U solids. If a lower stability constant for UO2(OH)2(aq) is used (as in D. Turner's MINTEQ database), saturation with schoepite results.

9e. As in 9e, but raise NO3- concentration to 8.3e-5 molal (the original concentration in Sample A of Sylwester et al.'s paper). Since NO3- is used as charge balance, there shouldn't be any difference in the results for 9d and 9e:





10. The following calculations relate to the solutions used in preparing EXAFS samples discussed in the paper:

The Structure of Uranium (VI) Sorption Complexes on Silica, Alumina, and Montmorillonite

E. R. Sylwester*, E. A. Hudson, P. G. Allen

Glenn T. Seaborg Institute for Transactinium Science, Lawrence Livermore National Laboratory, L-231,

P.O. Box 808, Livermore, CA 94551, USA

The following table gives the experimental conditions:

Table 1. Summary of uranium sorption data

Sample	Sorbent	[NaCl] (molal)	Final pH	Initial $[UO_2^{2+}]$ (molal)	Final $[UO_2^{2+}]$ (molal)	Uranium Uptake (%)	Uranium Loading (moles of U per g of solid)
A	silica	0	6.46	4.15E-5	1.02E-6	97.5	4.05E-05
B	silica	0	3.14	0.979E-2	0.970E-2	0.92	9.00E-05
C	alumina	0	6.50	4.18E-5	4.62E-8	99.9	4.18E-05
D	alumina	0	3.48	0.991E-2	0.958E-2	3.33	3.30E-04
E	montmorillonite	0	3.24	0.987E-2	0.949E-2	3.85	3.80E-04
F	montmorillonite	0	4.11	1.00E-4	1.72E-7	99.8	9.98E-05
G	montmorillonite	0.01	4.11	0.979E-4	0.196E-4	80.0	7.83E-05
H	montmorillonite	0.10	4.06	1.00E-4	0.891E-4	10.9	1.09E-05
I	montmorillonite	0.10	6.41	1.02E-4	0.276E-4	72.9	7.44E-05

10a. Sample A, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

```
Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample A (Silica)

      Input:
      UO2++ = 4.15E-5 molal (initial concentration)
      NO3- = 8.30E-5 molal
      log fCO2 = -3.5 atm
      charge balance on H+

          Step #      0              Xi = 0.0000
          Temperature =  25.0 C      Pressure =  1.013 bars
          pH =  4.704                log fO2 =   -0.699
          Eh =   0.9404 volts        pe =  15.8977
          Ionic strength       =     0.000111
          Activity of water    =     1.000000
          Solvent mass         =     1.000000 kg
          Solution mass        =     1.000031 kg
          Solution density     =     1.013    g/cm3
          Chlorinity           =     0.000000 molal
```

Dissolved solids = 31 mg/kg sol'n

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
O2(aq)	0.0002528	8.088	1.0000	-3.5973
NO3-	8.300e-005	5.146	0.9878	-4.0863
UO2++	2.401e-005	6.484	0.9524	-4.6408
H+	2.001e-005	0.02017	0.9881	-4.7039
CO2(aq)	1.074e-005	0.4728	1.0000	-4.9689
UO2OH+	7.264e-006	2.085	0.9879	-5.1441
(UO2)2(OH)2++	3.258e-006	1.870	0.9524	-5.5083
(UO2)3(OH)5+	1.039e-006	0.9297	0.9879	-5.9888
HCO3-	2.487e-007	0.01517	0.9879	-6.6097
(UO2)3(OH)4++	9.674e-008	0.08495	0.9524	-7.0356
UO2CO3(aq)	6.167e-008	0.02035	1.0000	-7.2099
(UO2)2OH+++	5.792e-008	0.03226	0.8962	-7.2848
(UO2)4(OH)7+	2.624e-008	0.03147	0.9879	-7.5863

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
UO3:2H2O	-0.0662	Schoepite-dehy(1	-0.3360
Schoepite	-0.0662	Schoepite-dehy(.	-1.4392
Ice	-0.1387	Schoepite-dehy(.	-1.9572
UO2(OH)2(beta)	-0.1786	UO2CO3	-2.4198
Schoepite-dehy(.	-0.2496	Rutherfordine	-2.4401
UO3:.9H2O(alpha)	-0.2496	UO3(gamma)	-2.9402
Schoepite-dehy(.	-0.3299		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	7.242e-014	-13.140
NO2(g)	5.518e-017	-16.258
NO(g)	8.271e-023	-22.082
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	3.218e-066	-65.492
UO3(g)	6.593e-067	-66.181
UO2(g)	9.184e-120	-119.037
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	5.080e-204	-203.294
C2H4(g)	7.603e-239	-238.119
U(g)	6.590e-289	-288.181

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-7.194e-005	-7.194e-005	-0.07251		

H2O	55.51	55.51	1.000e+006
HCO3-	1.106e-005	1.106e-005	0.6747
NH3(aq)	8.300e-005	8.300e-005	1.413
O2(aq)	0.0004188	0.0004188	13.40
UO2++	4.150e-005	4.150e-005	11.21

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.106e-005	1.106e-005	0.1328		
Hydrogen	111.0	111.0	1.119e+005		
Nitrogen	8.300e-005	8.300e-005	1.163		
Oxygen	55.51	55.51	8.881e+005		
Uranium	4.150e-005	4.150e-005	9.878		

10b. Sample A, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 8.3e-5 (charge balance)
UO2++ total molality = 1.02e-6
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 9.5

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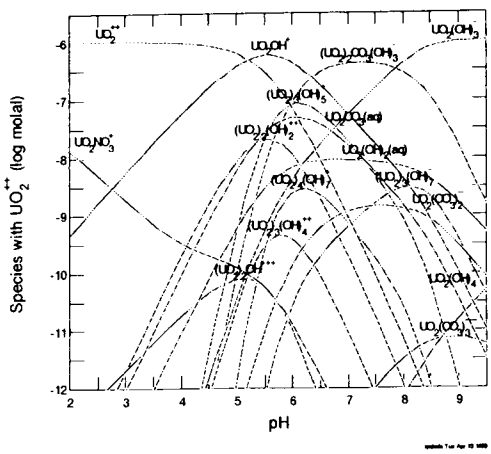
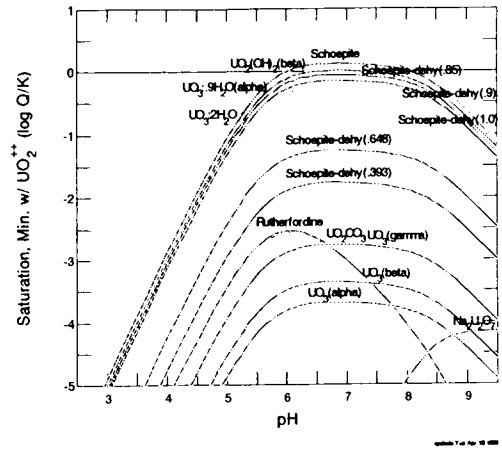




11a. Sample B, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample B (Silica)

```
Input:
UO2++ = 0.979E-2 molal (initial concentration)
NO3- = 1.958E-2 molal
log fCO2 = -3.5 atm
charge balance on H+

Step #      0                Xi = 0.0000
Temperature =   25.0 C       Pressure =   1.013 bars
pH =   3.186                 log fO2 =    -0.699
Eh =    1.0302 volts         pe =   17.4154
Ionic strength        =      0.029021
Activity of water     =      1.000000
Solvent mass          =      1.000000 kg
Solution mass         =      1.003885 kg
Solution density      =      1.013    g/cm3
Chlorinity            =      0.000000 molal
Dissolved solids      =          3870 mg/kg sol'n

No minerals in system.

Aqueous species        molality    mg/kg sol'n    act. coef.     log act.
-----------------------------------------------------------------------------
 NO3-                   0.01941         1199.       0.8445       -1.7853
 UO2++                 0.008626         2320.       0.5283       -2.3413
 H+                   0.0007421        0.7451       0.8775       -3.1863
 (UO2)2OH+++          0.0002557         141.9       0.2447       -4.2036
 O2(aq)               0.0002528         8.057       1.0000       -3.5973
 (UO2)2(OH)2++        0.0002150         122.9       0.5283       -3.9447
 UO2NO3+              0.0001674         55.38       0.8512       -3.8462
 UO2OH+              5.101e-005         14.58       0.8512       -4.3624
 CO2(aq)             1.074e-005        0.4709       1.0000       -4.9689
 (UO2)3(OH)4++       1.173e-006         1.026       0.5283       -6.2079
 HNO3(aq)            5.320e-007       0.03339       1.0000       -6.2741
 (UO2)3(OH)5+        2.461e-007        0.2194       0.8512       -6.6789
 UO2CO3(aq)          1.133e-008      0.003725       1.0000       -7.9458
  (only species > 1e-8 molal listed)

Mineral saturation states
```

	log Q/K		log Q/K
Ice	-0.1387	UO3:.9H2O(alpha)	-0.9855
Schoepite	-0.8021	Schoepite-dehy(.	-1.0658
UO3:2H2O	-0.8021	Schoepite-dehy(1	-1.0719
UO2(OH)2(beta)	-0.9145	Schoepite-dehy(.	-2.1751
Schoepite-dehy(.	-0.9855	Schoepite-dehy(.	-2.6931

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	3.141e-006	-5.503
NO2(g)	3.634e-013	-12.440
NO(g)	5.447e-019	-18.264
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	2.120e-062	-61.674
UO3(g)	1.211e-067	-66.917
UO2(g)	1.687e-120	-119.773
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	9.332e-205	-204.030
C2H4(g)	7.603e-239	-238.119
U(g)	1.211e-289	-288.917

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-0.01957	-0.01957	-19.65		
H2O	55.49	55.49	9.958e+005		
HCO3-	1.076e-005	1.076e-005	0.6542		
NH3(aq)	0.01958	0.01958	332.2		
O2(aq)	0.03941	0.03941	1256.		
UO2++	0.009790	0.009790	2633.		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.076e-005	1.076e-005	0.1288		
Hydrogen	111.0	111.0	1.115e+005		
Nitrogen	0.01958	0.01958	273.2		
Oxygen	55.59	55.59	8.859e+005		
Uranium	0.009790	0.009790	2321.		

11b. Sample B, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

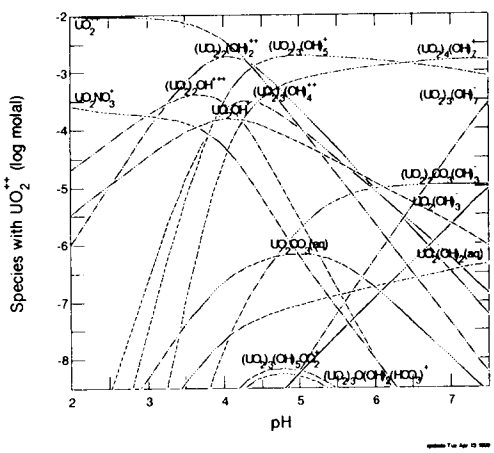
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat

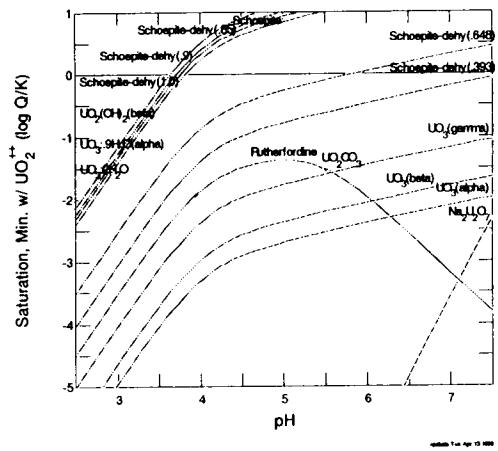
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .01958 (charge balance)
UO2++ total molality = .0097
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 9.5

[Did not converge over the full range of pH. Plotted only up to pH 7.5]





[At the final pH value (3.14), the solution is undersaturated with uranyl minerals.]

12a. Sample C, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample C (Alumina)

Input:
UO2++ = 4.18E-5 molal (initial concentration)
NO3- = 8.36E-5 molal
log fCO2 = -3.5 atm
charge balance on H+

```
Step #     0              Xi = 0.0000
Temperature =  25.0 C     Pressure =  1.013 bars
pH =  4.702               log fO2 =   -0.699
Eh =   0.9406 volts       pe =  15.8997
Ionic strength      =     0.000112
Activity of water   =     1.000000
Solvent mass        =     1.000000 kg
Solution mass       =     1.000031 kg
Solution density    =     1.013    g/cm3
Chlorinity          =     0.000000 molal
Dissolved solids    =           31 mg/kg sol'n
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
O2(aq)	0.0002528	8.088	1.0000	-3.5973
NO3-	8.360e-005	5.183	0.9878	-4.0832
UO2++	2.422e-005	6.540	0.9522	-4.6371
H+	2.011e-005	0.02026	0.9880	-4.7019
CO2(aq)	1.074e-005	0.4728	1.0000	-4.9689
UO2OH+	7.292e-006	2.093	0.9878	-5.1425
(UO2)2(OH)2++	3.284e-006	1.885	0.9522	-5.5049
(UO2)3(OH)5+	1.041e-006	0.9318	0.9878	-5.9879
HCO3-	2.475e-007	0.01510	0.9878	-6.6117
(UO2)3(OH)4++	9.743e-008	0.08555	0.9522	-7.0326
UO2CO3(aq)	6.162e-008	0.02034	1.0000	-7.2102
(UO2)2OH+++	5.866e-008	0.03268	0.8958	-7.2794
(UO2)4(OH)7+	2.628e-008	0.03151	0.9878	-7.5857

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
UO3:2H2O	-0.0665	Schoepite-dehy(1	-0.3363
Schoepite	-0.0665	Schoepite-dehy(.	-1.4395
Ice	-0.1387	Schoepite-dehy(.	-1.9575
UO2(OH)2(beta)	-0.1789	UO2CO3	-2.4201
Schoepite-dehy(.	-0.2499	Rutherfordine	-2.4404
UO3:.9H2O(alpha)	-0.2499	UO3(gamma)	-2.9405
Schoepite-dehy(.	-0.3302		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	7.415e-014	-13.130
NO2(g)	5.584e-017	-16.253
NO(g)	8.369e-023	-22.077
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	3.257e-066	-65.487
UO3(g)	6.588e-067	-66.181
UO2(g)	9.177e-120	-119.037
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	5.076e-204	-203.294
C2H4(g)	7.603e-239	-238.119
U(g)	6.585e-289	-288.181

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-7.254e-005	-7.254e-005	-0.07311		
H2O	55.51	55.51	1.000e+006		
HCO3-	1.106e-005	1.106e-005	0.6746		
NH3(aq)	8.360e-005	8.360e-005	1.424		
O2(aq)	0.0004200	0.0004200	13.44		
UO2++	4.180e-005	4.180e-005	11.29		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.106e-005	1.106e-005	0.1328		
Hydrogen	111.0	111.0	1.119e+005		
Nitrogen	8.360e-005	8.360e-005	1.171		
Oxygen	55.51	55.51	8.881e+005		
Uranium	4.180e-005	4.180e-005	9.949		

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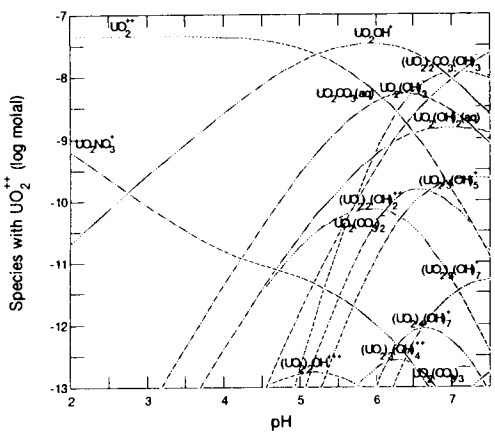
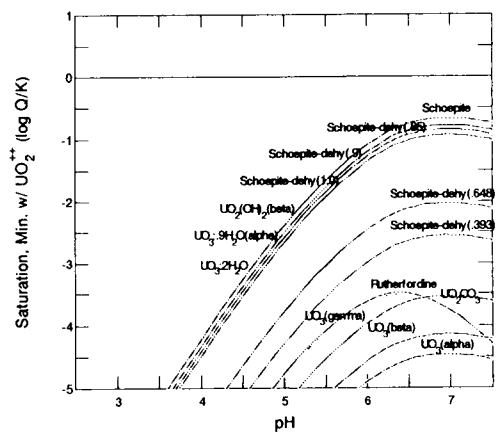
12b. Sample C, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 8.36e-5 (charge balance)
UO2++ total molality = 4.62e-8
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 9.5





13a. Sample D, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

```
Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample D (Alumina)

      Input:
      UO2++ = 0.991E-2 molal (final concentration)
      NO3- = 1.982E-2 molal
      log fCO2 = -3.5 atm
      charge balance on H+


          Step #      0              Xi = 0.0000
          Temperature =  25.0 C      Pressure =  1.013 bars
          pH =  3.183                log fO2 =   -0.699
          Eh =   1.0304 volts        pe =  17.4189
          Ionic strength       =     0.029377
          Activity of water    =     1.000000
          Solvent mass         =     1.000000 kg
```

```
        Solution mass        =    1.003933 kg
        Solution density     =    1.013    g/cm3
        Chlorinity           =    0.000000 molal
        Dissolved solids     =        3917 mg/kg sol'n
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.01965	1214.	0.8438	-1.7804
UO2++	0.008732	2349.	0.5266	-2.3374
H+	0.0007486	0.7515	0.8771	-3.1827
(UO2)2OH+++	0.0002600	144.3	0.2431	-4.1993
O2(aq)	0.0002528	8.057	1.0000	-3.5973
(UO2)2(OH)2++	0.0002160	123.5	0.5266	-3.9439
UO2NO3+	0.0001710	56.55	0.8505	-3.8373
UO2OH+	5.109e-005	14.61	0.8505	-4.3620
CO2(aq)	1.074e-005	0.4709	1.0000	-4.9689
(UO2)3(OH)4++	1.170e-006	1.023	0.5266	-6.2103
HNO3(aq)	5.424e-007	0.03405	1.0000	-6.2657
(UO2)3(OH)5+	2.430e-007	0.2166	0.8505	-6.6848
UO2CO3(aq)	1.125e-008	0.003697	1.0000	-7.9490

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Ice	-0.1387	UO3:.9H2O(alpha)	-0.9887
Schoepite	-0.8053	Schoepite-dehy(.	-1.0690
UO3:2H2O	-0.8053	Schoepite-dehy(1	-1.0751
UO2(OH)2(beta)	-0.9177	Schoepite-dehy(.	-2.1783
Schoepite-dehy(.	-0.9887	Schoepite-dehy(.	-2.6963

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	3.266e-006	-5.486
NO2(g)	3.706e-013	-12.431
NO(g)	5.554e-019	-18.255
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	2.161e-062	-61.665
UO3(g)	1.202e-067	-66.920
UO2(g)	1.675e-120	-119.776
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	9.265e-205	-204.033
C2H4(g)	7.603e-239	-238.119
U(g)	1.202e-289	-288.920

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg

```
H+                -0.01981      -0.01981       -19.89
H2O                  55.49         55.49  9.957e+005
HCO3-            1.076e-005    1.076e-005       0.6541
NH3(aq)             0.01982       0.01982        336.2
O2(aq)              0.03989       0.03989        1272.
UO2++             0.009910      0.009910        2665.

 Elemental composition                In fluid                    Sorbed
                 total moles     moles        mg/kg        moles        mg/kg
 ---------------------------------------------------------------------------
---
Carbon           1.076e-005    1.076e-005       0.1288
Hydrogen             111.0         111.0  1.115e+005
Nitrogen            0.01982       0.01982        276.5
Oxygen               55.59         55.59  8.859e+005
Uranium           0.009910      0.009910        2350.
```

13b. Sample D, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .01982 (charge balance)
UO2++ total molality = .00958
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 7

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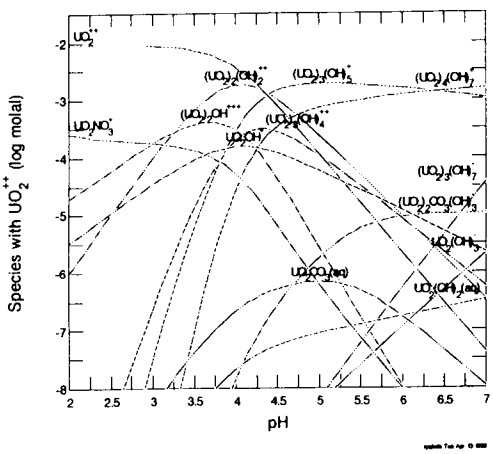

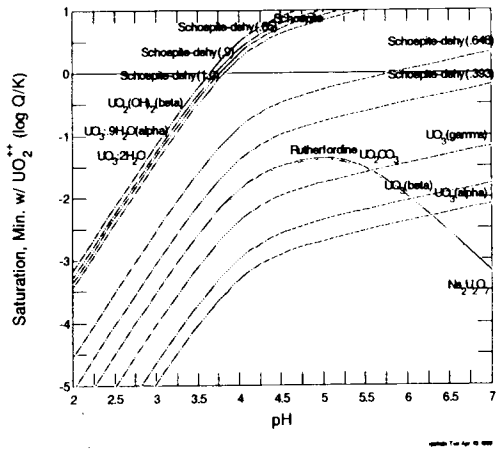

Note that at the final pH value (3.48), the solution undersaturated with schoepite.

