S/N 185E

ELECTRIC SCIENTIFIC NOTEBOOK # 185E

ELECTRIC
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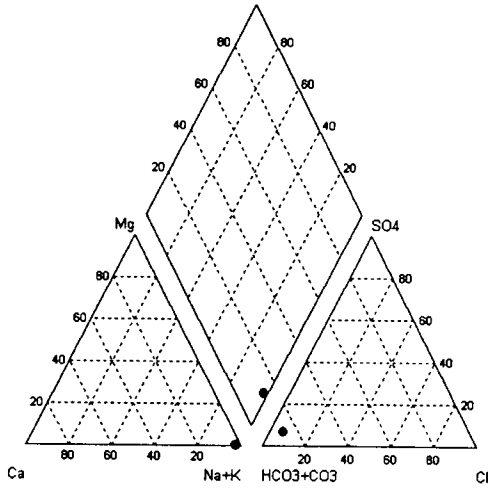
185E

VOL. 10

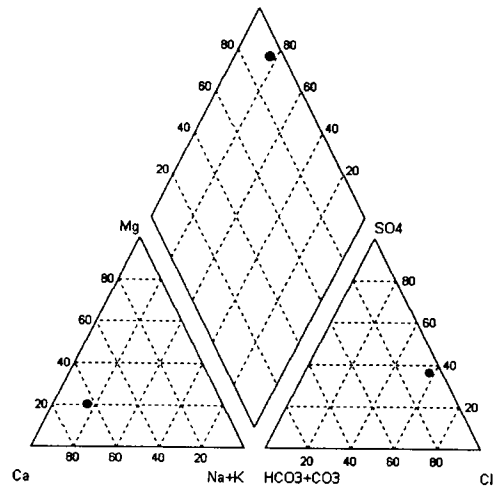
The entries in this electronic scientific notebook #185, Volume 10, document activities conducted during the Period September 14, 2001, through March 17, 2002, under the Evolution of the Near-field Environment Key Technical Issue (Project Number 20-1402-561).

September 25, 2001

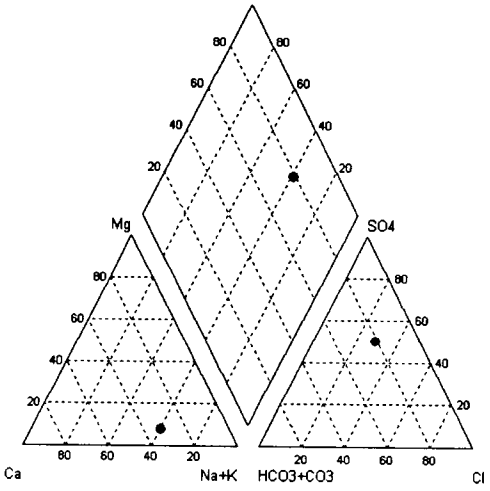
As indicated in scientific notebook #185 Volume 9, page 104, five Yucca Mountain groundwater compositions were selected for simulation of evaporation processes using the OLI ESP software. The compositions of the selected YM waters, listed previously in Volume 9, are also listed in the next page of this scientific notebook. Four of the listed waters are porewaters (see notebook #185 Vol. 9), and the fifth is the average J-13 well water composition reported by Harrar (1990). The OLI simulation was conducted by L. Yang and was documented in his scientific notebook.



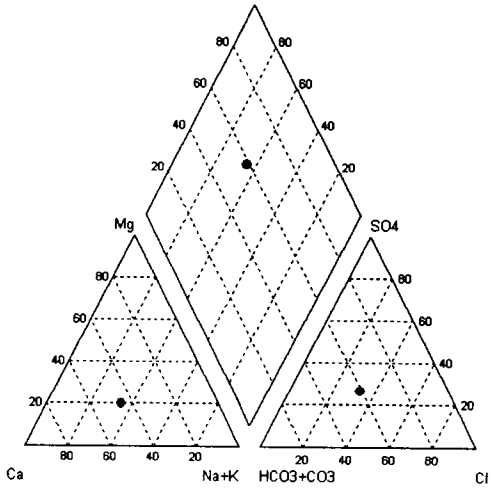
UZ-14/1542.3-1542.8



NRG-6/158.2-158.6



NRG-6/244.6-245.0



UZ-14/85.2-85.6

Yucca Mountain groundwaters selected for simulation of evaporation processes using the OLI ESP software.

Species	units	UZ-14/1542.3-1542.8	UZ-14/85.2-85.6	NRG-6/158.2-158.6
Ca^{2+}	mg/L	3.6	49.9	122
Mg^{2+}	mg/L	0.5	13.2	23.3
Na^{+}	mg/L	207	43.5	35.6
SiO_2(aq)	mg/L	143	89.8	97.4
Al^{3+}	mg/L	13.80	0.30	0.00
HCO_3^-	mg/L	384	131	34
CO_3^{2-}	mg/L	46	0	0
Cl^-	mg/L	20	60	185
NO_3^-	mg/L	4	22	32
SO_4^{2-}	mg/L	28	66	159
pH		8.6	6.9	6.8
charge bal.		1.02%	-0.91%	-0.26%
water type		Na-HCO3	Ca-Na-HCO3-Cl-SO4	Ca-Mg-Cl-SO4

Species	units	NRG-6/244.6-245.0	Average J13
Ca^{2+}	mg/L	33	13.00
Mg^{2+}	mg/L	4.9	2.01
Na^{+}	mg/L	72	45.80
K^{+}	mg/L		5.04
SiO_2(aq)	mg/L	51	61
Al^{3+}	mg/L	0.60	0
HCO_3^-	mg/L	61	128.90
CO_3^{2-}	mg/L	0	0
Cl^-	mg/L	49	7.14
NO_3^-	mg/L	40	8.78
SO_4^{2-}	mg/L	115	18.40
F^-	mg/L	na	2.18
pH		7.2	7.41
charge bal.		-2.26%	-0.31%
Water type		Na-Ca-SO4-Cl	Na-Ca-HCO3