14a. Sample E, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

```
Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample E
(Montmorillonite)

      Input:
      UO2++ = 0.987E-2 molal (initial concentration)
      NO3- = 1.974E-2 molal
      log fCO2 = -3.5 atm
      charge balance on H+


          Step #      0              Xi = 0.0000
          Temperature =  25.0 C      Pressure =  1.013 bars
          pH =  3.184                log fO2 =   -0.699
          Eh =   1.0304 volts        pe =  17.4178
          Ionic strength       =     0.029259
          Activity of water    =     1.000000
          Solvent mass         =     1.000000 kg
          Solution mass        =     1.003917 kg
          Solution density     =     1.013    g/cm3
          Chlorinity           =     0.000000 molal
          Dissolved solids     =         3901 mg/kg sol'n

  No minerals in system.

  Aqueous species        molality    mg/kg sol'n    act. coef.     log act.
 ---------------------------------------------------------------------------
   NO3-                   0.01957        1209.       0.8440        -1.7821
   UO2++                 0.008696        2339.       0.5272        -2.3387
   H+                   0.0007464       0.7494       0.8772        -3.1839
   (UO2)2OH+++          0.0002586        143.5       0.2436        -4.2007
   O2(aq)               0.0002528        8.057       1.0000        -3.5973
   (UO2)2(OH)2++        0.0002157        123.3       0.5272        -3.9442
   UO2NO3+              0.0001698        56.16       0.8507        -3.8403
```

UO2OH+	5.106e-005	14.60	0.8507	-4.3621
CO2(aq)	1.074e-005	0.4709	1.0000	-4.9689
(UO2)3(OH)4++	1.171e-006	1.024	0.5272	-6.2095
HNO3(aq)	5.389e-007	0.03383	1.0000	-6.2685
(UO2)3(OH)5+	2.440e-007	0.2176	0.8507	-6.6828
UO2CO3(aq)	1.127e-008	0.003706	1.0000	-7.9479

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Ice	-0.1387	UO3:.9H2O(alpha)	-0.9876
Schoepite	-0.8042	Schoepite-dehy(.	-1.0679
UO3:2H2O	-0.8042	Schoepite-dehy(1	-1.0740
UO2(OH)2(beta)	-0.9166	Schoepite-dehy(.	-2.1772
Schoepite-dehy(.	-0.9876	Schoepite-dehy(.	-2.6952

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	3.224e-006	-5.492
NO2(g)	3.682e-013	-12.434
NO(g)	5.518e-019	-18.258
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	2.147e-062	-61.668
UO3(g)	1.205e-067	-66.919
UO2(g)	1.679e-120	-119.775
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	9.287e-205	-204.032
C2H4(g)	7.603e-239	-238.119
U(g)	1.205e-289	-288.919

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-0.01973	-0.01973	-19.81		
H2O	55.49	55.49	9.958e+005		
HCO3-	1.076e-005	1.076e-005	0.6541		
NH3(aq)	0.01974	0.01974	334.9		
O2(aq)	0.03973	0.03973	1266.		
UO2++	0.009870	0.009870	2655.		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.076e-005	1.076e-005	0.1288		
Hydrogen	111.0	111.0	1.115e+005		
Nitrogen	0.01974	0.01974	275.4		
Oxygen	55.59	55.59	8.859e+005		
Uranium	0.009870	0.009870	2340.		

14b. Sample E, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .01974 (charge balance)
UO2++ total molality = .00949
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 7

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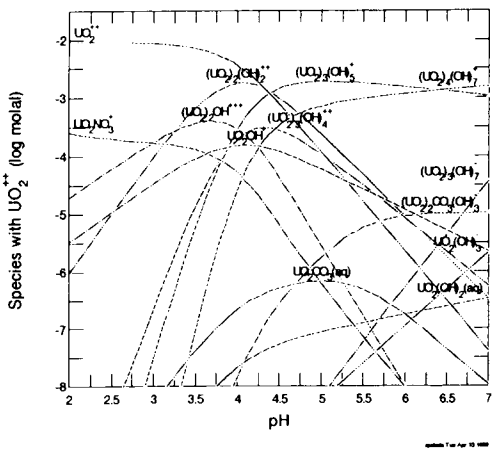
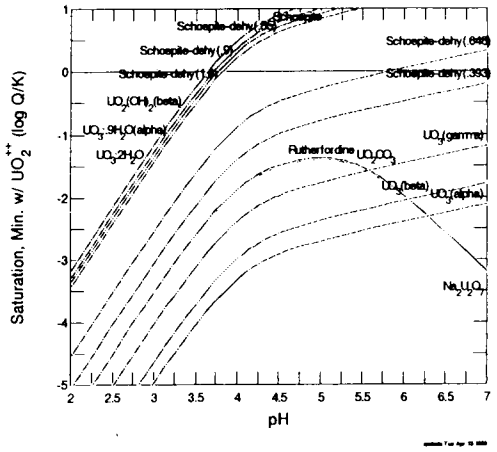




Note that at the final pH value (3.24), the solution is undersaturated with uranyl minerals.

15a. Sample F, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

```
Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample F
(Montmorillonite)

      Input:
      UO2++ = 1.0E-4 molal (initial concentration)
      NO3- = 2.0E-4 molal
      log fCO2 = -3.5 atm
      charge balance on H+


          Step #      0              Xi = 0.0000
          Temperature =  25.0 C      Pressure =  1.013 bars
          pH =  4.459                log fO2 =   -0.699
          Eh =   0.9549 volts        pe =  16.1426
          Ionic strength       =     0.000277
          Activity of water    =     1.000000
          Solvent mass         =     1.000000 kg
          Solution mass        =     1.000054 kg
          Solution density     =     1.013    g/cm3
          Chlorinity           =     0.000000 molal
          Dissolved solids     =           54 mg/kg sol'n

  No minerals in system.

  Aqueous species        molality    mg/kg sol'n    act. coef.     log act.
 ---------------------------------------------------------------------------
   O2(aq)                0.0002528         8.088       1.0000       -3.5973
   NO3-                  0.0002000         12.40       0.9809       -3.7074
   UO2++                6.735e-005         18.18       0.9264       -4.2049
   H+                   3.541e-005       0.03568       0.9815       -4.4590
   UO2OH+               1.135e-005         3.259       0.9810       -4.9532
   CO2(aq)              1.074e-005        0.4727       1.0000       -4.9689
   (UO2)2(OH)2++        8.070e-006         4.633       0.9264       -5.1263
```

(UO2)3(OH)5+	1.266e-006	1.134	0.9810	-5.9057
(UO2)2OH+++	2.610e-007	0.1454	0.8424	-6.6579
(UO2)3(OH)4++	2.117e-007	0.1859	0.9264	-6.7075
HCO3-	1.425e-007	0.008693	0.9810	-6.8546
UO2CO3(aq)	5.447e-008	0.01798	1.0000	-7.2638
(UO2)4(OH)7+	2.826e-008	0.03389	0.9810	-7.5572
UO2NO3+	2.380e-008	0.007902	0.9810	-7.6317

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
UO3:2H2O	-0.1201	Schoepite-dehy(1	-0.3899
Schoepite	-0.1201	Schoepite-dehy(.	-1.4931
Ice	-0.1387	Schoepite-dehy(.	-2.0111
UO2(OH)2(beta)	-0.2325	UO2CO3	-2.4737
Schoepite-dehy(.	-0.3035	Rutherfordine	-2.4940
UO3:.9H2O(alpha)	-0.3035	UO3(gamma)	-2.9941
Schoepite-dehy(.	-0.3838		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	1.281e-012	-11.893
NO2(g)	2.321e-016	-15.634
NO(g)	3.478e-022	-21.459
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	1.353e-065	-64.869
UO3(g)	5.823e-067	-66.235
UO2(g)	8.112e-120	-119.091
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	4.487e-204	-203.348
C2H4(g)	7.603e-239	-238.119
U(g)	5.821e-289	-288.235

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-0.0001891	-0.0001891	-0.1905		
H2O	55.51	55.51	9.999e+005		
HCO3-	1.094e-005	1.094e-005	0.6676		
NH3(aq)	0.0002000	0.0002000	3.406		
O2(aq)	0.0006528	0.0006528	20.89		
UO2++	0.0001000	0.0001000	27.00		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.094e-005	1.094e-005	0.1314		
Hydrogen	111.0	111.0	1.119e+005		

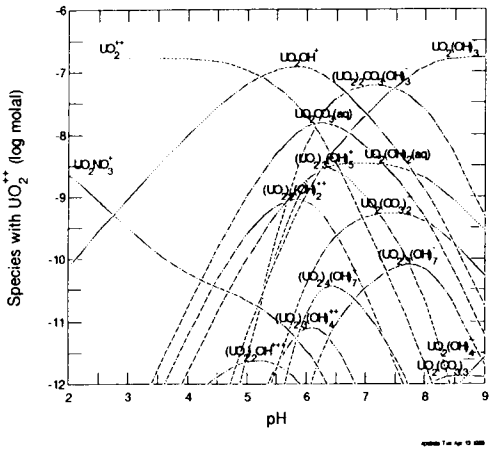
Nitrogen	0.0002000	0.0002000	2.801
Oxygen	55.51	55.51	8.881e+005
Uranium	0.0001000	0.0001000	23.80

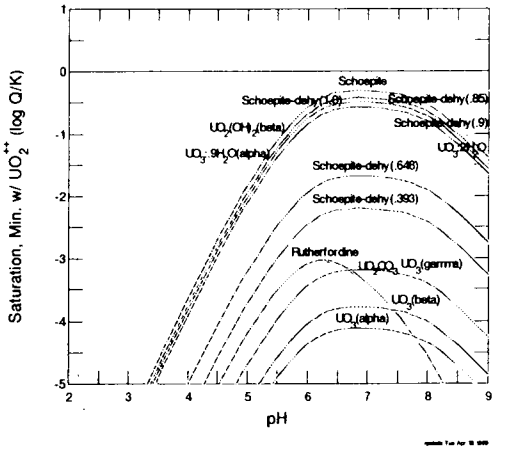
15b. Sample F, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 2e-4 (charge balance)
UO2++ total molality = 1.72e-7
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 9





Note that the solution is undersaturated with uranyl minerals throughout the pH range.

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April 14, 1999

The following documents additional GWB calculations of uranium speciation and mineral saturation for experimental conditions related to preparation of EXAFS samples (see Table 1 on page 149).

16a. Sample G, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

```
Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample G
(Montmorillonite)

      Input:
      UO2++ = 0.979E-4 molal (initial concentration)
      NO3- = 1.958E-4 molal
      log fCO2 = -3.5 atm
      charge balance on H+

          Step #     0              Xi = 0.0000
          Temperature =  25.0 C     Pressure =  1.013 bars
          pH =  4.465               log fO2 =   -0.699
          Eh =   0.9546 volts       pe =  16.1368
          Ionic strength      =     0.000271
          Activity of water   =     1.000000
          Solvent mass        =     1.000000 kg
          Solution mass       =     1.000053 kg
          Solution density    =     1.013    g/cm3
          Chlorinity          =     0.000000 molal
          Dissolved solids    =           53 mg/kg sol'n

 No minerals in system.

 Aqueous species        molality    mg/kg sol'n    act. coef.      log act.
-------------------------------------------------------------------------------
  O2(aq)                0.0002528         8.088      1.0000        -3.5973
  NO3-                  0.0001958         12.14      0.9811        -3.7165
  UO2++                6.573e-005         17.75      0.9272        -4.2151
  H+                   3.492e-005       0.03520      0.9817        -4.4649
  UO2OH+               1.124e-005         3.226      0.9812        -4.9575
  CO2(aq)              1.074e-005        0.4727      1.0000        -4.9689
  (UO2)2(OH)2++        7.905e-006         4.538      0.9272        -5.1349
  (UO2)3(OH)5+         1.263e-006         1.130      0.9812        -5.9069
  (UO2)2OH+++          2.519e-007        0.1403      0.8439        -6.6724
  (UO2)3(OH)4++        2.081e-007        0.1827      0.9272        -6.7146
  HCO3-                1.444e-007      0.008809      0.9812        -6.8487
  UO2CO3(aq)           5.467e-008       0.01804      1.0000        -7.2623
  (UO2)4(OH)7+         2.828e-008       0.03391      0.9812        -7.5567
  UO2NO3+              2.276e-008      0.007556      0.9812        -7.6511
   (only species > 1e-8 molal listed)

 Mineral saturation states
                     log Q/K                            log Q/K
-----------------------------------------------------------------
  UO3:2H2O           -0.1186        Schoepite-dehy(1   -0.3884
  Schoepite          -0.1186        Schoepite-dehy(.   -1.4916
  Ice                -0.1387        Schoepite-dehy(.   -2.0096
  UO2(OH)2(beta)     -0.2310        UO2CO3             -2.4722
  Schoepite-dehy(.   -0.3020        Rutherfordine      -2.4925
```

```
  UO3:.9H2O(alpha)  -0.3020        UO3(gamma)        -2.9926
  Schoepite-dehy(.  -0.3823
   (only minerals with log Q/K > -3 listed)

 Gases                 fugacity      log fug.
-----------------------------------------------
  O2(g)                    0.2000      -0.699
  H2O(g)                  0.02598      -1.585
  CO2(g)                0.0003162      -3.500
  N2(g)                1.195e-012     -11.923
  NO2(g)               2.242e-016     -15.649
  NO(g)                3.360e-022     -21.474
  H2(g)                6.267e-042     -41.203
  CO(g)                6.189e-049     -48.208
  NH3(g)               1.307e-065     -64.884
  UO3(g)               5.844e-067     -66.233
  UO2(g)               8.141e-120    -119.089
  CH4(g)               3.890e-146    -145.410
  C(g)                 3.246e-190    -189.489
  UO(g)                4.503e-204    -203.346
  C2H4(g)              7.603e-239    -238.119
  U(g)                 5.842e-289    -288.233

                                   In fluid                  Sorbed
 Original basis  total moles     moles       mg/kg        moles       mg/kg
-----------------------------------------------------------------------------
---
  H+              -0.0001849   -0.0001849     -0.1863
  H2O                  55.51        55.51  9.999e+005
  HCO3-           1.094e-005   1.094e-005      0.6677
  NH3(aq)          0.0001958    0.0001958       3.334
  O2(aq)           0.0006444    0.0006444       20.62
  UO2++           9.790e-005   9.790e-005       26.43

 Elemental composition             In fluid                  Sorbed
                total moles     moles       mg/kg        moles       mg/kg
-----------------------------------------------------------------------------
---
  Carbon          1.094e-005   1.094e-005      0.1314
  Hydrogen             111.0        111.0  1.119e+005
  Nitrogen         0.0001958    0.0001958       2.742
  Oxygen               55.51        55.51  8.881e+005
  Uranium         9.790e-005   9.790e-005       23.30
```

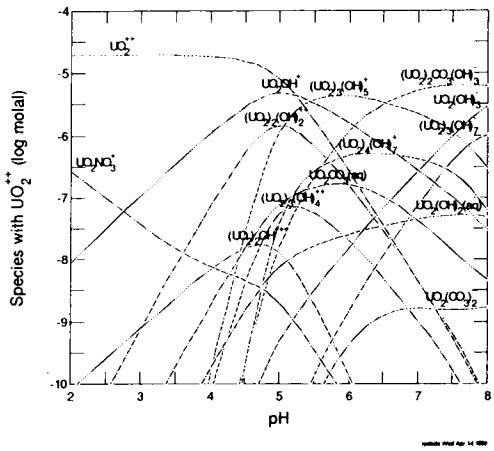
16b. Sample G, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

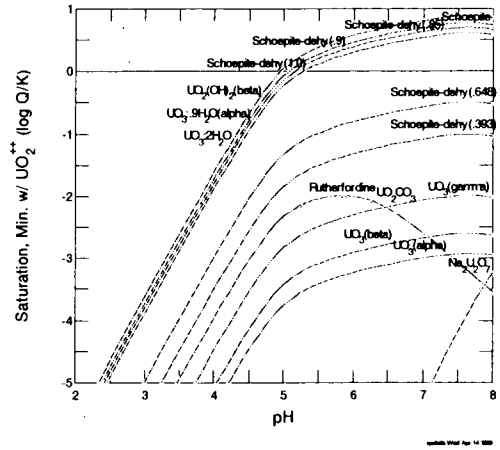
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:

H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .0001958 (charge balance)
UO2++ total molality = 1.96e-5
H+ pH = 2
Na+ total molality = 1e-4
CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 8





Note that at the final pH value (4.11), the solution is undersaturated with uranyl minerals.

17a. Sample H, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample H (Montmorillonite)

Input:
UO2++ = 1.0E-4 molal (initial concentration)
NO3- = 2.0E-4 molal
log fCO2 = -3.5 atm
charge balance on H+

```
Step #      0                Xi = 0.0000
Temperature =  25.0 C        Pressure =  1.013 bars
pH =  4.459                  log fO2 =   -0.699
Eh =   0.9549 volts          pe =  16.1426
Ionic strength        =      0.000277
Activity of water     =      1.000000
Solvent mass          =      1.000000 kg
Solution mass         =      1.000054 kg
Solution density      =      1.013    g/cm3
Chlorinity            =      0.000000 molal
Dissolved solids      =            54 mg/kg sol'n
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
O2(aq)	0.0002528	8.088	1.0000	-3.5973
NO3-	0.0002000	12.40	0.9809	-3.7074
UO2++	6.735e-005	18.18	0.9264	-4.2049
H+	3.541e-005	0.03568	0.9815	-4.4590
UO2OH+	1.135e-005	3.259	0.9810	-4.9532
CO2(aq)	1.074e-005	0.4727	1.0000	-4.9689
(UO2)2(OH)2++	8.070e-006	4.633	0.9264	-5.1263
(UO2)3(OH)5+	1.266e-006	1.134	0.9810	-5.9057
(UO2)2OH+++	2.610e-007	0.1454	0.8424	-6.6579
(UO2)3(OH)4++	2.117e-007	0.1859	0.9264	-6.7075
HCO3-	1.425e-007	0.008693	0.9810	-6.8546
UO2CO3(aq)	5.447e-008	0.01798	1.0000	-7.2638
(UO2)4(OH)7+	2.826e-008	0.03389	0.9810	-7.5572
UO2NO3+	2.380e-008	0.007902	0.9810	-7.6317

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
UO3:2H2O	-0.1201	Schoepite-dehy(1	-0.3899
Schoepite	-0.1201	Schoepite-dehy(.	-1.4931
Ice	-0.1387	Schoepite-dehy(.	-2.0111
UO2(OH)2(beta)	-0.2325	UO2CO3	-2.4737
Schoepite-dehy(.	-0.3035	Rutherfordine	-2.4940
UO3:.9H2O(alpha)	-0.3035	UO3(gamma)	-2.9941
Schoepite-dehy(.	-0.3838		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

```
-----------------------------------------------
  O2(g)                    0.2000      -0.699
  H2O(g)                  0.02598      -1.585
  CO2(g)                0.0003162      -3.500
  N2(g)                1.281e-012     -11.893
  NO2(g)               2.321e-016     -15.634
  NO(g)                3.478e-022     -21.459
  H2(g)                6.267e-042     -41.203
  CO(g)                6.189e-049     -48.208
  NH3(g)               1.353e-065     -64.869
  UO3(g)               5.823e-067     -66.235
  UO2(g)               8.112e-120    -119.091
  CH4(g)               3.890e-146    -145.410
  C(g)                 3.246e-190    -189.489
  UO(g)                4.487e-204    -203.348
  C2H4(g)              7.603e-239    -238.119
  U(g)                 5.821e-289    -288.235

                                    In fluid                  Sorbed
 Original basis  total moles     moles       mg/kg        moles       mg/kg
 ---------------------------------------------------------------------------
---
  H+              -0.0001891   -0.0001891     -0.1905
  H2O                  55.51        55.51  9.999e+005
  HCO3-            1.094e-005   1.094e-005      0.6676
  NH3(aq)           0.0002000    0.0002000       3.406
  O2(aq)            0.0006528    0.0006528       20.89
  UO2++             0.0001000    0.0001000       27.00

 Elemental composition              In fluid                  Sorbed
                 total moles     moles       mg/kg        moles       mg/kg
 ---------------------------------------------------------------------------
---
  Carbon           1.094e-005   1.094e-005      0.1314
  Hydrogen              111.0        111.0  1.119e+005
  Nitrogen          0.0002000    0.0002000       2.801
  Oxygen               55.51        55.51  8.881e+005
  Uranium           0.0001000    0.0001000       23.80
```

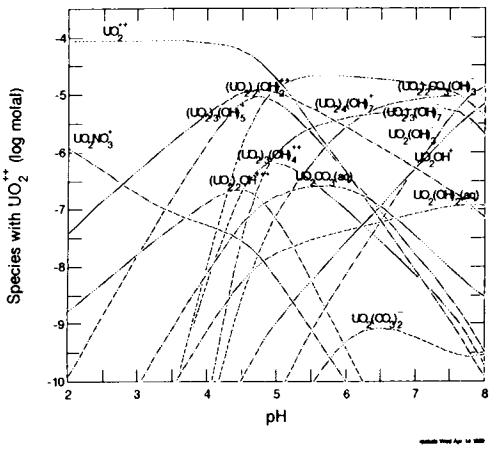
17b. Sample H, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

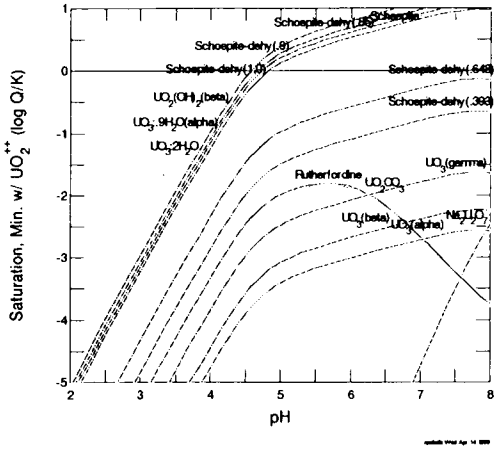
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = 2e-4 (charge balance)
UO2++ total molality = 8.91e-5
H+ pH = 2
Na+ total molality = 1e-4

CO2(g) (swapped for HCO3-) fugacity = .000316227766

Reactants:
Slide pH to 8
Note that at the final pH value (4.06), the solution is undersaturated with uranyl minerals.





18a. Sample I, based on initial U concentration [using D.Turner value for UO2(OH)2(aq)]

Geochemist's Workbench® 3.0 Equilibrium Calculation for Sample I (Montmorillonite)

Input:
UO2++ = 1.02E-4 molal (initial concentration)
NO3- = 2.04E-4 molal
log fCO2 = -3.5 atm
charge balance on H+

```
Step #      0              Xi = 0.0000
Temperature =  25.0 C      Pressure =  1.013 bars
pH =  4.454                log fO2 =   -0.699
Eh =   0.9552 volts        pe =  16.1481
Ionic strength       =     0.000282
Activity of water    =     1.000000
Solvent mass         =     1.000000 kg
Solution mass        =     1.000055 kg
Solution density     =     1.013    g/cm3
Chlorinity           =     0.000000 molal
Dissolved solids     =          55 mg/kg sol'n
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
O2(aq)	0.0002528	8.088	1.0000	-3.5973
NO3-	0.0002040	12.65	0.9808	-3.6989
UO2++	6.889e-005	18.60	0.9257	-4.1954
H+	3.586e-005	0.03614	0.9814	-4.4535
UO2OH+	1.146e-005	3.290	0.9809	-4.9491
CO2(aq)	1.074e-005	0.4727	1.0000	-4.9689
(UO2)2(OH)2++	8.227e-006	4.723	0.9257	-5.1183
(UO2)3(OH)5+	1.270e-006	1.137	0.9809	-5.9047
(UO2)2OH+++	2.697e-007	0.1502	0.8409	-6.6444
(UO2)3(OH)4++	2.150e-007	0.1888	0.9257	-6.7010
HCO3-	1.407e-007	0.008585	0.9809	-6.8601
UO2CO3(aq)	5.429e-008	0.01792	1.0000	-7.2653
(UO2)4(OH)7+	2.824e-008	0.03386	0.9809	-7.5576
UO2NO3+	2.481e-008	0.008238	0.9809	-7.6137

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
UO3:2H2O	-0.1216	Schoepite-dehy(1	-0.3914
Schoepite	-0.1216	Schoepite-dehy(.	-1.4946
Ice	-0.1387	Schoepite-dehy(.	-2.0126
UO2(OH)2(beta)	-0.2340	UO2CO3	-2.4752
Schoepite-dehy(.	-0.3050	Rutherfordine	-2.4955
UO3:.9H2O(alpha)	-0.3050	UO3(gamma)	-2.9956
Schoepite-dehy(.	-0.3853		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

O2(g)	0.2000	-0.699
H2O(g)	0.02598	-1.585
CO2(g)	0.0003162	-3.500
N2(g)	1.366e-012	-11.865
NO2(g)	2.397e-016	-15.620
NO(g)	3.592e-022	-21.445
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
NH3(g)	1.398e-065	-64.855
UO3(g)	5.803e-067	-66.236
UO2(g)	8.084e-120	-119.092
CH4(g)	3.890e-146	-145.410
C(g)	3.246e-190	-189.489
UO(g)	4.472e-204	-203.350
C2H4(g)	7.603e-239	-238.119
U(g)	5.801e-289	-288.237

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
H+	-0.0001931	-0.0001931	-0.1946		
H2O	55.51	55.51	9.999e+005		
HCO3-	1.094e-005	1.094e-005	0.6675		
NH3(aq)	0.0002040	0.0002040	3.474		
O2(aq)	0.0006608	0.0006608	21.14		
UO2++	0.0001020	0.0001020	27.54		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Carbon	1.094e-005	1.094e-005	0.1314		
Hydrogen	111.0	111.0	1.119e+005		
Nitrogen	0.0002040	0.0002040	2.857		
Oxygen	55.51	55.51	8.881e+005		
Uranium	0.0001020	0.0001020	24.28		

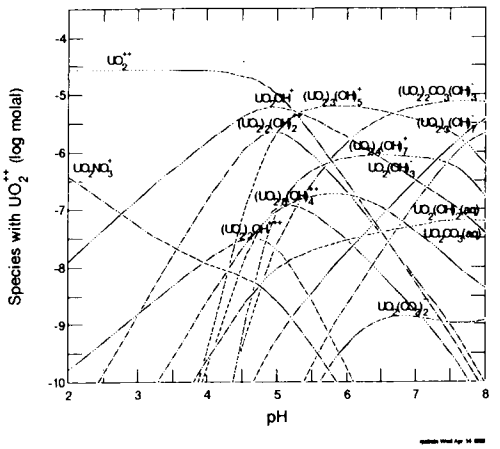
18b. Sample I, based on final U concentration, but using initial NO3- concentration (assumed not to sorb), precipitation suppressed:

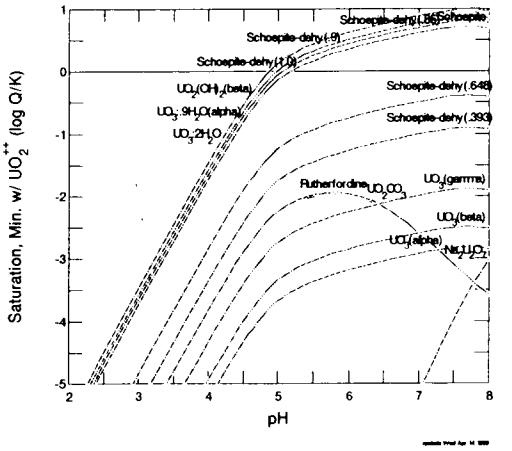
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\temp\gwb temp
Options: Debye-Huckel, no-precip

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
NO3- (swapped for NH3(aq)) total molality = .000204 (charge balance)
UO2++ total molality = 2.76e-5
H+ pH = 2
Na+ total molality = 1e-4

CO2(g) (swapped for HCO3-) fugacity = .000316227766

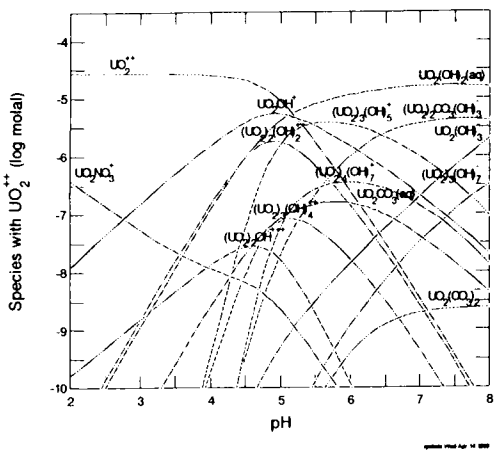
Reactants:
Slide pH to 8

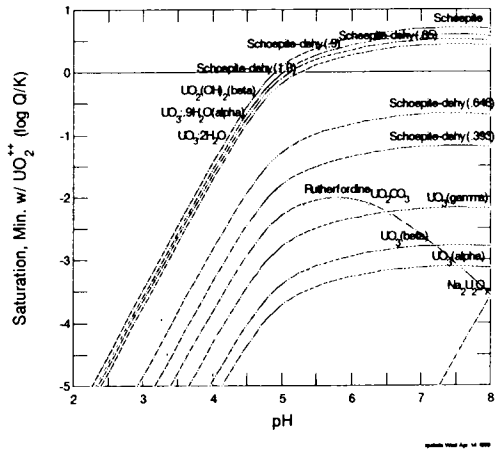




Note that at the final pH value (6.41), the solution is supersaturated with schoepite minerals.

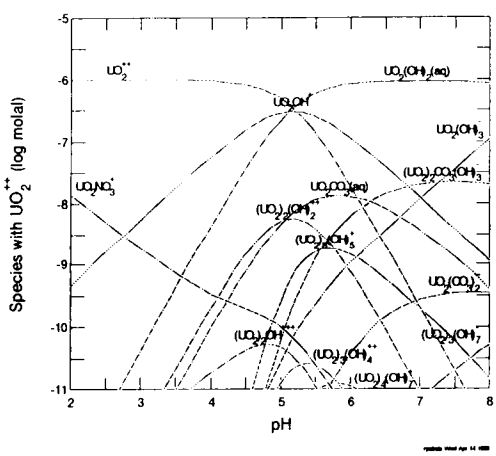
18b-2. Same as 18b, but using V8.R6 thermo.dat:

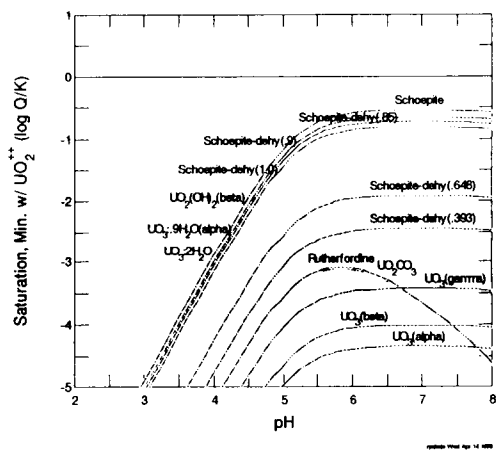




Note that, as in 18b, the solution is supersaturated with schoepite at the final pH (6.41) value.

19. Same as 10a, but using V8.R6 thermo.dat:





Note that by using a higher stability constant for UO2(OH)2(aq) [as in the V8.R6 thermo.dat], the solution is calculated to be undersaturated with uranyl minerals.

May 19, 1999

The information presented in the following pages were taken from the DOE Yucca Mountain Project web site. Of interest are data on the chemistry of saturated zone waters in the vicinity of Yucca Mountain. Of particular importance are DOE results that indicate the presence of reducing conditions in the saturated zone. Reducing environments are favorable for retardation of radionuclides due to lower solubility and higher sorption.

YMP Home | 30-Day Changes | TDM Dev Team

Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_006 DATA REPORT

TABLE DESCRIPTION:
Sodium Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method.

ROW#	Q	SODIUM ABUNDANC E mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	ACTIVITY
1	Y	19.78	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998	Pumping
2	Y	21.28	UE-25 WT #17	SPC00510023	WT-011	06/04/1998	Bailer 1306'
3	Y	20.41	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
4	Y	20.87	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
5	Y	23.26	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
6	Y	20.57	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
7	Y	20.36	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
8	Y	24.41	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998	Pumping
9	Y	21.76	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998	Pumping
10	Y	20.32	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998	Pumping
11	Y	20.08	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998	Pumping
12	Y	20.26	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998	Pumping
13	Y	13.94	USW WT-24	SPC00509801	WT-004**	10/22/1997	Pumping
14	Y	18.15	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998	Pumping

15	Y	20.68	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	20.31	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	20.10	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	20.24	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	20.06	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

s98311_001 DATA REPORT

TABLE DESCRIPTION:
Calcium Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method.

ROW#	Q	CALCIUM ABUNDAN CE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	ACTIVITY
1	Y	11.73	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998	Pumping
2	Y	11.42	UE-25 WT #17	SPC00510023	WT-011	06/04/1998	Bailer 1306'
3	Y	11.15	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
4	Y	11.64	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
5	Y	11.56	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
6	Y	11.80	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
7	Y	11.53	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
8	Y	12.67	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998	Pumping
9	Y	14.59	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998	Pumping
10	Y	9.18	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998	Pumping
11	Y	8.59	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998	Pumping
12	Y	8.07	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998	Pumping

13	Y	21.71	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	10.29	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	10.90	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	11.07	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	11.00	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	10.92	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	10.84	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_007 DATA REPORT

TABLE DESCRIPTION:
Potassium abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method. ND = not detected. N/M = not measured.

ROW#	Q	POTASSIUM ABUNDANCE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	ACTIVITY
1	Y	4.51	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998	Pumping
2	Y	3.30	UE-25 WT #17	SPC00510023	WT-011	06/04/1998	Bailer 1306'
3	Y	ND	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
4	Y	N/M	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998	Bailer 1306'
5	Y	5.34	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
6	Y	N/M	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
7	Y	ND	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	Bailer 1350'
8	Y	3.29	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998	Pumping
9	Y	2.56	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998	Pumping

10	Y	1.44	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998 Pumping
11	Y	3.20	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998 Pumping
12	Y	2.25	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998 Pumping
13	Y	3.36	USW WT-24	SPC00509801	WT-004**	10/22/1997 Pumping
14	Y	3.81	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998 Pumping
15	Y	4.60	UE-25 WT #3	SPC00510101	WT-023	06/22/1998 Pumping
16	Y	4.40	UE-25 WT #3	SPC00510102	WT-024	06/22/1998 Pumping
17	Y	4.27	UE-25 WT #3	SPC00510103	WT-025	06/22/1998 Pumping
18	Y	4.29	UE-25 WT #3	SPC00510104	WT-026	06/22/1998 Pumping
19	Y	4.71	UE-25 WT #3	SPC00510035	WT-055	06/23/1998 Pumping

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Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_005 DATA REPORT

TABLE DESCRIPTION:
Magnesium Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method.