The following table lists the results of L.Yang's OLI simulations:

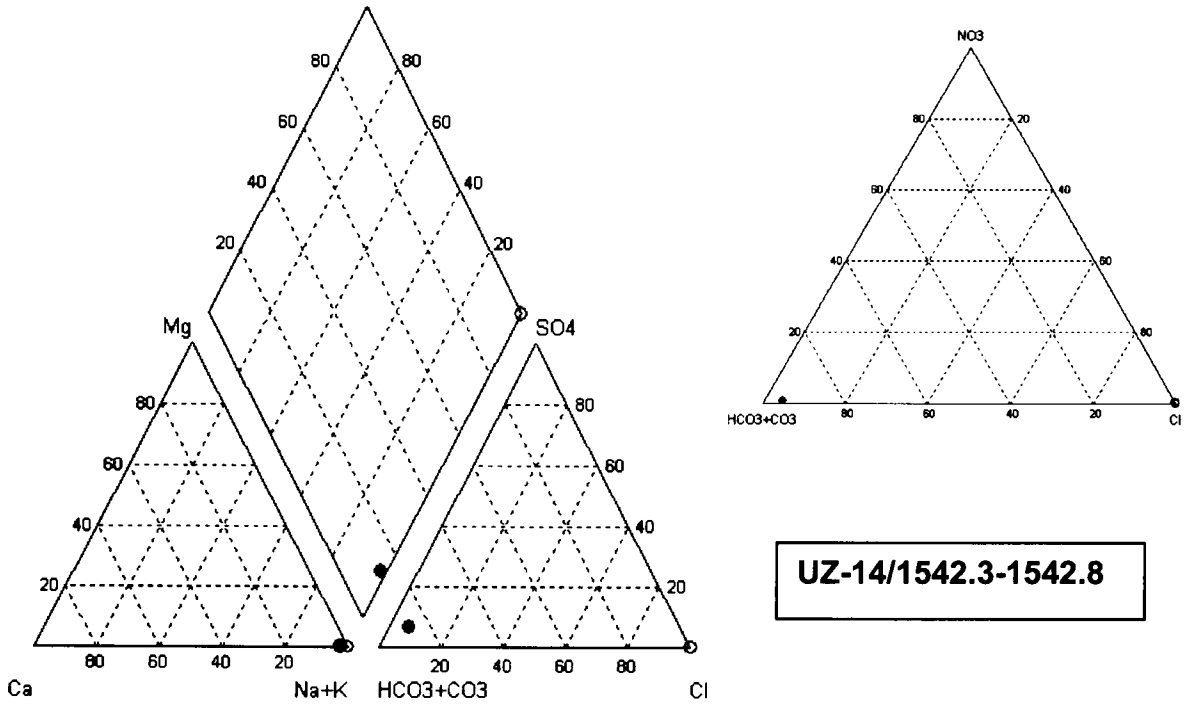
Row #		Molals(>1e-7)	UZ_A #1	UZ_A #2	UZ_B #1	UZ_B #2	NRG_A #1	NRG_A #2	NRG_B #1	NRG_B #2	AVG_J13#1	AVG_J13#2
2	2	H2F2										
3	3	CO2	1.12E-07	1.3E-06		2.6E-06		4.1799E-06		not conv.		2.8392E-06
4	4	H2SO4										
5	5	HCL										
6	7	HNO3				2.17E-07						
7	11	CASO4			0.000325	0.000324	0.0001548	0.00015048	0.0002886			
8	12	ALOH3										
9	13	KCL									0.02851099	0.08603887
10	15	MGCO3		9.5E-07		1.28E-06		5.8403E-07				9.6148E-07
11	16	MGH2SIO4	3.09E-07	2.9E-07	4E-07	4E-07	1.907E-07	1.8544E-07	3.556E-07		3.9004E-07	3.0221E-07
12	17	MGSO4			9.98E-06	0.000437	0.0001239	0.00019906	3.989E-06			
13	18	NAF									0.11345541	0.04404628
14	19	NAHCO3	0.024407	0.09164	7.23E-06	4.78E-05		4.3188E-07	7.391E-06		0.01800816	0.09456722
15	20	NAHSIO3	4.682643	1.06684	0.003832	0.000579	6.268E-06	5.3217E-06	0.0087038		10.1026735	1.15355488
16	21	NANO3	0.042275	0.07129	0.110955	0.111682	2.12E-05	2.6575E-05	0.0993088		0.01446812	0.03134128
17	23	CACO3	8.74E-07	8.1E-07	1.13E-06	1.13E-06		5.2451E-07	1.006E-06		1.1032E-06	8.5478E-07
18	24	SIO2	0.001901	0.00169	0.002552	0.002545	0.0016208	0.00156709	0.002289		0.00219956	0.00214024
19	25	CAH2SIO4	1.37E-07		4.89E-07				9.651E-07		5.042E-07	
20	26	OHION	0.01998	0.00393	1.17E-05	1.77E-06	5.993E-07	5.5703E-07	2.804E-05		0.04849589	0.00303368
21	31	ALION										
22	32	ALOH2ION										
23	33	ALOH4ION	0.00549	0.00035	1.17E-05	1.78E-06			3.226E-05			
24	34	ALOHION										
25	35	ALSO42ION										
26	36	ALSO4ION										
27	37	CAFION										
28	38	CAHCO3ION			6.02E-06	3.98E-05	2.281E-06	0.00019446	2.701E-06			
29	39	CAHSIO3ION	1.84E-07		0.000781	0.000118	0.0014388	0.00096673	0.0007044		1.9414E-07	
30	40	CAION			0.107076	0.107546	2.0081512	1.55090884	0.0600947			
31	41	CANO3ION	2.43E-07	3.3E-07	2.184817	2.180375	1.1428547	1.13387246	0.6860565			1.3698E-07
32	42	CAOHION			6.53E-05	9.81E-06	0.0001757	0.0001188	5.825E-05			
33	43	CLION	4.174277	3.39829	4.791008	4.768404	9.3320722	9.24763396	3.8509559		2.9511929	6.4177514
34	44	CO3ION	0.820127	0.8021	1.55E-07	1.57E-07			4.069E-07		1.13044947	0.34479776
35	45	FION									0.13546363	0.03765619
36	46	H2SIO4ION	0.039129	0.00232					1.178E-07		0.27109204	0.00483229
37	47	H3SIO4ION	0.375021	0.07507	0.000272	4.1E-05	2.162E-06	1.9645E-06	0.000559		1.30610994	0.16319869
38	48	HCO3ION	0.012392	0.04686	3.14E-06	2.08E-05		1.0215E-06	3.337E-06		0.01191509	0.07401834
39	50	HION					7.066E-07	7.9551E-07				
40	51	HSO4ION										