ROW#	Q	MAGNESIUM ABUNDANCE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE ACTIVITY
1	Y	0.42	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998 Pumping
2	Y	1.01	UE-25 WT #17	SPC00510023	WT-011	06/04/1998 Bailer 1306'
3	Y	1.41	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998 Bailer 1306'
4	Y	1.45	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998 Bailer 1306'
5	Y	1.19	UE-25 WT #17	SPC00510025	WT-013	06/04/1998 Bailer 1350'
6	Y	1.18	UE-25 WT #17	SPC00510025	WT-013	06/04/1998 Bailer 1350'
7	Y	1.18	UE-25 WT #17	SPC00510025	WT-013	06/04/1998 Bailer 1350'

8	Y	1.18	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998
Pumping						
9	Y	1.94	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998
Pumping						
10	Y	0.94	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998
Pumping						
11	Y	0.87	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998
Pumping						
12	Y	0.83	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998
Pumping						
13	Y	1.52	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	1.10	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	1.10	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	1.10	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	1.10	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	1.11	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	1.12	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_008 DATA REPORT

TABLE DESCRIPTION:
Lithium Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method. ND = not detected. NC = present but below detection limit.

ROW#	Q	LITHIUM ABUNDAN CE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE
ACTIVITY						
1	Y	0.02	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998
Pumping						
2	Y	0.15	UE-25 WT #17	SPC00510023	WT-011	06/04/1998
Bailer 1306'						
3	Y	ND	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
4	Y	0.11	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
5	Y	0.17	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						

6	Y	0.10	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
7	Y	ND	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
8	Y	0.19	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998
Pumping						
9	Y	0.14	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998
Pumping						
10	Y	0.06	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998
Pumping						
11	Y	0.06	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998
Pumping						
12	Y	0.07	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998
Pumping						
13	Y	NC	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	0.02	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	0.03	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	0.03	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	0.04	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	0.04	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	0.04	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_004 DATA REPORT

TABLE DESCRIPTION:
Iron Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method. NC = present but below detection limit.

ROW#	Q	IRON ABUNDANCE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE ACTIVITY
1	Y	0.60	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998
Pumping						
2	Y	1.16	UE-25 WT #17	SPC00510023	WT-011	06/04/1998
Bailer 1306'						
3	Y	0.78	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
4	Y	0.85	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						

5	Y	0.05	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
6	Y	1.82	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
7	Y	1.73	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
8	Y	2.13	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998
Pumping						
9	Y	0.03	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998
Pumping						
10	Y	0.01	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998
Pumping						
11	Y	0.04	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998
Pumping						
12	Y	0.16	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998
Pumping						
13	Y	0.50	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	0.27	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	NC	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	NC	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	NC	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	NC	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	NC	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

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Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98311_003 DATA REPORT

TABLE DESCRIPTION:
Manganese Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method. NC = present but below detection limit.

ROW#	Q	MANGANESE ABUNDANCE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	ACTIVITY
1	Y	0.16	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998	Pumping

2	Y	0.42	UE-25 WT #17	SPC00510023	WT-011	06/04/1998
Bailer 1306'						
3	Y	0.34	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
4	Y	0.37	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
5	Y	0.40	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
6	Y	0.44	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
7	Y	0.38	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
8	Y	0.42	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998
Pumping						
9	Y	0.73	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998
Pumping						
10	Y	0.40	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998
Pumping						
11	Y	0.41	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998
Pumping						
12	Y	0.41	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998
Pumping						
13	Y	0.11	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	0.09	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	NC	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	NC	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	NC	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	NC	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	NC	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

s98311_002 DATA REPORT

TABLE DESCRIPTION:
Silicon Abundance data of ground water samples using Inductively Coupled Plasma-Atomic Emission Spectrometry from UE-25 WT #3, UE-25 WT #17, and USW WT-24, from 10/22/1997 to 06/23/1998.

TDIF: 307213

DTN: LAAM831311AQ98.002

FOOTNOTES: * = filtered method. ** = filtered and acidified method.

****

ROW#	Q	SILICON ABUNDAN CE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE ACTIVITY

****

1	Y	22.15	UE-25 WT #17	SPC00510019	WT-005**	01/27/1998
Pumping						
2	Y	15.60	UE-25 WT #17	SPC00510023	WT-011	06/04/1998
Bailer 1306'						
3	Y	15.97	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
4	Y	15.08	UE-25 WT #17	SPC00510024	WT-012**	06/04/1998
Bailer 1306'						
5	Y	20.44	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
6	Y	17.14	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
7	Y	17.23	UE-25 WT #17	SPC00510025	WT-013	06/04/1998
Bailer 1350'						
8	Y	24.71	UE-25 WT #17	SPC00510116	WT-037*	07/01/1998
Pumping						
9	Y	20.57	UE-25 WT #17	SPC00510118	WT-039*	07/01/1998
Pumping						
10	Y	24.62	UE-25 WT #17	SPC00510120	WT-041*	07/01/1998
Pumping						
11	Y	23.69	UE-25 WT #17	SPC00510122	WT-043*	07/01/1998
Pumping						
12	Y	22.90	UE-25 WT #17	SPC00510123	WT-044*	07/01/1998
Pumping						
13	Y	21.51	USW WT-24	SPC00509801	WT-004**	10/22/1997
Pumping						
14	Y	26.11	UE-25 WT #3	SPC00510020	WT-008**	02/05/1998
Pumping						
15	Y	33.46	UE-25 WT #3	SPC00510101	WT-023	06/22/1998
Pumping						
16	Y	32.66	UE-25 WT #3	SPC00510102	WT-024	06/22/1998
Pumping						
17	Y	32.86	UE-25 WT #3	SPC00510103	WT-025	06/22/1998
Pumping						
18	Y	32.75	UE-25 WT #3	SPC00510104	WT-026	06/22/1998
Pumping						
19	Y	32.00	UE-25 WT #3	SPC00510035	WT-055	06/23/1998
Pumping						

s98310_001 DATA REPORT

TABLE DESCRIPTION:
Chloride Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to 07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Date and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage designators. Condition is sample treatment.

****

ROW#	Q	CHLORIDE ABUNDANCE mg/L	METHOD	LOCATION	CONDITION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME
1	Y	6.33	Pumping	UE-25 WT #17	Filtered/Acidified	SPC00510019	WT-005	01/27/1998	19:00
2	Y	6.76	Pumping	UE-25 WT #17	Unfiltered	SPC00510018	WT-006	01/27/1998	19:00
3	Y	6.97	Pumping	UE-25 WT #17	Unfiltered	SPC00509798	WT-007	01/28/1998	09:00
4	Y	15.61	Bailer	UE-25 WT #17	Unfiltered, 1306*	SPC00510023	WT-011	06/04/1998	nm
5	Y	15.77	Bailer	UE-25 WT #17	Unfiltered, 1350*	SPC00510025	WT-013	06/04/1998	nm
6	Y	15.80	Pumping	UE-25 WT #17	Unfiltered	SPC00510115	WT-036	07/01/1998	09:22
7	Y	16.36	Pumping	UE-25 WT #17	Filtered	SPC00510116	WT-037	07/01/1998	09:22
8	Y	8.77	Pumping	UE-25 WT #17	Unfiltered	SPC00510117	WT-038	07/01/1998	10:52
9	Y	9.39	Pumping	UE-25 WT #17	Filtered	SPC00510118	WT-039	07/01/1998	10:52
10	Y	5.83	Pumping	UE-25 WT #17	Unfiltered	SPC00510119	WT-040	07/01/1998	13:52
11	Y	5.78	Pumping	UE-25 WT #17	Filtered	SPC00510120	WT-041	07/01/1998	13:52
12	Y	5.89	Pumping	UE-25 WT #17	Unfiltered	SPC00510121	WT-042	07/01/1998	14:45
13	Y	6.03	Pumping	UE-25 WT #17	Filtered	SPC00510122	WT-043	07/01/1998	14:45
14	Y	6.09	Pumping	UE-25 WT #17	Filtered	SPC00510123	WT-044	07/01/1998	15:20
15	Y	6.57	Pumping	UE-25 WT #17	Unfiltered	SPC00510124	WT-045	07/01/1998	15:20
16	Y	9.07	Pumping	USW WT-24	Unfiltered	SPC00509802	WT-001	10/22/1997	10:00
17	Y	6.00	Pumping	UE-25 WT #3	Unfiltered	SPC00510022	WT-010	02/05/1998	19:00
18	Y	6.73	Pumping	UE-25 WT #3	Unfiltered	SPC00510035	WT-055	06/23/1998	nm

s98310_002 DATA REPORT

TABLE DESCRIPTION:
Bromide Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to 07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Data and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage

designators. Condition is sample treatment.

ROW#	Q	BROMIDE ABUNDAN CE mg/L	METHOD	LOCATION	CONDITION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME
1	Y	nm	Pumping	UE-25 WT #17	Filtered/Acidified	SPC00510019	WT-005	01/27/1998	19:00
2	Y	0.19	Pumping	UE-25 WT #17	Unfiltered	SPC00510018	WT-006	01/27/1998	19:00
3	Y	0.20	Pumping	UE-25 WT #17	Unfiltered	SPC00509798	WT-007	01/28/1998	09:00
4	Y	2.78	Bailer	UE-25 WT #17	Unfiltered, 1306*	SPC00510023	WT-011	06/04/1998	nm
5	Y	2.91	Bailer	UE-25 WT #17	Unfiltered, 1350*	SPC00510025	WT-013	06/04/1998	nm
6	Y	2.88	Pumping	UE-25 WT #17	Unfiltered	SPC00510115	WT-036	07/01/1998	09:22
7	Y	2.94	Pumping	UE-25 WT #17	Filtered	SPC00510116	WT-037	07/01/1998	09:22
8	Y	1.16	Pumping	UE-25 WT #17	Unfiltered	SPC00510117	WT-038	07/01/1998	10:52
9	Y	1.28	Pumping	UE-25 WT #17	Filtered	SPC00510118	WT-039	07/01/1998	10:52
10	Y	0.16	Pumping	UE-25 WT #17	Unfiltered	SPC00510119	WT-040	07/01/1998	13:52
11	Y	0.15	Pumping	UE-25 WT #17	Filtered	SPC00510120	WT-041	07/01/1998	13:52
12	Y	0.18	Pumping	UE-25 WT #17	Unfiltered	SPC00510121	WT-042	07/01/1998	14:45
13	Y	0.19	Pumping	UE-25 WT #17	Filtered	SPC00510122	WT-043	07/01/1998	14:45
14	Y	0.22	Pumping	UE-25 WT #17	Filtered	SPC00510123	WT-044	07/01/1998	15:20
15	Y	0.26	Pumping	UE-25 WT #17	Unfiltered	SPC00510124	WT-045	07/01/1998	15:20
16	Y	0.13	Pumping	USW WT-24	Unfiltered	SPC00509802	WT-001	10/22/1997	10:00
17	Y	0.04	Pumping	UE-25 WT #3	Unfiltered	SPC00510022	WT-010	02/05/1998	19:00
18	Y	0.04	Pumping	UE-25 WT #3	Unfiltered	SPC00510035	WT-055	06/23/1998	nm

s98310_003 DATA REPORT

TABLE DESCRIPTION:
Fluoride Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to 07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Date and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage designators. Condition is sample treatment.

ROW#	Q	FLUORIDE ABUNDANCE mg/L	METHOD	LOCATION	CONDITION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME
1	Y	nm	Pumping	UE-25 WT #17	Filtered/Acidified	SPC00510019	WT-005	01/27/1998	19:00
2	Y	nm	Pumping	UE-25 WT #17	Unfiltered	SPC00510018	WT-006	01/27/1998	19:00
3	Y	nm	Pumping	UE-25 WT #17	Unfiltered	SPC00509798	WT-007	01/28/1998	09:00
4	Y	2.51	Bailer	UE-25 WT #17	Unfiltered, 1306*	SPC00510023	WT-011	06/04/1998	nm
5	Y	2.51	Bailer	UE-25 WT #17	Unfiltered, 1350*	SPC00510025	WT-013	06/04/1998	nm
6	Y	2.89	Pumping	UE-25 WT #17	Unfiltered	SPC00510115	WT-036	07/01/1998	09:22
7	Y	3.32	Pumping	UE-25 WT #17	Filtered	SPC00510116	WT-037	07/01/1998	09:22
8	Y	4.01	Pumping	UE-25 WT #17	Unfiltered	SPC00510117	WT-038	07/01/1998	10:52
9	Y	4.50	Pumping	UE-25 WT #17	Filtered	SPC00510118	WT-039	07/01/1998	10:52
10	Y	3.42	Pumping	UE-25 WT #17	Unfiltered	SPC00510119	WT-040	07/01/1998	13:52
11	Y	3.41	Pumping	UE-25 WT #17	Filtered	SPC00510120	WT-041	07/01/1998	13:52
12	Y	3.22	Pumping	UE-25 WT #17	Unfiltered	SPC00510121	WT-042	07/01/1998	14:45
13	Y	3.41	Pumping	UE-25 WT #17	Filtered	SPC00510122	WT-043	07/01/1998	14:45
14	Y	3.44	Pumping	UE-25 WT #17	Filtered	SPC00510123	WT-044	07/01/1998	15:20
15	Y	3.41	Pumping	UE-25 WT #17	Unfiltered	SPC00510124	WT-045	07/01/1998	15:20
16	Y	nm	Pumping	USW WT-24	Unfiltered	SPC00509802	WT-001	10/22/1997	10:00
17	Y	2.24	Pumping	UE-25 WT #3	Unfiltered	SPC00510022	WT-010	02/05/1998	19:00
18	Y	4.44	Pumping	UE-25 WT #3	Unfiltered	SPC00510035	WT-055	06/23/1998	nm

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View Unit Descriptions

s98310_004 DATA REPORT

TABLE DESCRIPTION:
Nitrate Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to

07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Date and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage designators. Condition is sample treatment.

ROW#	Q	NITRATE CE mg/L	ABUNDAN	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME	METHOD	CONDITION
1	Y	nm		UE-25 WT #17	SPC00510019	WT-005	01/27/1998	19:00	Pumping	Filtered/Acidified
2	Y	nm		UE-25 WT #17	SPC00510018	WT-006	01/27/1998	19:00	Pumping	Unfiltered
3	Y	nm		UE-25 WT #17	SPC00509798	WT-007	01/28/1998	09:00	Pumping	Unfiltered
4	Y	0.07		UE-25 WT #17	SPC00510023	WT-011	06/04/1998	nm	Bailer	Unfiltered, 1306*
5	Y	nd		UE-25 WT #17	SPC00510025	WT-013	06/04/1998	nm	Bailer	Unfiltered, 1350*
6	Y	nm		UE-25 WT #17	SPC00510115	WT-036	07/01/1998	09:22	Pumping	Unfiltered
7	Y	nm		UE-25 WT #17	SPC00510116	WT-037	07/01/1998	09:22	Pumping	Filtered
8	Y	nm		UE-25 WT #17	SPC00510117	WT-038	07/01/1998	10:52	Pumping	Unfiltered
9	Y	0.49		UE-25 WT #17	SPC00510118	WT-039	07/01/1998	10:52	Pumping	Filtered
10	Y	4.92		UE-25 WT #17	SPC00510119	WT-040	07/01/1998	13:52	Pumping	Unfiltered
11	Y	4.96		UE-25 WT #17	SPC00510120	WT-041	07/01/1998	13:52	Pumping	Filtered
12	Y	4.93		UE-25 WT #17	SPC00510121	WT-042	07/01/1998	14:45	Pumping	Unfiltered
13	Y	5.03		UE-25 WT #17	SPC00510122	WT-043	07/01/1998	14:45	Pumping	Filtered
14	Y	4.99		UE-25 WT #17	SPC00510123	WT-044	07/01/1998	15:20	Pumping	Filtered
15	Y	4.99		UE-25 WT #17	SPC00510124	WT-045	07/01/1998	15:20	Pumping	Unfiltered
16	Y	nm		USW WT-24	SPC00509802	WT-001	10/22/1997	10:00	Pumping	Unfiltered
17	Y	5.70		UE-25 WT #3	SPC00510022	WT-010	02/05/1998	19:00	Pumping	Unfiltered
18	Y	5.62		UE-25 WT #3	SPC00510035	WT-055	06/23/1998	nm	Pumping	Unfiltered

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Yucca Mountain Site Characterization Project
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View Unit Descriptions

s98310_005 DATA REPORT

TABLE DESCRIPTION:
Phosphate Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to 07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Date and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage designators. Condition is sample treatment.

ROW#	Q	PHOSPHATE ABUNDANCE mg/L	LOCATION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME	METHOD	CONDITION
1	Y	< 0.1	UE-25 WT #17	SPC00510019	WT-005	01/27/1998	19:00	Pumping	Filtered/Acidified
2	Y	< 0.1	UE-25 WT #17	SPC00510018	WT-006	01/27/1998	19:00	Pumping	Unfiltered
3	Y	< 0.1	UE-25 WT #17	SPC00509798	WT-007	01/28/1998	09:00	Pumping	Unfiltered
4	Y	< 0.1	UE-25 WT #17	SPC00510023	WT-011	06/04/1998	nm	Bailer	Unfiltered, 1306*
5	Y	< 0.1	UE-25 WT #17	SPC00510025	WT-013	06/04/1998	nm	Bailer	Unfiltered, 1350*
6	Y	< 0.1	UE-25 WT #17	SPC00510115	WT-036	07/01/1998	09:22	Pumping	Unfiltered
7	Y	< 0.1	UE-25 WT #17	SPC00510116	WT-037	07/01/1998	09:22	Pumping	Filtered
8	Y	< 0.1	UE-25 WT #17	SPC00510117	WT-038	07/01/1998	10:52	Pumping	Unfiltered
9	Y	< 0.1	UE-25 WT #17	SPC00510118	WT-039	07/01/1998	10:52	Pumping	Filtered
10	Y	< 0.1	UE-25 WT #17	SPC00510119	WT-040	07/01/1998	13:52	Pumping	Unfiltered
11	Y	< 0.1	UE-25 WT #17	SPC00510120	WT-041	07/01/1998	13:52	Pumping	Filtered
12	Y	< 0.1	UE-25 WT #17	SPC00510121	WT-042	07/01/1998	14:45	Pumping	Unfiltered
13	Y	< 0.1	UE-25 WT #17	SPC00510122	WT-043	07/01/1998	14:45	Pumping	Filtered
14	Y	< 0.1	UE-25 WT #17	SPC00510123	WT-044	07/01/1998	15:20	Pumping	Filtered
15	Y	< 0.1	UE-25 WT #17	SPC00510124	WT-045	07/01/1998	15:20	Pumping	Unfiltered
16	Y	< 0.1	USW WT-24	SPC00509802	WT-001	10/22/1997	10:00	Pumping	Unfiltered
17	Y	< 0.1	UE-25 WT #3	SPC00510022	WT-010	02/05/1998	19:00	Pumping	Unfiltered
18	Y	< 0.1	UE-25 WT #3	SPC00510035	WT-055	06/23/1998	nm	Pumping	Unfiltered

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View Unit Descriptions

s98310_006 DATA REPORT

TABLE DESCRIPTION:
Sulfate Abundance data of groundwater samples, using ion chromatography analysis, from UE-25 WT #3, UE-25 WT #17 and USW WT-24, 10/22/1997 to 07/01/1998.