41	52	KION									1.87558722	5.90929245
42	53	KSO4ION									0.00312734	0.00251503
43	54	MGFION										
44	55	MGHCO3ION			4.38E-07	0.000127	4.33E-06	0.000609				
45	56	MGHSIO3ION		2.379E-07	8.13E-05	0.000537	0.003906	0.004337	3.3E-05			1.9289E-07
46	57	MGION			0.000248	0.010787	1.512397	1.945774	4.52E-05			
47	58	MGOHION			2.85E-05	0.000188	0.001997	0.002232	1.14E-05			
48	59	NA2FION									0.23050426	0.14650483
49	60	NACO3ION	0.1634097	0.1330334							0.33279167	0.28252563
50	61	NAION	11.124239	13.516901	10.44812	10.45521	1.149296	1.121734	12.71917		7.67206614	8.25988461
51	62	NASO4ION	0.0006428	0.0005802	0.000711	0.000715	2.47E-06	3.21E-06	0.001804		0.00112452	0.0009786
52	63	NO3ION	4.5217498	8.0461782	7.956995	8.004133	0.008664	0.009744	9.135558		2.08059691	6.55724343
53	66	SO4ION	0.06638	0.1018922	0.049773	0.049974	1.34E-05	1.66E-05	0.268687		0.05213133	0.0387731
		Total Na+	16.037617	14.880291	10.56363	10.56823	1.149326	1.121769	12.829	0	18.4850918	10.0134033
		Total K+	0	0	0	0	0	0	0	0	1.90722556	5.99784635
		Total Ca2+	1.438E-06	1.141E-06	2.293071	2.288414	3.152777	2.686212	0.747207	0	1.8015E-06	9.9176E-07
		Total Mg2+	3.091E-07	1.478E-06	0.000369	0.012077	1.518428	1.953152	9.4E-05	0	3.9004E-07	1.4566E-06
		Total Al3+	0.0054897	0.0003453	1.17E-05	1.78E-06	0	0	3.23E-05	0	0	0
		Total SiO2	5.0986952	1.1459206	0.007519	0.00382	0.006974	0.006878	0.012291	0	11.6820761	1.3237266
		Total Cl-	4.1742772	3.3982851	4.791008	4.768404	9.332072	9.247634	3.850956	0	2.97970389	6.50379027
		Total NO3-	4.5640256	8.1174726	10.25277	10.29619	1.151539	1.143643	9.920923	0	2.09506504	6.58858484
		Total SO42-	0.0670228	0.1024724	0.050818	0.051451	0.000295	0.000369	0.270783	0	0.0563832	0.04226672
		Total CO32-	0.9835375	0.935139	1.29E-06	2.57E-06	0	1.11E-06	1.41E-06	0	1.46324224	0.62732521
		Total HCO3-	0.0367992	0.1385016	1.68E-05	0.000235	6.61E-06	0.000805	1.34E-05	0	0.02992325	0.16858556
		Total F-	0	0	0	0	0	0	0	0	0.4794233	0.22820729
Molal conc:		Na+ ion	11.124239	13.516901	10.44812	10.45521	1.149296	1.121734	12.71917	0	7.67206614	8.25988461
		K+ ion	0	0	0	0	0	0	0	0	1.87558722	5.90929245
		Ca2+ ion	0	0	0.107076	0.107546	2.008151	1.550909	0.060095	0	0	0
		Mg2+ ion	0	0	0.000248	0.010787	1.512397	1.945774	4.52E-05	0	0	0
		Silica ions	0.4160517	0.0790756	0.002824	0.002586	0.001623	0.001569	0.002848	0	1.57940154	0.17017123
		Al-OH ions	0.0054897	0.0003453	1.17E-05	1.78E-06	0	0	3.23E-05	0	0	0
		Cl- ion	4.1742772	3.3982851	4.791008	4.768404	9.332072	9.247634	3.850956	0	2.9511929	6.4177514
		NO3- ion	4.5217498	8.0461782	7.956995	8.004133	0.008664	0.009744	9.135558	0	2.08059691	6.55724343
		SO42- ion	0.06638	0.1018922	0.049773	0.049974	1.34E-05	1.66E-05	0.268687	0	0.05213133	0.0387731
		CO32- ion	0.8201269	0.8021038	1.55E-07	1.57E-07	0	0	4.07E-07	0	1.13044947	0.34479776
		HCO3- ion	0.0123922	0.0468641	3.14E-06	2.08E-05	0	1.02E-06	3.34E-06	0	0.01191509	0.07401834
		F- ion	0	0	0	0	0	0	0	0	0.13546363	0.03765619
		Charge bal.	0.6428062	0.2175819	-2.18478	-2.18063	-1.15037	-1.14231	-0.68444	0	2.00332323	0.31536597

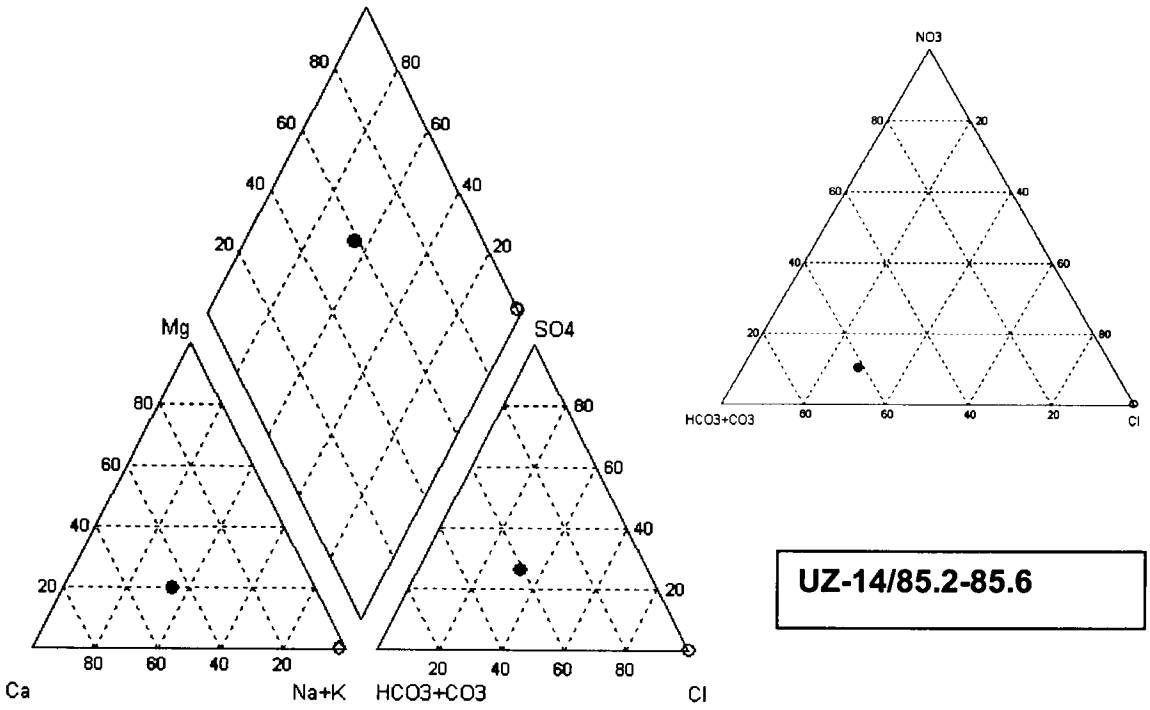
mg/L values:	Na+ ion	255746.26	310753.56	240202.3	240365.3	26422.32	25788.65	292413.8	0	176380.801	189894.747
	K+ ion	0	0	0	0	0	0	0	0	73331.7092	231041.516
	Ca2+ ion	0	0	4291.603	4310.445	80486.7	62160.43	2408.596	0	0	0
	Mg2+ ion	0	0	6.036149	262.1829	36758.81	47292.03	1.097886	0	0	0
	Silica ions	24997.637	4751.1022	169.6753	155.3797	97.51234	94.27361	171.1211	0	94895.1827	10224.3979
	Al-OH ions	148.12216	9.3170169	0.316292	0.047894	0	0	0.870317	0	0	0
	Cl- ion	147990.65	120479.4	169855.6	169054.2	330850	327856.4	136527.9	0	104628.642	227528.54
	NO3- ion	280.36658	498.89524	493.3655	496.2883	0.537175	0.604184	566.4411	0	129.005331	406.575322
	SO42- ion	6.3761943	9.7873524	4.780953	4.800311	0.001288	0.001598	25.80895	0	5.00752719	3.72438923
	CO32- ion	49.214175	48.132645	9.32E-06	9.4E-06	0	0	2.44E-05	0	67.8360119	20.6906241
	HCO3- ion	0.7561213	2.8594618	0.000192	0.001268	0	6.23E-05	0.000204	0	0.72701091	4.51630299
	F- ion	0	0	0	0	0	0	0	0	2.57353803	0.71539228
Column#	Molals(>1e-7)	UZ_A #1	UZ_A #2	UZ_B #1	UZ_B #2	NRG_A #1	NRG_A #2	NRG_B #1	NRG_B #2	AVG_J13#1	AVG_J13#2

Note that the charge balance values listed in the previous page are in equivalents per liter.