TDIF: 307210

DTN: LAAM831311AQ98.001

FOOTNOTES: Date and Time are collection date and time, respectively. Method is collection method. nm = not measured. * denotes footage designators. Condition is sample treatment.

ROW#	Q	SULFATE ABUNDAN CE mg/L	METHOD	LOCATION	CONDITION	SPC NUMBER	SAMPLE NUMBER	DATE	TIME
1	Y	18.79	Pumping	UE-25 WT #17	Filtered/Acidified	SPC00510019	WT-005	01/27/1998	19:00
2	Y	20.30	Pumping	UE-25 WT #17	Unfiltered	SPC00510018	WT-006	01/27/1998	19:00
3	Y	21.88	Pumping	UE-25 WT #17	Unfiltered	SPC00509798	WT-007	01/28/1998	09:00
4	Y	10.58	Bailer	UE-25 WT #17	Unfiltered, 1306*	SPC00510023	WT-011	06/04/1998	nm
5	Y	14.44	Bailer	UE-25 WT #17	Unfiltered, 1350*	SPC00510025	WT-013	06/04/1998	nm
6	Y	0.37	Pumping	UE-25 WT #17	Unfiltered	SPC00510115	WT-036	07/01/1998	09:22
7	Y	0.62	Pumping	UE-25 WT #17	Filtered	SPC00510116	WT-037	07/01/1998	09:22
8	Y	10.86	Pumping	UE-25 WT #17	Unfiltered	SPC00510117	WT-038	07/01/1998	10:52
9	Y	11.72	Pumping	UE-25 WT #17	Filtered	SPC00510118	WT-039	07/01/1998	10:52
10	Y	19.99	Pumping	UE-25 WT #17	Unfiltered	SPC00510119	WT-040	07/01/1998	13:52
11	Y	19.82	Pumping	UE-25 WT #17	Filtered	SPC00510120	WT-041	07/01/1998	13:52
12	Y	19.45	Pumping	UE-25 WT #17	Unfiltered	SPC00510121	WT-042	07/01/1998	14:45
13	Y	19.43	Pumping	UE-25 WT #17	Filtered	SPC00510122	WT-043	07/01/1998	14:45
14	Y	19.19	Pumping	UE-25 WT #17	Filtered	SPC00510123	WT-044	07/01/1998	15:20
15	Y	19.75	Pumping	UE-25 WT #17	Unfiltered	SPC00510124	WT-045	07/01/1998	15:20
16	Y	17.29	Pumping	USW WT-24	Unfiltered	SPC00509802	WT-001	10/22/1997	10:00
17	Y	19.05	Pumping	UE-25 WT #3	Unfiltered	SPC00510022	WT-010	02/05/1998	19:00
18	Y	19.72	Pumping	UE-25 WT #3	Unfiltered	SPC00510035	WT-055	06/23/1998	nm

View Unit Descriptions

s98312_002 DATA REPORT

TABLE DESCRIPTION:
EH data of downhole measurements from UE-25 WT #17, 05/06/1998 and 07/15/1998.

TDIF: 307214

DTN: LAAM831311AQ98.003

FOOTNOTES: nm = not measured.

ROW#	Q	EH	LOCATION	DATE	TEMPERATURE	DEPTH	MEASUREMENT
		mV			°C	ft	
1	Y	nm	UE-25 WT #17	05/06/1998	nm	1100	Measured going down
2	Y	nm	UE-25 WT #17	05/06/1998	nm	1200	Measured going down
3	Y	nm	UE-25 WT #17	05/06/1998	nm	1227	Measured going down
4	Y	nm	UE-25 WT #17	05/06/1998	nm	1257	Measured going down
5	Y	nm	UE-25 WT #17	05/06/1998	nm	1267	Measured going down
6	Y	nm	UE-25 WT #17	05/06/1998	nm	1277	Measured going down
7	Y	nm	UE-25 WT #17	05/06/1998	nm	1280	Measured going down
8	Y	452	UE-25 WT #17	05/06/1998	28.0	1287	Measured going down
9	Y	nm	UE-25 WT #17	05/06/1998	nm	1288	Measured going down
10	Y	nm	UE-25 WT #17	05/06/1998	nm	1289	Measured going down
11	Y	nm	UE-25 WT #17	05/06/1998	nm	1290	Measured going down
12	Y	nm	UE-25 WT #17	05/06/1998	nm	1291	Measured going down
13	Y	nm	UE-25 WT #17	05/06/1998	nm	1294	Measured going down
14	Y	72	UE-25 WT #17	05/06/1998	30.8	1300	Measured going down
15	Y	-70	UE-25 WT #17	05/06/1998	30.9	1310	Measured going down
16	Y	-104	UE-25 WT #17	05/06/1998	31.0	1320	Measured going down
17	Y	-118	UE-25 WT #17	05/06/1998	31.1	1330	Measured going down
18	Y	-121	UE-25 WT #17	05/06/1998	31.2	1340	Measured going down
19	Y	-121	UE-25 WT #17	05/06/1998	31.2	1350	Measured going down
20	Y	-117	UE-25 WT #17	05/06/1998	31.2	1360	Measured going down
21	Y	-104	UE-25 WT #17	05/06/1998	31.3	1370	Measured going down

22	Y	270	UE-25 WT #17	05/06/1998	30.1	
1100			Measured coming up			
23	Y	274	UE-25 WT #17	05/06/1998	30.6	
1200			Measured coming up			
24	Y	271	UE-25 WT #17	05/06/1998	30.7	
1227			Measured coming up			
25	Y	243	UE-25 WT #17	05/06/1998	30.9	
1257			Measured coming up			
26	Y	242	UE-25 WT #17	05/06/1998	30.9	
1267			Measured coming up			
27	Y	242	UE-25 WT #17	05/06/1998	31.0	
1277			Measured coming up			
28	Y	nm	UE-25 WT #17	05/06/1998	nm	
1280			Measured coming up			
29	Y	237	UE-25 WT #17	05/06/1998	31.0	
1287			Measured coming up			
30	Y	231	UE-25 WT #17	05/06/1998	31.0	
1288			Measured coming up			
31	Y	229	UE-25 WT #17	05/06/1998	31.0	
1289			Measured coming up			
32	Y	nm	UE-25 WT #17	05/06/1998	nm	
1290			Measured coming up			
33	Y	156	UE-25 WT #17	05/06/1998	31.1	
1291			Measured coming up			
34	Y	-63	UE-25 WT #17	05/06/1998	31.2	
1294			Measured coming up			
35	Y	-68	UE-25 WT #17	05/06/1998	31.2	
1300			Measured coming up			
36	Y	-72	UE-25 WT #17	05/06/1998	31.2	
1310			Measured coming up			
37	Y	-70	UE-25 WT #17	05/06/1998	31.2	
1320			Measured coming up			
38	Y	-94	UE-25 WT #17	05/06/1998	31.2	
1330			Measured coming up			
39	Y	-96	UE-25 WT #17	05/06/1998	31.2	
1340			Measured coming up			
40	Y	-118	UE-25 WT #17	05/06/1998	31.3	
1350			Measured coming up			
41	Y	-77	UE-25 WT #17	05/06/1998	31.3	
1360			Measured coming up			
42	Y	-104	UE-25 WT #17	05/06/1998	31.3	
1370			Measured coming up			
43	Y	nm	UE-25 WT #17	07/15/1998	nm	
1100			Measured going down			
44	Y	nm	UE-25 WT #17	07/15/1998	nm	
1200			Measured going down			
45	Y	nm	UE-25 WT #17	07/15/1998	nm	
1227			Measured going down			
46	Y	nm	UE-25 WT #17	07/15/1998	nm	
1257			Measured going down			
47	Y	nm	UE-25 WT #17	07/15/1998	nm	
1267			Measured going down			
48	Y	nm	UE-25 WT #17	07/15/1998	nm	
1277			Measured going down			
49	Y	433	UE-25 WT #17	07/15/1998	28.8	
1280			Measured going down			
50	Y	nm	UE-25 WT #17	07/15/1998	nm	
1287			Measured going down			
51	Y	nm	UE-25 WT #17	07/15/1998	nm	
1288			Measured going down			
52	Y	nm	UE-25 WT #17	07/15/1998	nm	
1289			Measured going down			
53	Y	432	UE-25 WT #17	07/15/1998	29.1	
1290			Measured going down			
54	Y	nm	UE-25 WT #17	07/15/1998	nm	
1291			Measured going down			
55	Y	nm	UE-25 WT #17	07/15/1998	nm	
1294			Measured going down			
56	Y	-2	UE-25 WT #17	07/15/1998	30.9	
1300			Measured going down			

57	Y	-4	UE-25 WT #17	07/15/1998	31.2	1310
			Measured going down			
58	Y	6	UE-25 WT #17	07/15/1998	31.2	1320
			Measured going down			
59	Y	21	UE-25 WT #17	07/15/1998	31.2	1330
			Measured going down			
60	Y	7	UE-25 WT #17	07/15/1998	31.3	1340
			Measured going down			
61	Y	-4	UE-25 WT #17	07/15/1998	31.3	1350
			Measured going down			
62	Y	-10	UE-25 WT #17	07/15/1998	31.3	1360
			Measured going down			
63	Y	-36	UE-25 WT #17	07/15/1998	31.4	1370
			Measured going down			
64	Y	nm	UE-25 WT #17	07/15/1998	nm	1100
			Measured coming up			
65	Y	nm	UE-25 WT #17	07/15/1998	nm	1200
			Measured coming up			
66	Y	nm	UE-25 WT #17	07/15/1998	nm	1227
			Measured coming up			
67	Y	nm	UE-25 WT #17	07/15/1998	nm	1257
			Measured coming up			
68	Y	nm	UE-25 WT #17	07/15/1998	nm	1267
			Measured coming up			
69	Y	nm	UE-25 WT #17	07/15/1998	nm	1277
			Measured coming up			
70	Y	nm	UE-25 WT #17	07/15/1998	nm	1280
			Measured coming up			
71	Y	nm	UE-25 WT #17	07/15/1998	nm	1287
			Measured coming up			
72	Y	nm	UE-25 WT #17	07/15/1998	nm	1288
			Measured coming up			
73	Y	nm	UE-25 WT #17	07/15/1998	nm	1289
			Measured coming up			
74	Y	nm	UE-25 WT #17	07/15/1998	nm	1290
			Measured coming up			
75	Y	nm	UE-25 WT #17	07/15/1998	nm	1291
			Measured coming up			
76	Y	nm	UE-25 WT #17	07/15/1998	nm	1294
			Measured coming up			
77	Y	nm	UE-25 WT #17	07/15/1998	nm	1300
			Measured coming up			
78	Y	-52	UE-25 WT #17	07/15/1998	31.2	1310
			Measured coming up			
79	Y	nm	UE-25 WT #17	07/15/1998	nm	1320
			Measured coming up			
80	Y	nm	UE-25 WT #17	07/15/1998	nm	1330
			Measured coming up			
81	Y	-9	UE-25 WT #17	07/15/1998	31.3	1340
			Measured coming up			
82	Y	nm	UE-25 WT #17	07/15/1998	nm	1350
			Measured coming up			
83	Y	nm	UE-25 WT #17	07/15/1998	nm	1360
			Measured coming up			
84	Y	-36	UE-25 WT #17	07/15/1998	31.4	1370
			Measured coming up			

s98312_001 DATA REPORT

TABLE DESCRIPTION:
PH data of downhole measurements from UE-25 WT #17, 05/06/1998 and 07/15/1998.

TDIF: 307214

DTN: LAAM831311AQ98.003

FOOTNOTES: nm = not measured.

ROW#	Q	PH	LOCATION	DATE	TEMPERATURE	DEPTH	MEASUREMENT
					°C	ft	
1	Y	nm	UE-25 WT #17	05/06/1998	nm	1100	Measured going down
2	Y	nm	UE-25 WT #17	05/06/1998	nm	1200	Measured going down
3	Y	nm	UE-25 WT #17	05/06/1998	nm	1227	Measured going down
4	Y	nm	UE-25 WT #17	05/06/1998	nm	1257	Measured going down
5	Y	nm	UE-25 WT #17	05/06/1998	nm	1267	Measured going down
6	Y	nm	UE-25 WT #17	05/06/1998	nm	1277	Measured going down
7	Y	nm	UE-25 WT #17	05/06/1998	nm	1280	Measured going down
8	Y	nm	UE-25 WT #17	05/06/1998	nm	1287	Measured going down
9	Y	nm	UE-25 WT #17	05/06/1998	nm	1288	Measured going down
10	Y	nm	UE-25 WT #17	05/06/1998	nm	1289	Measured going down
11	Y	7.00	UE-25 WT #17	05/06/1998	27.8	1290	Measured going down
12	Y	nm	UE-25 WT #17	05/06/1998	nm	1291	Measured going down
13	Y	nm	UE-25 WT #17	05/06/1998	nm	1294	Measured going down
14	Y	7.07	UE-25 WT #17	05/06/1998	31.0	1300	Measured going down
15	Y	7.09	UE-25 WT #17	05/06/1998	31.0	1310	Measured going down
16	Y	7.06	UE-25 WT #17	05/06/1998	31.1	1320	Measured going down
17	Y	7.06	UE-25 WT #17	05/06/1998	31.2	1330	Measured going down
18	Y	7.04	UE-25 WT #17	05/06/1998	31.3	1340	Measured going down
19	Y	7.02	UE-25 WT #17	05/06/1998	31.3	1350	Measured going down
20	Y	7.03	UE-25 WT #17	05/06/1998	31.3	1360	Measured going down
21	Y	7.03	UE-25 WT #17	05/06/1998	31.4	1370	Measured going down
22	Y	nm	UE-25 WT #17	07/15/1998	nm	1100	Measured going down
23	Y	nm	UE-25 WT #17	07/15/1998	nm	1200	Measured going down
24	Y	nm	UE-25 WT #17	07/15/1998	nm	1227	Measured going down

25	Y	nm	UE-25 WT #17	07/15/1998	nm	
1257			Measured going down			
26	Y	nm	UE-25 WT #17	07/15/1998	nm	
1267			Measured going down			
27	Y	nm	UE-25 WT #17	07/15/1998	nm	
1277			Measured going down			
28	Y	nm	UE-25 WT #17	07/15/1998	nm	
1280			Measured going down			
29	Y	nm	UE-25 WT #17	07/15/1998	nm	
1287			Measured going down			
30	Y	nm	UE-25 WT #17	07/15/1998	nm	
1288			Measured going down			
31	Y	nm	UE-25 WT #17	07/15/1998	nm	
1289			Measured going down			
32	Y	7.22	UE-25 WT #17	07/15/1998	31.1	
1290			Measured going down			
33	Y	nm	UE-25 WT #17	07/15/1998	nm	
1291			Measured going down			
34	Y	nm	UE-25 WT #17	07/15/1998	nm	
1294			Measured going down			
35	Y	7.2	UE-25 WT #17	07/15/1998	31.2	
1300			Measured going down			
36	Y	7.21	UE-25 WT #17	07/15/1998	31.3	
1310			Measured going down			
37	Y	7.22	UE-25 WT #17	07/15/1998	31.3	
1320			Measured going down			
38	Y	7.22	UE-25 WT #17	07/15/1998	31.3	
1330			Measured going down			
39	Y	7.23	UE-25 WT #17	07/15/1998	31.4	
1340			Measured going down			
40	Y	7.22	UE-25 WT #17	07/15/1998	31.4	
1350			Measured going down			
41	Y	7.23	UE-25 WT #17	07/15/1998	31.4	
1360			Measured going down			
42	Y	7.23	UE-25 WT #17	07/15/1998	31.4	
1370			Measured going down			
43	Y	nm	UE-25 WT #17	07/15/1998	nm	
1100			Measured coming up			
44	Y	nm	UE-25 WT #17	07/15/1998	nm	
1200			Measured coming up			
45	Y	nm	UE-25 WT #17	07/15/1998	nm	
1227			Measured coming up			
46	Y	nm	UE-25 WT #17	07/15/1998	nm	
1257			Measured coming up			
47	Y	nm	UE-25 WT #17	07/15/1998	nm	
1267			Measured coming up			
48	Y	nm	UE-25 WT #17	07/15/1998	nm	
1277			Measured coming up			
49	Y	nm	UE-25 WT #17	07/15/1998	nm	
1280			Measured coming up			
50	Y	nm	UE-25 WT #17	07/15/1998	nm	
1287			Measured coming up			
51	Y	nm	UE-25 WT #17	07/15/1998	nm	
1288			Measured coming up			
52	Y	nm	UE-25 WT #17	07/15/1998	nm	
1289			Measured coming up			
53	Y	nm	UE-25 WT #17	07/15/1998	nm	
1290			Measured coming up			
54	Y	nm	UE-25 WT #17	07/15/1998	nm	
1291			Measured coming up			
55	Y	nm	UE-25 WT #17	07/15/1998	nm	
1294			Measured coming up			
56	Y	nm	UE-25 WT #17	07/15/1998	nm	
1300			Measured coming up			
57	Y	7.19	UE-25 WT #17	07/15/1998	31.3	
1310			Measured coming up			
58	Y	nm	UE-25 WT #17	07/15/1998	nm	
1320			Measured coming up			
59	Y	nm	UE-25 WT #17	07/15/1998	nm	
1330			Measured coming up			

60	Y	7.21	UE-25 WT #17	07/15/1998	31.4	
1340		Measured coming up				
61	Y	nm	UE-25 WT #17	07/15/1998	nm	
1350		Measured coming up				
62	Y	nm	UE-25 WT #17	07/15/1998	nm	
1360		Measured coming up				
63	Y	7.23	UE-25 WT #17	07/15/1998	31.4	
1370		Measured coming up				

Yucca Mountain Site Characterization Project
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s98313_002 DATA REPORT

TABLE DESCRIPTION:
EH data of downhole measurements from UE-25 WT #3, 05/07/1998 and 06/30/1998.

TDIF: 307215

DTN: LAAM831311AQ98.004

FOOTNOTES: nm = not measured.

****

ROW#	Q	EH	LOCATION	DATE	TEMPERATURE °C	DEPTH ft	MEASUREMENT
1	Y	nm	UE-25 WT #3	05/07/1998	nm	950	Measured going down
2	Y	nm	UE-25 WT #3	05/07/1998	nm	970	Measured going down
3	Y	nm	UE-25 WT #3	05/07/1998	nm	980	Measured going down
4	Y	nm	UE-25 WT #3	05/07/1998	nm	990	Measured going down
5	Y	352	UE-25 WT #3	05/07/1998	33.1	1000	Measured going down
6	Y	349	UE-25 WT #3	05/07/1998	33.2	1010	Measured going down
7	Y	348	UE-25 WT #3	05/07/1998	33.2	1020	Measured going down
8	Y	347	UE-25 WT #3	05/07/1998	33.3	1030	Measured going down
9	Y	357	UE-25 WT #3	05/07/1998	33.3	1040	Measured going down
10	Y	358	UE-25 WT #3	05/07/1998	33.4	1050	Measured going down
11	Y	383	UE-25 WT #3	05/07/1998	33.4	1060	Measured going down

12 Y 377 UE-25 WT #3 05/07/1998 33.5
1070 Measured going down
13 Y 374 UE-25 WT #3 05/07/1998 33.5
1080 Measured going down
14 Y 372 UE-25 WT #3 05/07/1998 33.6
1090 Measured going down
15 Y 371 UE-25 WT #3 05/07/1998 33.6
1100 Measured going down
16 Y nm UE-25 WT #3 05/07/1998 nm
1110 Measured going down
17 Y nm UE-25 WT #3 05/07/1998 nm
950 Measured coming up
18 Y nm UE-25 WT #3 05/07/1998 nm
970 Measured coming up
19 Y nm UE-25 WT #3 05/07/1998 nm
980 Measured coming up
20 Y 348 UE-25 WT #3 05/07/1998 33.2
990 Measured coming up
21 Y nm UE-25 WT #3 05/07/1998 nm
1000 Measured coming up
22 Y nm UE-25 WT #3 05/07/1998 nm
1010 Measured coming up
23 Y nm UE-25 WT #3 05/07/1998 nm
1020 Measured coming up
24 Y 344 UE-25 WT #3 05/07/1998 33.4
1030 Measured coming up
25 Y nm UE-25 WT #3 05/07/1998 nm
1040 Measured coming up
26 Y 348 UE-25 WT #3 05/07/1998 33.4
1050 Measured coming up
27 Y nm UE-25 WT #3 05/07/1998 nm
1060 Measured coming up
28 Y nm UE-25 WT #3 05/07/1998 nm
1070 Measured coming up
29 Y nm UE-25 WT #3 05/07/1998 nm
1080 Measured coming up
30 Y nm UE-25 WT #3 05/07/1998 nm
1090 Measured coming up
31 Y 371 UE-25 WT #3 05/07/1998 33.6
1100 Measured coming up
32 Y nm UE-25 WT #3 05/07/1998 nm
1110 Measured coming up
33 Y 447 UE-25 WT #3 06/30/1998 30.7
950 Measured going down
34 Y 449 UE-25 WT #3 06/30/1998 31
970 Measured going down
35 Y nm UE-25 WT #3 06/30/1998 nm
980 Measured going down
36 Y 356 UE-25 WT #3 06/30/1998 32.7
990 Measured going down
37 Y 341 UE-25 WT #3 06/30/1998 33
1000 Measured going down
38 Y 330 UE-25 WT #3 06/30/1998 33.1
1010 Measured going down
39 Y 326 UE-25 WT #3 06/30/1998 33.1
1020 Measured going down
40 Y 325 UE-25 WT #3 06/30/1998 33.2
1030 Measured going down
41 Y 324 UE-25 WT #3 06/30/1998 33.3
1040 Measured going down
42 Y 326 UE-25 WT #3 06/30/1998 33.3
1050 Measured going down
43 Y 327 UE-25 WT #3 06/30/1998 33.4
1060 Measured going down
44 Y 347 UE-25 WT #3 06/30/1998 33.4
1070 Measured going down
45 Y 335 UE-25 WT #3 06/30/1998 33.4
1080 Measured going down
46 Y 329 UE-25 WT #3 06/30/1998 33.5
1090 Measured going down

47	Y	325	UE-25 WT #3	06/30/1998	33.5	1100
			Measured going down			
48	Y	nm	UE-25 WT #3	06/30/1998	nm	1110
			Measured going down			
49	Y	nm	UE-25 WT #3	06/30/1998	nm	950
			Measured coming up			
50	Y	nm	UE-25 WT #3	06/30/1998	nm	970
			Measured coming up			
51	Y	nm	UE-25 WT #3	06/30/1998	nm	980
			Measured coming up			
52	Y	nm	UE-25 WT #3	06/30/1998	nm	990
			Measured coming up			
53	Y	nm	UE-25 WT #3	06/30/1998	nm	1000
			Measured coming up			
54	Y	nm	UE-25 WT #3	06/30/1998	33.2	1010
			Measured coming up			
55	Y	nm	UE-25 WT #3	06/30/1998	nm	1020
			Measured coming up			
56	Y	nm	UE-25 WT #3	06/30/1998	nm	1030
			Measured coming up			
57	Y	nm	UE-25 WT #3	06/30/1998	33.3	1040
			Measured coming up			
58	Y	nm	UE-25 WT #3	06/30/1998	nm	1050
			Measured coming up			
59	Y	nm	UE-25 WT #3	06/30/1998	nm	1060
			Measured coming up			
60	Y	320	UE-25 WT #3	06/30/1998	33.4	1070
			Measured coming up			
61	Y	nm	UE-25 WT #3	06/30/1998	nm	1080
			Measured coming up			
62	Y	nm	UE-25 WT #3	06/30/1998	nm	1090
			Measured coming up			
63	Y	325	UE-25 WT #3	06/30/1998	33.5	1100
			Measured coming up			
64	Y	nm	UE-25 WT #3	06/30/1998	nm	1110
			Measured coming up			

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s98313_001 DATA REPORT

TABLE DESCRIPTION:
PH data of downhole measurements from UE-25 WT #3, 05/07/1998 and 06/30/1998.

TDIF: 307215

DTN: LAAM831311AQ98.004

FOOTNOTES: nm = not measured.

****

ROW#	Q	PH	LOCATION	DATE	TEMPERATURE °C	DEPTH	MEASUREMENT

ft

****

1	Y	nm	UE-25 WT #3	05/07/1998	nm	
950			Measured going down			
2	Y	nm	UE-25 WT #3	05/07/1998	nm	
970			Measured going down			
3	Y	nm	UE-25 WT #3	05/07/1998	nm	
980			Measured going down			
4	Y	nm	UE-25 WT #3	05/07/1998	nm	
990			Measured going down			
5	Y	7.09	UE-25 WT #3	05/07/1998	32.3	
1000			Measured going down			
6	Y	7.08	UE-25 WT #3	05/07/1998	32.6	
1010			Measured going down			
7	Y	7.07	UE-25 WT #3	05/07/1998	32.8	
1020			Measured going down			
8	Y	7.07	UE-25 WT #3	05/07/1998	32.9	
1030			Measured going down			
9	Y	7.06	UE-25 WT #3	05/07/1998	33.2	
1040			Measured going down			
10	Y	7.05	UE-25 WT #3	05/07/1998	33.3	
1050			Measured going down			
11	Y	7.04	UE-25 WT #3	05/07/1998	33.4	
1060			Measured going down			
12	Y	7.03	UE-25 WT #3	05/07/1998	33.4	
1070			Measured going down			
13	Y	7.03	UE-25 WT #3	05/07/1998	33.5	
1080			Measured going down			
14	Y	7.02	UE-25 WT #3	05/07/1998	33.5	
1090			Measured going down			
15	Y	7.01	UE-25 WT #3	05/07/1998	33.6	
1100			Measured going down			
16	Y	7.00	UE-25 WT #3	05/07/1998	33.6	
1110			Measured going down			
17	Y	6.27	UE-25 WT #3	06/30/1998	29.7	
950			Measured going down			
18	Y	nm	UE-25 WT #3	06/30/1998	nm	
970			Measured going down			
19	Y	6.29	UE-25 WT #3	06/30/1998	29.7	
980			Measured going down			
20	Y	nm	UE-25 WT #3	06/30/1998	nm	
990			Measured going down			
21	Y	7.38	UE-25 WT #3	06/30/1998	32.9	
1000			Measured going down			
22	Y	7.36	UE-25 WT #3	06/30/1998	33.1	
1010			Measured going down			
23	Y	7.36	UE-25 WT #3	06/30/1998	33.2	
1020			Measured going down			
24	Y	7.36	UE-25 WT #3	06/30/1998	33.2	
1030			Measured going down			
25	Y	7.35	UE-25 WT #3	06/30/1998	33.3	
1040			Measured going down			
26	Y	7.33	UE-25 WT #3	06/30/1998	33.4	
1050			Measured going down			
27	Y	7.33	UE-25 WT #3	06/30/1998	33.4	
1060			Measured going down			
28	Y	7.32	UE-25 WT #3	06/30/1998	33.5	
1070			Measured going down			
29	Y	7.29	UE-25 WT #3	06/30/1998	33.5	
1080			Measured going down			
30	Y	7.26	UE-25 WT #3	06/30/1998	33.6	
1090			Measured going down			
31	Y	7.28	UE-25 WT #3	06/30/1998	33.6	
1100			Measured going down			
32	Y	nm	UE-25 WT #3	06/30/1998	nm	
1110			Measured going down			
33	Y	nm	UE-25 WT #3	06/30/1998	nm	
950			Measured coming up			

34	Y	nm	UE-25 WT #3	06/30/1998	nm	
970		Measured coming up				
35	Y	nm	UE-25 WT #3	06/30/1998	nm	
980		Measured coming up				
36	Y	nm	UE-25 WT #3	06/30/1998	nm	
990		Measured coming up				
37	Y	nm	UE-25 WT #3	06/30/1998	nm	
1000		Measured coming up				
38	Y	7.36	UE-25 WT #3	06/30/1998	33.3	
1010		Measured coming up				
39	Y	nm	UE-25 WT #3	06/30/1998	nm	
1020		Measured coming up				
40	Y	nm	UE-25 WT #3	06/30/1998	nm	
1030		Measured coming up				
41	Y	7.33	UE-25 WT #3	06/30/1998	33.4	
1040		Measured coming up				
42	Y	nm	UE-25 WT #3	06/30/1998	nm	
1050		Measured coming up				
43	Y	nm	UE-25 WT #3	06/30/1998	nm	
1060		Measured coming up				
44	Y	7.31	UE-25 WT #3	06/30/1998	33.5	
1070		Measured coming up				
45	Y	nm	UE-25 WT #3	06/30/1998	nm	
1080		Measured coming up				
46	Y	nm	UE-25 WT #3	06/30/1998	nm	
1090		Measured coming up				
47	Y	7.28	UE-25 WT #3	06/30/1998	33.6	
1100		Measured coming up				
48	Y	nm	UE-25 WT #3	06/30/1998	nm	
1110		Measured coming up				

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s98315_001 DATA REPORT

TABLE DESCRIPTION:
Geochemical field measurements of pumped water samples from UE-25 WT #17, 01/27/1998.

TDIF: 307216

DTN: LAAM831311AQ98.005

FOOTNOTES: Geochemical measurements are static measurments obtained on pumped water samples in open containers open to the atmosphere during analysis. Oxygen Abundance is dissolved oxygen. Temperature is air temperature. Alkalinity as CaCO3. nm indicates not measured.

ROW#	Q	LOCATION	DEPTH ft	OXYGEN ABUND. mg/L	EH mV	PH	SPEC. CONDUCT. microSiemens per cm	SOLUTION TEMP. Centigrade	TEMPERATURE Centigrade
1	Y	UE-25 WT#17	1646	1.2	nm	nm	261	27	19.5
2	Y	UE-25 WT#17	1655	1.4	nm	7.14	244	27.7	19.2
3	Y	UE-25 WT#17	1715	2.2	nm	nm	243	29.6	18.2
4	Y	UE-25 WT#17	1730	2.6	64	7.24	246	29.1	18.3
5	Y	UE-25 WT#17	1745	3	87	7.37	296	28.4	18.6
6	Y	UE-25 WT#17	1800	3.2	81	7.47	246	28.8	18.8
7	Y	UE-25 WT#17	1815	3.3	76	7.49	243	29.5	19.2
8	Y	UE-25 WT#17	1830	3.2	79	7.49	247	29.1	18.6
9	Y	UE-25 WT#17	1845	3.3	72	7.55	245	29.8	18.6
10	Y	UE-25 WT#17	1900	4	nm	nm	250	29	18.6

ROW#	Q	LOCATION	DEPTH ft	NITRITE ABUND. mg/L	NITRATE ABUND. mg/L	TOTAL IRON mg/L	MANGANESE ABUND. mg/L	ALKALINITY mg/L
1	Y	UE-25 WT#17	1646	nm	nm	nm	nm	nm

2	Y	UE-25 WT#17	1655	nm	nm	nm	nm	nm
3	Y	UE-25 WT#17	1715	nm	nm	nm	nm	nm
4	Y	UE-25 WT#17	1730	nm	nm	nm	nm	nm
5	Y	UE-25 WT#17	1745	0	0.5	nm	nm	nm
6	Y	UE-25 WT#17	1800	nm	nm	3.6	nm	nm
7	Y	UE-25 WT#17	1815	0	nm	3.5	nm	nm
8	Y	UE-25 WT#17	1830	nm	4.5	3.4	nm	nm
9	Y	UE-25 WT#17	1845	nm	nm	nm	0.2	nm
10	Y	UE-25 WT#17	1900	nm	nm	nm	nm	100

Yucca Mountain Site Characterization Project
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s98314_008 DATA REPORT

TABLE DESCRIPTION:
Alkalinity data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static measurements in an open beaker. Alkalinity is CaCO3. Temperature is air temperature. nm = not measured.

ROW#	Q	ALKALINITY mg/L	LOCATION	TIME	TEMPERATURE ^oC
1	Y	nm	UE-25 WT #3	16:20	17.5
2	Y	nm	UE-25 WT #3	16:55	18.5
3	Y	nm	UE-25 WT #3	17:17	19.3
4	Y	nm	UE-25 WT #3	17:30	20
5	Y	nm	UE-25 WT #3	17:47	20
6	Y	97	UE-25 WT #3	18:05	20

s98314_004 DATA REPORT

TABLE DESCRIPTION:
Specific Conductance data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker. nm = not measured.

ROW#	Q	SPECIFIC CONDUCTANCE µS/cm	LOCATION	TIME	SOLUTION TEMPERATURE ^oC
1	Y	303	UE-25 WT #3	16:20	31
2	Y	287	UE-25 WT #3	16:55	29.5
3	Y	nm	UE-25 WT #3	17:17	30.5
4	Y	290	UE-25 WT #3	17:30	30
5	Y	286	UE-25 WT #3	17:47	30
6	Y	297	UE-25 WT #3	18:05	31.5

s98314_002 DATA REPORT

TABLE DESCRIPTION:
Eh data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker.

ROW#	Q	EH mV	LOCATION	TIME	SOLUTION TEMPERATURE ^oC
1	Y	264	UE-25 WT #3	16:20	31
2	Y	278	UE-25 WT #3	16:55	29.5
3	Y	268	UE-25 WT #3	17:17	30.5
4	Y	268	UE-25 WT #3	17:30	30
5	Y	272	UE-25 WT #3	17:47	30
6	Y	268	UE-25 WT #3	18:05	31.5

s98314_007 DATA REPORT

TABLE DESCRIPTION:
Total Iron data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker. Temperature is air temperature. nm = not measured.

ROW#	Q	TOTAL IRON mg/L	LOCATION	TIME	TEMPERATURE ^oC
1	Y	nm	UE-25 WT #3	16:20	17.5
2	Y	0	UE-25 WT #3	16:55	18.5
3	Y	nm	UE-25 WT #3	17:17	19.3
4	Y	nm	UE-25 WT #3	17:30	20
5	Y	nm	UE-25 WT #3	17:47	20
6	Y	nm	UE-25 WT #3	18:05	20

s98314_006 DATA REPORT

TABLE DESCRIPTION:
Nitrate Abundance data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker. Temperature is air temperature. nm = not measured.

ROW#	Q	NITRATE ABUNDAN	LOCATION	TIME	TEMPERATURE

		CE mg/L			^oC
1	Y	3.3	UE-25 WT #3	16:20	17.5
2	Y	3.1	UE-25 WT #3	16:55	18.5
3	Y	3.1	UE-25 WT #3	17:17	19.3
4	Y	nm	UE-25 WT #3	17:30	20
5	Y	nm	UE-25 WT #3	17:47	20
6	Y	3.3	UE-25 WT #3	18:05	20

s98314_005 DATA REPORT

TABLE DESCRIPTION:
Nitrite Abundance data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker. Temperature is air temperature. nm = not measured.

ROW#	Q	NITRITE ABUNDANCE mg/L	LOCATION	TIME	TEMPERATURE ^oC
1	Y	0	UE-25 WT #3	16:20	17.5
2	Y	0	UE-25 WT #3	16:55	18.5
3	Y	nm	UE-25 WT #3	17:17	19.3
4	Y	nm	UE-25 WT #3	17:30	20
5	Y	0	UE-25 WT #3	17:47	20
6	Y	nm	UE-25 WT #3	18:05	20

s98314_001 DATA REPORT

TABLE DESCRIPTION:
Dissolved Oxygen Abundance data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker.

ROW#	Q	OXYGEN ABUNDANCE mg/L	LOCATION	TIME	SOLUTION TEMPERATURE ^oC
1	Y	3.8	UE-25 WT #3	16:20	31
2	Y	5	UE-25 WT #3	16:55	29.5
3	Y	4.8	UE-25 WT #3	17:17	30.5
4	Y	5.2	UE-25 WT #3	17:30	30
5	Y	5.2	UE-25 WT #3	17:47	30
6	Y	5	UE-25 WT #3	18:05	31.5

s98314_003 DATA REPORT

TABLE DESCRIPTION:
pH data of pumped water from UE-25 WT #3, 02/05/1998 to 09/09/1998.

TDIF: 307217

DTN: LAAM831311AQ98.006

FOOTNOTES: The data are static field measurements in an open beaker.

ROW#	Q	PH	LOCATION	TIME	SOLUTION TEMPERATURE ^oC
1	Y	7.6	UE-25 WT #3	16:20	31
2	Y	7.38	UE-25 WT #3	16:55	29.5
3	Y	7.25	UE-25 WT #3	17:17	30.5
4	Y	7.39	UE-25 WT #3	17:30	30
5	Y	7.32	UE-25 WT #3	17:47	30
6	Y	7.41	UE-25 WT #3	18:05	31.5

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s98316_001 DATA REPORT

TABLE DESCRIPTION:
Flow-thru cell and static measurements of water from UE-25 WT #3, 06/22/1998.