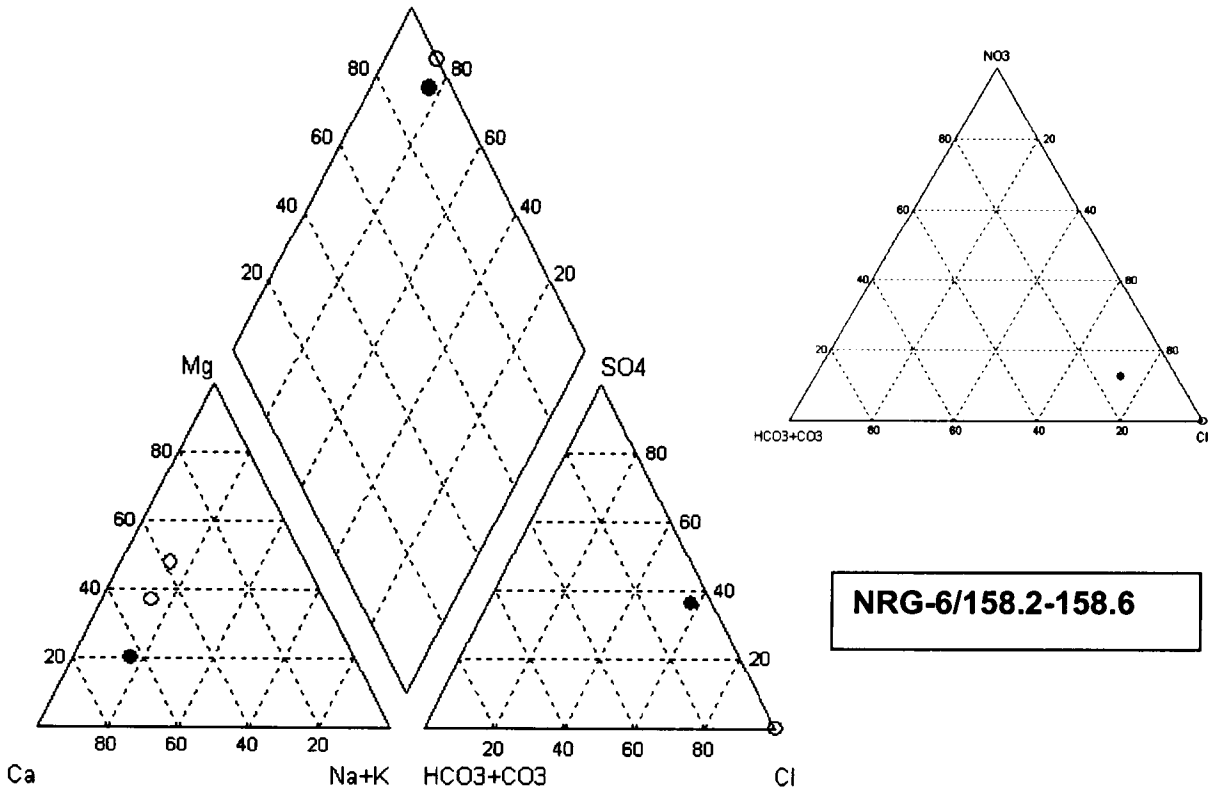
The following plots compare the initial YM water composition with the composition after evaporation at 110 °C at constant atmospheric pressure of 0.85, which is the approximate atmospheric pressure at Yucca Mountain. Two calculations for each composition were made by L. Yang. One calculation adjusted the initial total aqueous carbonate concentration such that the initial pCO2 is equal to ~1.02×10^{-3} bar, the pCO2 estimated for the YM geochemical system. The other calculation did not make such an adjustment. The initial compositions are plotted as solid circles, whereas the evaporated compositions are plotted as open circles. Note that the two calculations for each YM water composition resulted in very close values and may not be distinguishable in the plots.