TDIF: 307218

DTN: LAAM831311AQ98.007

FOOTNOTES: In the Oxygen Abundance, Eh, pH, Specific Conductance, and Solution Temperature columns analysis made on flow-thru samples as they flowed directly from the pump outlet through a cell, so as to avoid contact with air during the analysis; in all other columns, analyses that were made on static samples which were collected from the pump outlet and analyzed in an open container. Oxygen abundance is dissolved oxygen. Solution Temperature is attributal to Oxygen Abundance, Eh, pH, and Specific Conductance. Temperature is air temperature and is attributal to all other columns. Alkalinity as CaCO3. nm = not measured. Iron + 2 (Ferrous Iron) is attributal to Total Iron only.

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ROW#	Q	LOCATION	DEPTH ft	OXYGEN mg/L	EH mV	PH	SPEC. CONDUCT.	SOLUTION TEMP.	TEMPERATURE
1	Y	UE-25 WT #3	1222	5.6	307	7.61	290	31.6	29
2	Y	UE-25 WT #3	1320	6.5	327	7.55	291	32.9	nm
3	Y	UE-25 WT #3	1422	6.4	345	7.33	290	33	nm
4	Y	UE-25 WT #3	1451	6.4	275	7.4	291	32.9	nm
5	Y	UE-25 WT #3	1500	6.3	273	7.37	291	33	nm
6	Y	UE-25 WT #3	1515	3.7	356	7.14	291	32.8	nm
7	Y	UE-25 WT #3	1520	nm	nm	nm	nm	nm	nm
8	Y	UE-25 WT #3	1522	4.4	422	7.16	291	32.8	nm

ROW#	Q	LOCATION	DEPTH ft	NITRITE ABUND. mg/L	NITRATE ABUND. mg/L	TOTAL IRON mg/L	IRON+2 mg/L	MANGANESE ABUND. mg/L	ALKALINITY mg/L

1	Y	UE-25 WT #3	1222	0.003	5.28	0.15	0	0.005	88
2	Y	UE-25 WT #3	1320	0	3.96	0.09	0.01	0.007	90
3	Y	UE-25 WT #3	1422	0.007	5.28	0.05	0.01	0.004	87
4	Y	UE-25 WT #3	1451	nm	nm	nm	nm	nm	nm
5	Y	UE-25 WT #3	1500	nm	nm	nm	nm	nm	nm
6	Y	UE-25 WT #3	1515	nm	nm	nm	nm	nm	nm
7	Y	UE-25 WT #3	1520	0	7.04	0.03	0	0	88
8	Y	UE-25 WT #3	1522	nm	nm	nm	nm	nm	nm

s98317_001 DATA REPORT

TABLE DESCRIPTION:
Analysis of bailed samples from UE-25 WT #17, 06/04/1998.

TDIF: 307219

DTN: LAAM831311AQ98.008

FOOTNOTES: Data values are static field measurements in an open beaker. Oxygen Abundance is dissolved oxygen. Solution Temperature is attributal to Oxygen Abundance, Eh, pH, and Specific Conductance. Temperature is air temperature . Iron + 2 (Ferrous Iron) is attributal to Total Iron only. Alkalinity as CaCO3. nm indicates not measured.

****

ROW#	Q	LOCATION	DEPTH ft	OXYGEN ABUND. mg/L	EH mV	PH	SPEC. COND. microSiemens per cm	SOLUTION TEMP. Centigrade	TEMPERATURE Centigrade
1	Y	UE-25 WT#17	1306	1.5	147	6.96	nm	nm	nm
2	Y	UE-25 WT#17	1350	0	46	7.03	nm	nm	nm

ROW#	Q	LOCATION	DEPTH	NITRITE ABUND.	NITRATE ABUND.	TOTAL IRON	IRON+2	MANGANESE ABUND.	ALKALINITY

				ft	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
1	Y	UE-25	WT#17	1306	0	0	4	0.79	0	nm
2	Y	UE-25	WT#17	1350	0.053	0	4	1.62	nm	nm

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Yucca Mountain Site Characterization Project
Technical Data Management

View Unit Descriptions

s98318_003 DATA REPORT

TABLE DESCRIPTION:
Specific Conductance data from flow-thru cell measurements of pumped water samples from UE-25 WT #17, 07/01/1998 to 09/08/1998.

TDIF: 307220

DTN: LAAM831311AQ98.009

FOOTNOTES: Time is flow-thru time. In the Condition column, Flow-thru = flow-thru cell, static = measurement in open beaker. Solution Temperature is pH probe. nm = not measured.

ROW#	Q	SPECIFIC CONDUCTANCE µS/cm	LOCATION	TIME	SOLUTION TEMPERATURE °C	CONDITION
1	Y	368	UE-25 WT #17	10:48	27.3	Flow-thru
2	Y	353	UE-25 WT #17	10:54	27.5	Flow-thru
3	Y	346	UE-25 WT #17	11:00	27.8	Flow-thru
4	Y	344	UE-25 WT #17	11:05	28.3	Flow-thru
5	Y	336	UE-25 WT #17	11:15	28.7	Flow-thru
6	Y	335	UE-25 WT #17	11:25	29.1	Flow-thru
7	Y	327	UE-25 WT #17	11:30	29.1	Flow-thru
8	Y	318	UE-25 WT #17	11:40	29.1	Flow-thru
9	Y	309	UE-25 WT #17	11:50	29.0	Flow-thru
10	Y	307	UE-25 WT #17	12:00	29.5	Flow-thru
11	Y	305	UE-25 WT #17	12:12	28.3	Flow-thru
12	Y	nm	UE-25 WT #17	12:12	nm	Static
13	Y	305	UE-25 WT #17	12:21	28.2	Flow-thru
14	Y	306	UE-25 WT #17	12:27	28.2	Flow-thru
15	Y	302	UE-25 WT #17	12:42	28.3	Flow-thru

16	Y	299		UE-25 WT #17	13:00	28.7
17	Y	293	Flow-thru	UE-25 WT #17	13:25	28.8
18	Y	288	Flow-thru	UE-25 WT #17	13:47	28.6
19	Y	285	Flow-thru	UE-25 WT #17	14:00	28.6
20	Y	285	Flow-thru	UE-25 WT #17	14:15	28.6
21	Y	285	Flow-thru	UE-25 WT #17	14:30	28.6
22	Y	284	Flow-thru	UE-25 WT #17	14:45	29.0
23	Y	283	Flow-thru	UE-25 WT #17	15:00	29.5
24	Y	290	Flow-thru	UE-25 WT #17	15:15	29.6
25	Y	283	Flow-thru	UE-25 WT #17	15:30	29.7
26	Y	284	Flow-thru	UE-25 WT #17	15:45	29.7

s98318_002 DATA REPORT

TABLE DESCRIPTION:
Eh data from flow-thru cell measurements of pumped water samples from UE-25 WT #17, 07/01/1998 to 09/08/1998.

TDIF: 307220

DTN: LAAM831311AQ98.009

FOOTNOTES: Time is flow-thru analysis time. In the Condition column, Flow-thru = flow-thru cell, static = measurement in open beaker. Solution Temperature is pH probe. nm = not measured.

****

ROW#	Q	EH mV	LOCATION	TIME	SOLUTION TEMPERATURE °C	CONDITION
1	Y	-34	UE-25 WT #17	10:48	27.3	Flow-thru
2	Y	-33	UE-25 WT #17	10:54	27.5	Flow-thru
3	Y	-34	UE-25 WT #17	11:00	27.8	Flow-thru
4	Y	-38	UE-25 WT #17	11:05	28.3	Flow-thru
5	Y	-43	UE-25 WT #17	11:15	28.7	Flow-thru
6	Y	-40	UE-25 WT #17	11:25	29.1	Flow-thru
7	Y	-43	UE-25 WT #17	11:30	29.1	Flow-thru
8	Y	-55	UE-25 WT #17	11:40	29.1	Flow-thru
9	Y	-60	UE-25 WT #17	11:50	29.0	Flow-thru
10	Y	-56	UE-25 WT #17	12:00	29.5	Flow-thru

11	Y	-52	UE-25 WT #17	12:12	28.3	Flow-thru
12	Y	nm	UE-25 WT #17	12:12	nm	Static
13	Y	-60	UE-25 WT #17	12:21	28.2	Flow-thru
14	Y	-65	UE-25 WT #17	12:27	28.2	Flow-thru
15	Y	-65	UE-25 WT #17	12:42	28.3	Flow-thru
16	Y	-58	UE-25 WT #17	13:00	28.7	Flow-thru
17	Y	-48	UE-25 WT #17	13:25	28.8	Flow-thru
18	Y	-40	UE-25 WT #17	13:47	28.6	Flow-thru
19	Y	-34	UE-25 WT #17	14:00	28.6	Flow-thru
20	Y	-35	UE-25 WT #17	14:15	28.6	Flow-thru
21	Y	-40	UE-25 WT #17	14:30	28.6	Flow-thru
22	Y	-35	UE-25 WT #17	14:45	29.0	Flow-thru
23	Y	-35	UE-25 WT #17	15:00	29.5	Flow-thru
24	Y	-39	UE-25 WT #17	15:15	29.6	Flow-thru
25	Y	-33	UE-25 WT #17	15:30	29.7	Flow-thru
26	Y	-23	UE-25 WT #17	15:45	29.7	Flow-thru

s98318_004 DATA REPORT

TABLE DESCRIPTION:
Dissolved Oxygen Abundance data from flow-thru cell measurements of pumped water samples from UE-25 WT #17, 07/01/1998 to 09/08/1998.

TDIF: 307220

DTN: LAAM831311AQ98.009

FOOTNOTES: Time is flow-thru analysis time. In the Condition column, Flow-thru = flow-thru cell, static = measurement in open beaker. Solution Temperature is pH probe. nm = not measured.

ROW#	Q	OXYGEN ABUNDANCE mg/L	LOCATION	TIME	SOLUTION TEMPERATURE °C	CONDITION
1	Y	0.0	UE-25 WT #17	10:48	27.3	Flow-thru
2	Y	0.0	UE-25 WT #17	10:54	27.5	Flow-thru
3	Y	0.0	UE-25 WT #17	11:00	27.8	Flow-thru
4	Y	0.0	UE-25 WT #17	11:05	28.3	Flow-thru

5	Y	0.0	UE-25 WT #17	11:15	28.7	Flow-thru
6	Y	0.0	UE-25 WT #17	11:25	29.1	Flow-thru
7	Y	0.0	UE-25 WT #17	11:30	29.1	Flow-thru
8	Y	0.0	UE-25 WT #17	11:40	29.1	Flow-thru
9	Y	0.0	UE-25 WT #17	11:50	29.0	Flow-thru
10	Y	0.0	UE-25 WT #17	12:00	29.5	Flow-thru
11	Y	0.0	UE-25 WT #17	12:12	28.3	Flow-thru
12	Y	nm	UE-25 WT #17	12:12	nm	Static
13	Y	0.0	UE-25 WT #17	12:21	28.2	Flow-thru
14	Y	0.0	UE-25 WT #17	12:27	28.2	Flow-thru
15	Y	0.0	UE-25 WT #17	12:42	28.3	Flow-thru
16	Y	0.0	UE-25 WT #17	13:00	28.7	Flow-thru
17	Y	0.0	UE-25 WT #17	13:25	28.8	Flow-thru
18	Y	0.0	UE-25 WT #17	13:47	28.6	Flow-thru
19	Y	0.0	UE-25 WT #17	14:00	28.6	Flow-thru
20	Y	0.0	UE-25 WT #17	14:15	28.6	Flow-thru
21	Y	0.0	UE-25 WT #17	14:30	28.6	Flow-thru
22	Y	0.0	UE-25 WT #17	14:45	29.0	Flow-thru
23	Y	0.0	UE-25 WT #17	15:00	29.5	Flow-thru
24	Y	0.0	UE-25 WT #17	15:15	29.6	Flow-thru
25	Y	0.0	UE-25 WT #17	15:30	29.7	Flow-thru
26	Y	0.0	UE-25 WT #17	15:45	29.7	Flow-thru

s98318_001 DATA REPORT

TABLE DESCRIPTION:
pH data from flow-thru cell measurements of pumped water samples from UE-25 WT #17, 07/01/1998 to 09/08/1998.

TDIF: 307220

DTN: LAAM831311AQ98.009

FOOTNOTES: Time is flow-thru analysis time. Solution Temperature is pH probe. In the Condition column, Flow-thru = flow-thru cell, static = measurement in open beaker. nm = not measured.

****

ROW#	Q	PH	LOCATION	TIME	SOLUTION TEMPERATURE °C	CONDITION

****

1	Y	6.72	UE-25 WT #17	10:48	27.3	Flow-thru
2	Y	6.68	UE-25 WT #17	10:54	27.5	Flow-thru
3	Y	6.66	UE-25 WT #17	11:00	27.8	Flow-thru
4	Y	6.64	UE-25 WT #17	11:05	28.3	Flow-thru
5	Y	6.62	UE-25 WT #17	11:15	28.7	Flow-thru
6	Y	6.57	UE-25 WT #17	11:25	29.1	Flow-thru
7	Y	6.57	UE-25 WT #17	11:30	29.1	Flow-thru
8	Y	6.52	UE-25 WT #17	11:40	29.1	Flow-thru
9	Y	6.53	UE-25 WT #17	11:50	29.0	Flow-thru
10	Y	6.51	UE-25 WT #17	12:00	29.5	Flow-thru
11	Y	6.45	UE-25 WT #17	12:12	28.3	Flow-thru
12	Y	7.14	UE-25 WT #17	12:12	nm	Static
13	Y	6.48	UE-25 WT #17	12:21	28.2	Flow-thru
14	Y	6.46	UE-25 WT #17	12:27	28.2	Flow-thru
15	Y	6.48	UE-25 WT #17	12:42	28.3	Flow-thru
16	Y	6.40	UE-25 WT #17	13:00	28.7	Flow-thru
17	Y	6.36	UE-25 WT #17	13:25	28.8	Flow-thru
18	Y	6.26	UE-25 WT #17	13:47	28.6	Flow-thru
19	Y	6.17	UE-25 WT #17	14:00	28.6	Flow-thru
20	Y	6.13	UE-25 WT #17	14:15	28.6	Flow-thru
21	Y	6.07	UE-25 WT #17	14:30	28.6	Flow-thru
22	Y	6.06	UE-25 WT #17	14:45	29.0	Flow-thru
23	Y	6.07	UE-25 WT #17	15:00	29.5	Flow-thru
24	Y	6.11	UE-25 WT #17	15:15	29.6	Flow-thru
25	Y	6.13	UE-25 WT #17	15:30	29.7	Flow-thru
26	Y	6.12	UE-25 WT #17	15:45	29.7	Flow-thru

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s98319_001 DATA REPORT

TABLE DESCRIPTION:
Static measurement data for samples from UE-25 WT #17, 07/01/1998.

TDIF: 307221

DTN: LAAM831311AQ98.010

FOOTNOTES: Oxygen Abundance is dissolved oxygen. Temperature is air temperature. Iron + 2 (Ferrous Iron) is attributal to Total Iron only. Alkalinity as CaCO3. nm indicates not measured. OR indicates Over Range.

****

ROW#	Q	LOCATION	DEPTH ft	OXYGEN ABUND. mg/L	EH mV	PH	SPEC. COND.	SOLUTION TEMP. Centigrade	TEMPERATURE Centigrade
1	Y	UE-25 WT #17	922	nm	nm	nm	nm	nm	nm
2	Y	UE-25 WT #17	922	nm	nm	nm	nm	nm	nm
3	Y	UE-25 WT #17	922	nm	nm	nm	nm	nm	nm
4	Y	UE-25 WT #17	930	0	10	6.46	353	27	nm
5	Y	UE-25 WT #17	1052	0	nm	nm	nm	nm	nm
6	Y	UE-25 WT #17	1352	nm	nm	nm	nm	nm	nm
7	Y	UE-25 WT #17	1352	nm	nm	nm	nm	nm	nm
8	Y	UE-25 WT #17	1445	nm	nm	nm	nm	nm	nm
9	Y	UE-25 WT #17	1520	nm	nm	nm	nm	nm	nm

ROW#	Q	LOCATION	DEPTH	NITRITE ABUND.	NITRATE ABUND.	TOTAL IRON	IRON+2	MANGANESE ABUND.	ALKALINITY	COMMENTS

			ft	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	
1	Y	UE-25 WT #17	922	0	0	OR	OR	0.52	nm	
2	Y	UE-25 WT #17	922	0	0	3.3	1.4	0.44	110	Sample filtered and diluted
3	Y	UE-25 WT #17	922	nm	nm	3.14	0.55	nm	87	Sample filtered
4	Y	UE-25 WT #17	930	nm	nm	nm	nm	nm	nm	
5	Y	UE-25 WT #17	1052	0.03	0.31	0.13	0.07	0.64	116	Sample filtered
6	Y	UE-25 WT #17	1352	0.02	0.88	0.25	0.17	0.41	88	Sample filtered
7	Y	UE-25 WT #17	1352	nm	nm	8.8	2.3	nm	nm	Sample diluted
8	Y	UE-25 WT #17	1445	0.03	2.42	0.29	0.27	0.37	84	Sample filtered
9	Y	UE-25 WT #17	1520	0.04	2.59	0.43	0.43	0.35	88	Sample filtered