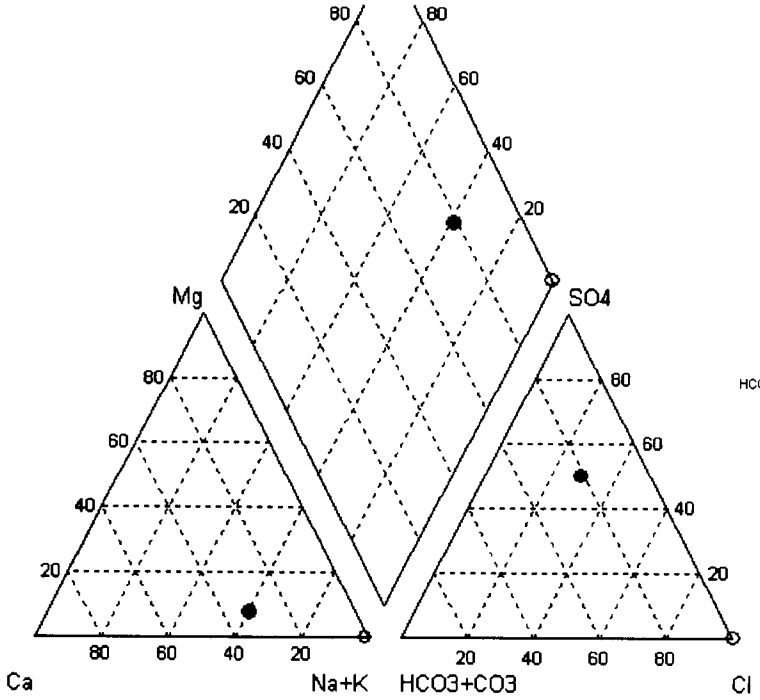
UZ-14/1542.3-1542.8

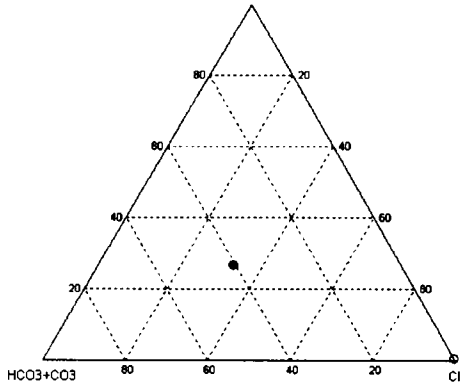


UZ-14/85.2-85.6

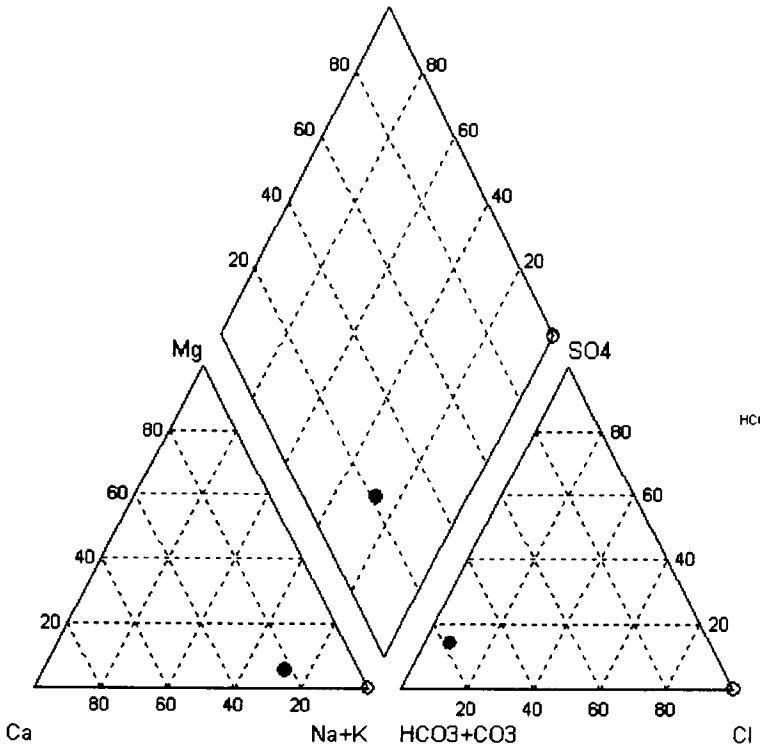


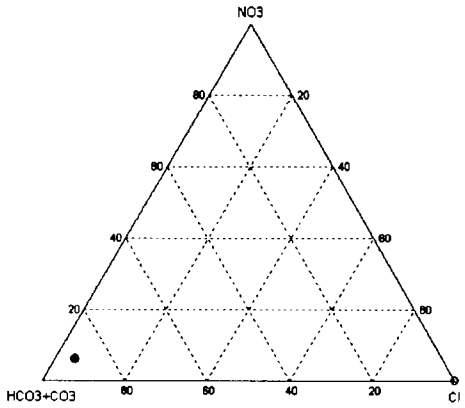
NRG-6/158.2-158.6





NRG-6/244.6-245.0





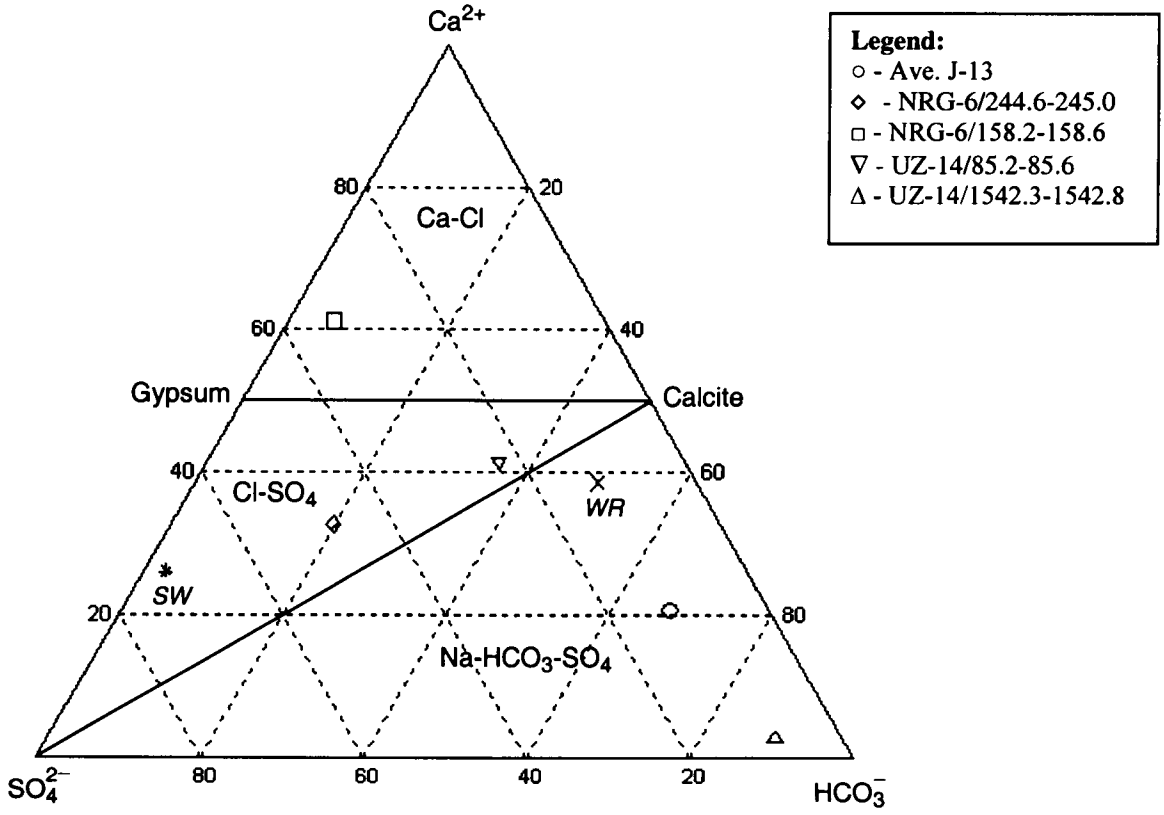
Average J-13

October 1, 2001

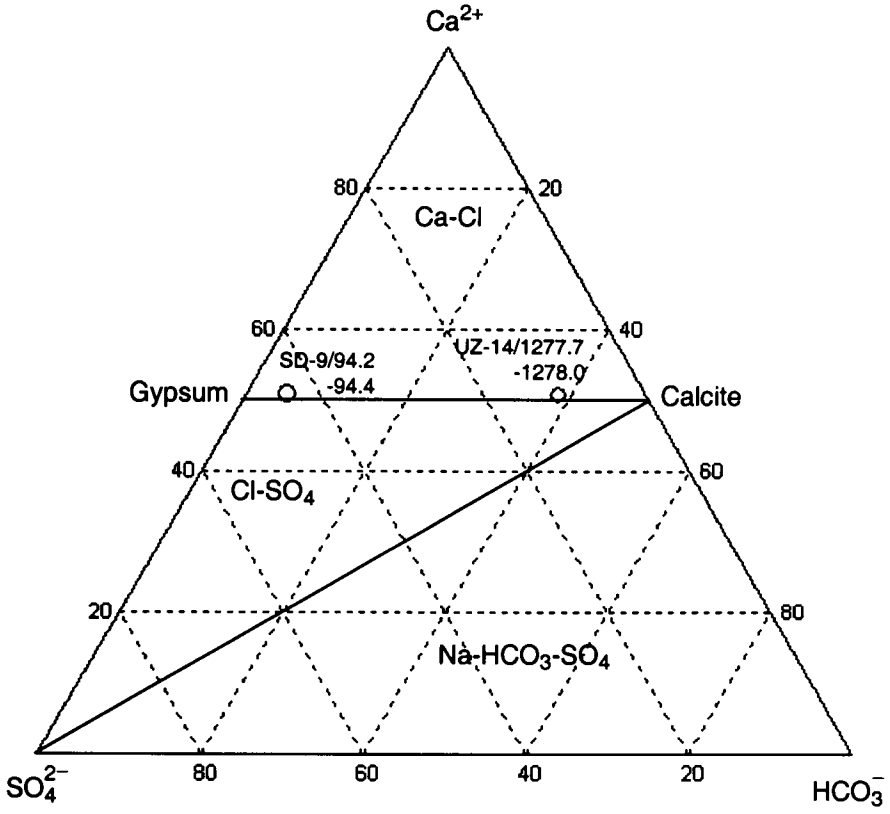
The following is the chemical divide analysis to determine the potential evolution of the YM waters upon evaporation. See discussion of chemical divide approach in Rosenberg et al. (2001; Applied Geochemistry **16**, 1231-1240). Two of the waters evolve into a Na-HCO3-CO3 brine, whereas three evolve into brines rich in Mg-Ca-Cl.

SampleID	**Ave-J13 Harrar**		**NRG-6/158.2-158.6**		**NRG-6/244.6**		**UZ-14/1542.3**		**UZ-14-85.2-85.6**	
Water Type	Na-Ca-HCO3		Ca-Mg-Cl-SO4		Na-Ca-SO4-Cl		Na-HCO3		Ca-Na-HCO3-Cl-SO4	
Reference	Harrar et al. 1990		Yang et al. 1998		Yang et al. 1998		Yang et al. 1996		Yang et al. 1996	
Ph (Lab)	7.41		6.8		7.2		8.6		6.9	
Cations	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)
Na+	4.58E+01	1.99E+00	3.56E+01	1.55E+00	7.20E+01	3.13E+00	2.07E+02	9.00E+00	4.35E+01	1.89E+00
K+	5.04E+00	1.29E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mg++	2.01E+00	1.65E-01	2.33E+01	1.92E+00	4.90E+00	4.03E-01	5.00E-01	4.11E-02	1.32E+01	1.09E+00
Ca++	1.30E+01	6.49E-01	1.22E+02	6.09E+00	3.30E+01	1.65E+00	3.60E+00	1.80E-01	4.99E+01	2.49E+00
Anions	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)