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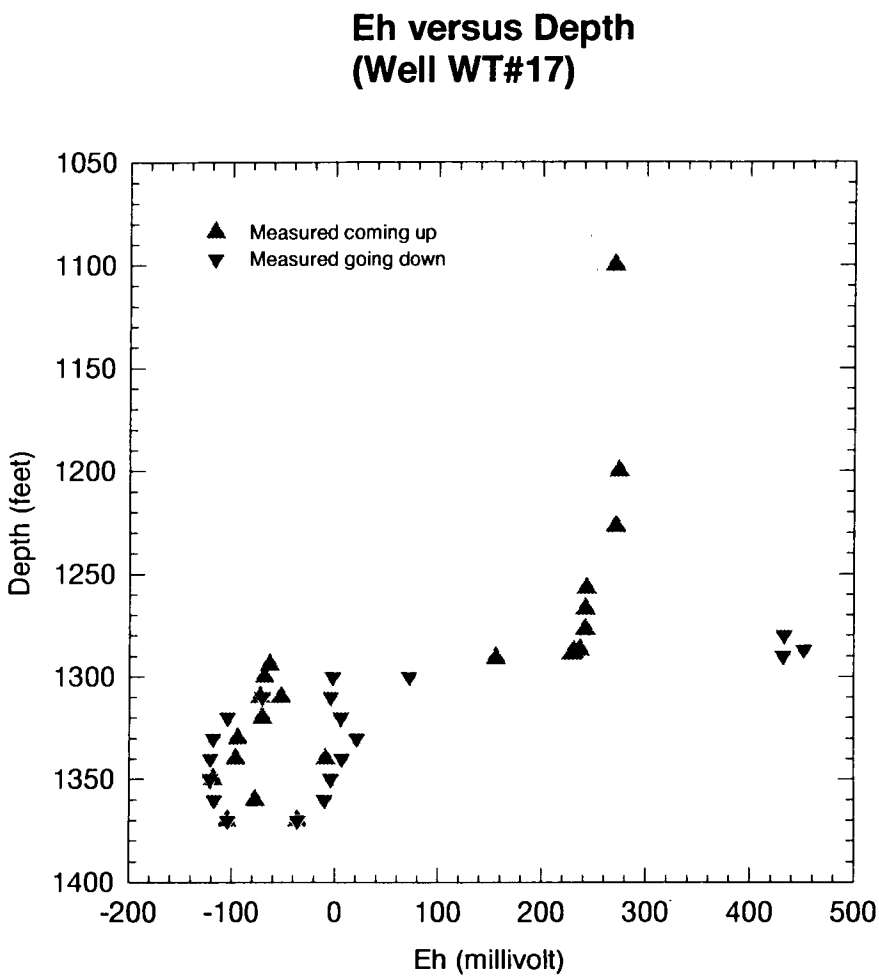
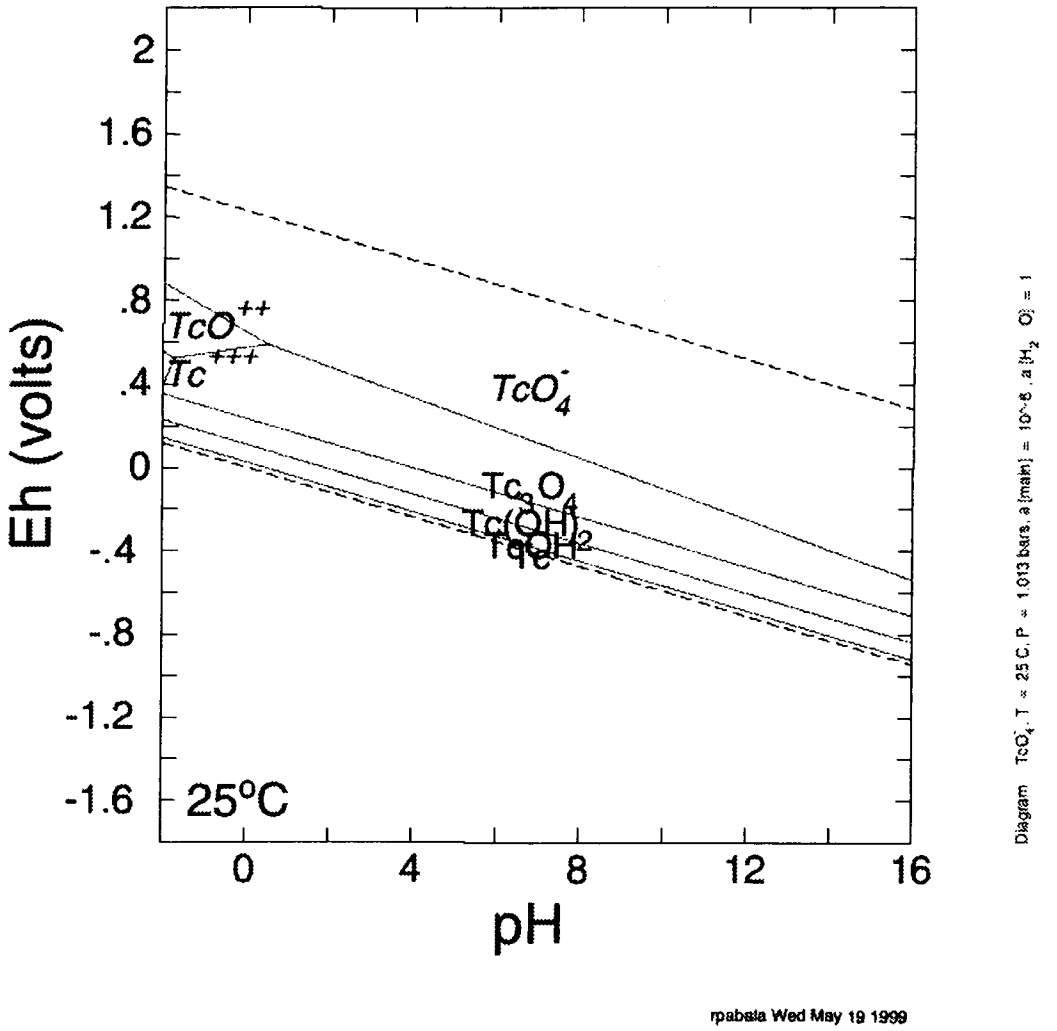
The following plots Eh versus depth for well WT#17. Data were taken from the s98312_001 data report listed on page 197 to 199. The pH values measured for WT#17 ranged from 6.27 to 7.38; temperatures ranged from 29.7 to 33.6 C.



Below about 1275 ft, there is a steep redox gradient that indicates reducing conditions at depth. These conditions could influence the solubility and retardation of multivalent radionuclides, such as Tc-99.

Below is an Eh-pH diagram for the technetium system at a technetium activity equal to 10E-6 molal, temperature of 25 C, and pressure of 1 atm. The figure was calculated using GWB and the EQ3 V8.R6 database.



The Eh-pH diagram and the Eh data from Well WT#17 indicate that reduction of Tc from +7 to +4 state could occur, thereby reducing the mobility of technetium in YM groundwater.

The following is the GWB Act2.output file for the Eh-pH calculation. The thermo.dat file indicates that the technetiumt thermodynamic data came from (i) Rard, J.A., 1983, Critical review of the chemistry and thermodynamics of technetium and some of its inorganic compounds and aqueous species: LLNL, UCRL-53440, 86p.; and (ii) Rard, J.A., 1984, Errata sheet to UCRL-53440: Unpub. note, 1p.

:

--Output from Act2 activity-activity diagram generator--

Temperature is 25 C; Pressure is 1.013 bars

pH plotted on the X axis from -2 to 16
Eh (volts) (swapped for O2(aq)) plotted on the Y axis from -1.8 to 2.2

Stability limits of water

Reaction	Log K	Equation
H2(g) = 2*e- + 2*H+	-.000351	Y =-.05916 *X - .0001556
O2(g) + 4*e- + 4*H+ = 2*H2O	83.11	Y =-.05916 *X + 1.229

Calculating diagram for TcO4-

Basis species	Activity/Fugacity	
TcO4-	1e-8	(main species)
H2O	1	(solvent)
e-	-on Y-axis-	
H+	-on X-axis-	

Species and minerals in main system

	Activity	Reaction	Log K
TcO4-	1e-8	TcO4- = TcO4-	0.0000
Tc+++	1e-8	Tc+++ + 4*H2O = TcO4- + 4*e- + 8*H+	-38.3899
TcO++	1e-8	TcO++ + 3*H2O = TcO4- + 3*e- + 6*H+	-32.9970
TcO4--	1e-8	TcO4-- = TcO4- + e-	10.3187
TcO4---	1e-8	TcO4--- = TcO4- + 2*e-	20.2869
(TcO(OH)2)2(aq)	5e-9	(TcO(OH)2)2(aq) + 2*H2O = 2*TcO4- + 6*e- + 8*H+	-65.8669
H2TcO4(aq)	1e-8	H2TcO4(aq) = TcO4- + e- + 2*H+	1.3138
HTcO4-	1e-8	HTcO4- = TcO4- + e- + H+	1.6116
TcO(OH)2(aq)	1e-8	TcO(OH)2(aq) + H2O = TcO4- + 3*e- + 4*H+	-29.6749
TcOOH+	1e-8	TcOOH+ + 2*H2O = TcO4- + 3*e- + 5*H+	-31.8615
HTcO4	1	HTcO4 = TcO4- + H+	5.9566
Tc	1	Tc + 4*H2O = TcO4- + 7*e- + 8*H+	-56.9257
Tc(OH)2	1	Tc(OH)2 + 2*H2O = TcO4- + 5*e- + 6*H+	-54.6195
Tc(OH)3	1	Tc(OH)3 + H2O = TcO4- + 4*e- + 5*H+	-47.6324
Tc2O7	1	Tc2O7 + H2O = 2*TcO4- + 2*H+	13.1077
Tc3O4	1	Tc3O4 + 8*H2O = 3*TcO4- + 13*e- + 16*H+	-155.8978
Tc4O7	1	Tc4O7 + 9*H2O = 4*TcO4- + 14*e- + 18*H+	-168.7887

```
  TcO2:2H2O(am)     1          TcO2:2H2O(am)  = TcO4-  + 3*e-  + 4*H+                    -
37.2289
  TcO3              1          TcO3  + H2O  = TcO4-  + e-  + 2*H+                          -
12.8296
  TcOH              1          TcOH  + 3*H2O  = TcO4-  + 6*e-  + 7*H+                      -
56.4909
  Tc2O7(g)          1.013      Tc2O7(g)  + H2O  = 2*TcO4-  + 2*H+
21.3593
 ---------------------------------------------------------------------------------------------
------
```

Solid-Aqueous Diagram

	pH(1)	Eh (vo(1)	pH(2)	Eh (vo(2)	Equation	Type
TcO4-	-2.000	0.887	1.109	0.520	2	Lower
	1.109	0.520	16.000	-0.565	15	Lower
Tc+++	-2.000	0.556	-1.134	0.453	21	Upper
	-2.000	0.250	-1.416	0.319	31	Lower
	-1.416	0.319	-1.134	0.453	34	Lower
TcO++	-2.000	0.887	1.109	0.520	2	Upper
	-2.000	0.556	-1.134	0.453	21	Lower
	-1.134	0.453	1.109	0.520	52	Lower
Tc	-2.000	0.144	16.000	-0.921	173	Upper
Tc(OH)2	-2.000	0.250	-1.416	0.319	31	Upper
	-1.416	0.319	16.000	-0.711	177	Upper
	-2.000	0.229	16.000	-0.836	181	Lower
Tc3O4	-1.416	0.319	-1.134	0.453	34	Upper
	-1.134	0.453	1.109	0.520	52	Upper
	1.109	0.520	16.000	-0.565	15	Upper
	-1.416	0.319	16.000	-0.711	177	Lower
TcOH	-2.000	0.229	16.000	-0.836	181	Upper
	-2.000	0.144	16.000	-0.921	173	Lower

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5/21/99

The following figure are the speciation and mineral saturation for a uranium(6+) solution calculated using GWB. The run conditions are:

Temperature is 25 C

Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat

Working directory: d:\

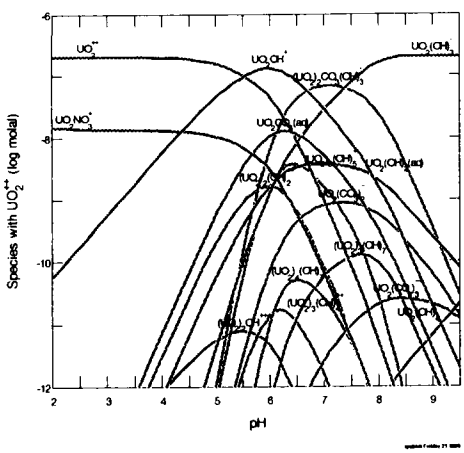
Options: Debye-Huckel

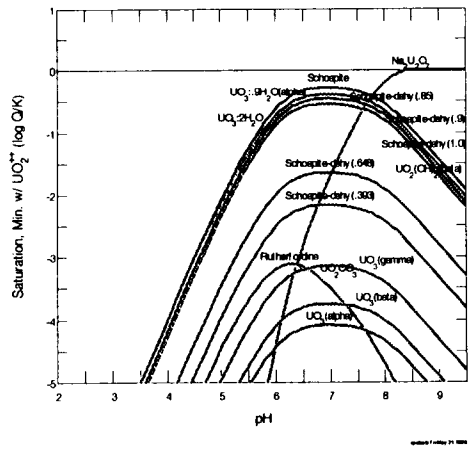
Basis is:

H2O	1 kg solvent
O2(g) (swapped for O2(aq))	fugacity = .2
CO2(g) (swapped for HCO3-)	fugacity = .000316227766
NO3- (swapped for NH3(aq))	total molality = 4.2e-7 (charge balance)
UO2++	total molality = 2.1e-7
Na+	total molality = .1
H+	pH = 2

Reactants:

Slide pH to 10





Note that the above calculations and results are the same as those presented as calculation #7 on page 146 and 147. The output file for the GWB run indicates that fCO2(g) for each run step was not fixed; actually fCO2(g) decreased with each step. **The total number of moles of carbon, however, was the same for all time steps. Thus, GWB operates differently from runs in which a single speciation calculation is done at a fixed pH and fixed fCO2. Using the "slide" capability gives different results, UNLESS fCO2 IS EXPLICITLY FIXED.**

To demonstrate the difference between using the "fix" option and not using it, another calculation was done as in the previous one, but specifying "fix f CO2(g)". The run conditions are as follows:

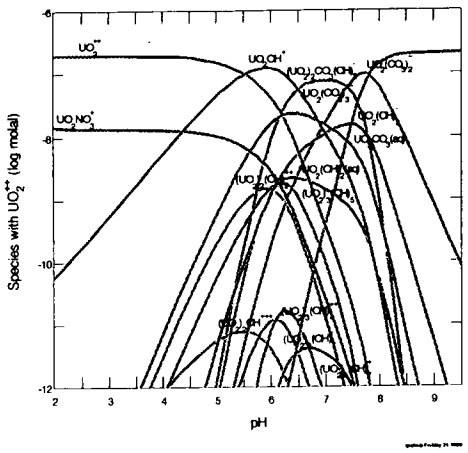
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\
Options: Debye-Huckel

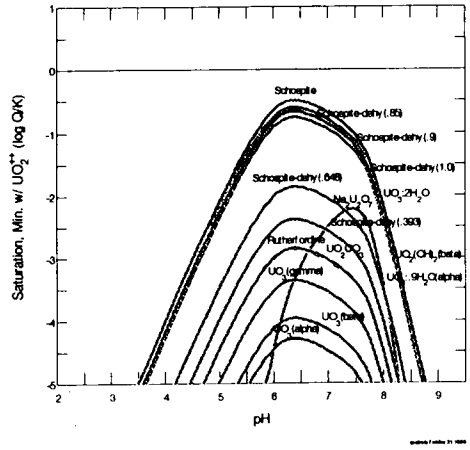
Basis is:

H2O	1 kg solvent
O2(g) (swapped for O2(aq))	fugacity = .2
CO2(g) (swapped for HCO3-)	fugacity = .000316227766
NO3- (swapped for NH3(aq))	total molality = 4.2e-7 (charge balance)
UO2++	total molality = 2.1e-7
Na+	total molality = .1
H+	pH = 2

Reactants:
Slide pH to 10
Fix fugacity of CO2(g)

The resulting speciation and mineral saturation are as follows:





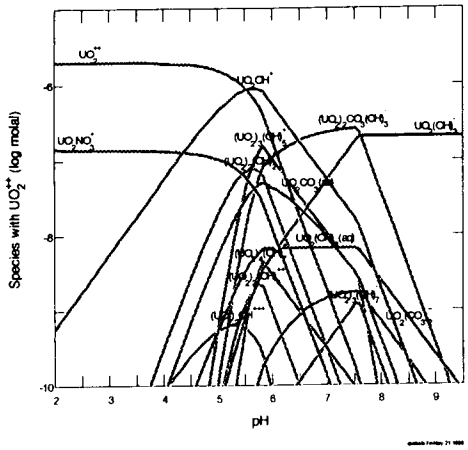
A calculation was done for the following conditions:

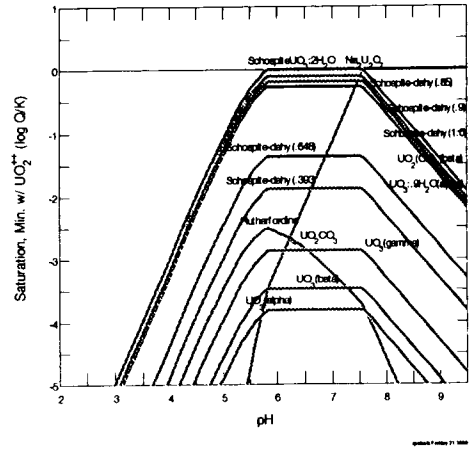
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\
Options: Debye-Huckel

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
CO2(g) (swapped for HCO3-) fugacity = .000316227766
NO3- (swapped for NH3(aq)) total molality = 4.2e-6 (charge balance)
UO2++ total molality = 2.1e-6
Na+ total molality = .1
H+ pH = 2

Reactants:
Slide pH to 10

Note the thermo.dat file that uses a lower stability constant for UO2(OH)2(aq) neutral species was used in the calculations. The resulting speciation and mineral saturation are:





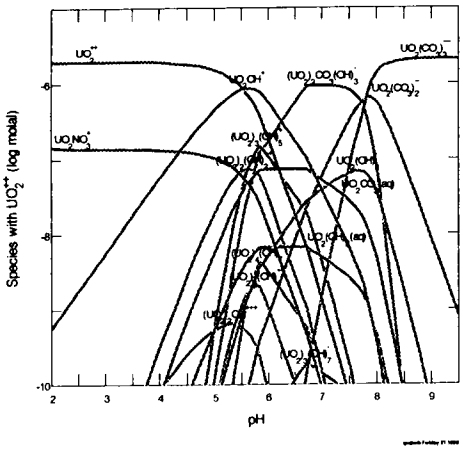
Another calculation that explicitly specified a fixed CO2 fugacity was run. The run conditions were:

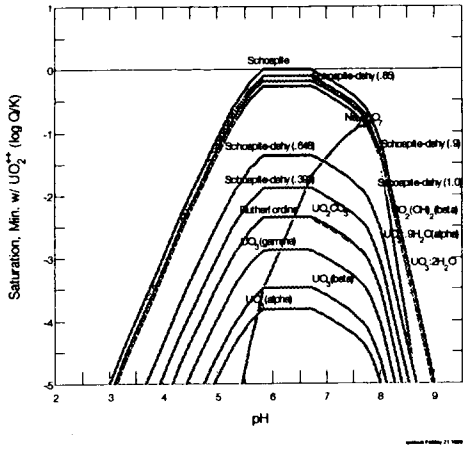
Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\DTurner\thermo.dat
Working directory: d:\
Options: Debye-Huckel

Basis is:
H2O 1 kg solvent
O2(g) (swapped for O2(aq)) fugacity = .2
CO2(g) (swapped for HCO3-) fugacity = .000316227766
NO3- (swapped for NH3(aq)) total molality = 4.2e-6 (charge balance)
UO2++ total molality = 2.1e-6
Na+ total molality = .1
H+ pH = 2

Reactants:
Slide pH to 10
Fix fugacity of CO2(g)

The resulting speciation and mineral saturation are :





Entries into Scientific Notebook No. 278 for the period April 1, 1999, to June 30, 1999, have been made by

7/16/99

Roberto T. Pabalan / Date

No original entry into this Scientific Notebook has been removed.