F-	2.18E+00	1.15E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cl-	7.14E+00	2.01E-01	1.85E+02	5.22E+00	4.90E+01	1.38E+00	2.00E+01	5.64E-01	6.00E+01	1.69E+00
SO4--	1.84E+01	3.83E-01	1.59E+02	3.31E+00	1.15E+02	2.39E+00	2.80E+01	5.83E-01	6.60E+01	1.37E+00
NO3-	8.78E+00	1.42E-01	3.20E+01	5.16E-01	4.00E+01	6.45E-01	4.00E+00	6.45E-02	2.20E+01	3.55E-01
HCO3-	1.29E+02	2.11E+00	3.40E+01	5.57E-01	6.10E+01	1.00E+00	3.84E+02	6.29E+00	1.31E+02	2.15E+00
CO3--	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.60E+01	1.53E+00	0.00E+00	0.00E+00
Chemical divide analysis:										
alkalinity =		2.11E+00		5.57E-01		1.00E+00		7.83E+00		2.15E+00
Is Ca2+>alk?		no		yes		yes		no		yes
If no (i.e., Ca<alk), then is Mg < remaining alkalinity?		yes NaHCO3-CO3						yes NaHCO3-CO3		
If yes (i.e., Ca>alk), then is remaining Ca>SO4?				yes, gyp precips. Na-Ca-Mg-Cl brine		no Na-Mg-SO4-Cl brine				no Na-Mg-SO4-Cl brine

The following is a ternary Ca^{2+}-SO_4^{2-}-HCO_3^- phase diagram, in mole-equivalents, patterned after the diagram from Spencer and Hardie (1990) to illustrate the "chemical divide" approach of Hardie and Eugster (1970). The body of the diagram is the primary stability field for calcite; gypsum and anhydrite stability fields are along the Ca2+-SO42- join. Lines from calcite to gypsum/anhydrite and from calcite to SO42- are chemical divides for the system which separate Ca-Cl, Cl-SO4, and Na-HCO3-SO4 type waters. Average river water (WR) has a Na-HCO3-SO4 composition, and modern seawater (SW) is a Cl-SO4 water. The initial compositions of the five YM water compositions simulated using OLI are also plotted.



The following figure plots the composition of SD-9/94.2-94.4 and UZ-14/1277.7-1278.0 waters in the ternary Ca-SO4-HCO3 plot. The figure shows that the two compositions plot in the Ca-Cl field. To determine if the chemical divide approach is consistent with the OLI ESP simulations, I will provide the compositions to L.Yang and have him simulate the evaporation of the two waters.



The compositions are:

Database: D:\Workdir\Documents\NEARFLD\WP Water Chem\Salt Precipitate Analysis\SALT ANALYSES.HC3

SampleID	SD-9/94.2-94.4		SampleID	UZ-14/1277.7-1278	
Water Type	Ca-SO4-Cl		Water Type	Ca-Na-Cl-HCO3	
Ph (Lab)	6.2		Ph (Lab)	not avail.	
Cations	(mg/l)	(meq/l)	Cations	(mg/l)	(meq/l)
Na+	4.30E+01	1.87E+00	Na+	4.50E+01	1.96E+00
K+	0.00E+00	0.00E+00	K+	0.00E+00	0.00E+00
Mg++	2.40E+01	1.97E+00	Mg++	5.10E+00	4.20E-01
Ca++	1.25E+02	6.24E+00	Ca++	7.40E+01	3.69E+00
Anions	(mg/l)	(meq/l)	Anions	(mg/l)	(meq/l)

F-	0.00E+00	0.00E+00
Cl-	1.70E+02	4.80E+00
SO4--	2.60E+02	5.41E+00
NO3-	1.10E+01	1.77E-01
HCO3-	3.70E+01	6.07E-01
CO3--	0.00E+00	0.00E+00

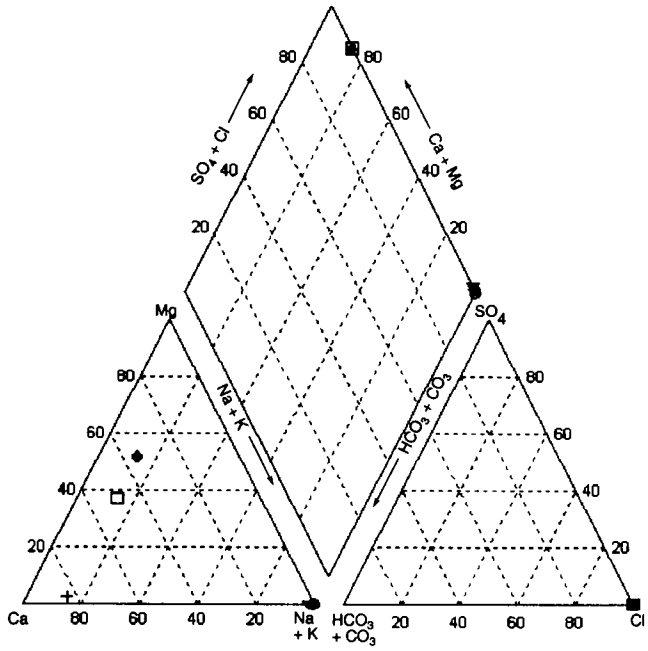
Uncharged	(mg/l)
SiO2	74
Al	0

F-	0.00E+00	0.00E+00
Cl-	1.30E+02	3.67E+00
SO4--	3.80E+01	7.91E-01
NO3-	1.50E+01	2.42E-01
HCO3-	1.70E+02	2.79E+00
CO3--	0.00E+00	0.00E+00

Uncharged	(mg/l)
SiO2	38
Al	0

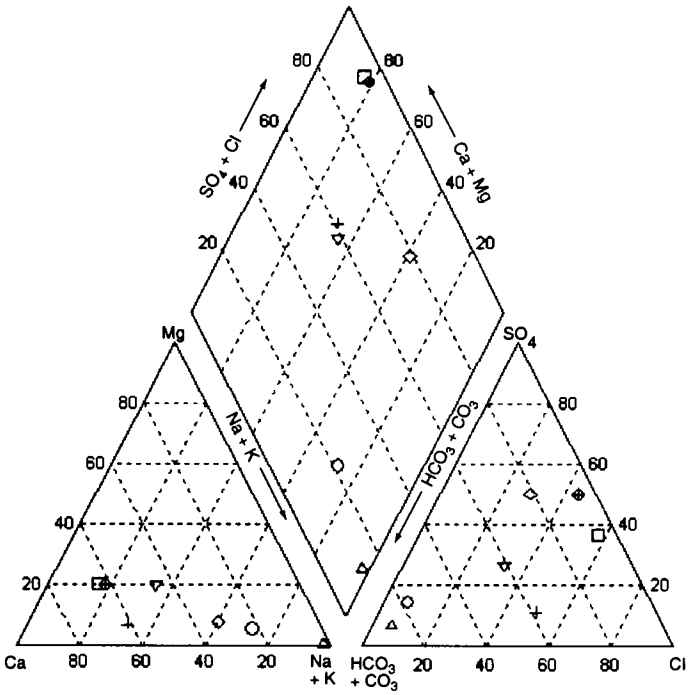
October 16, 2001

The following is a plot of the final YM water compositions after evaporation at 110 C. The results plotted are for the cases in which the pCO2 was not constrained (evap-1 in L.Yang's notebook). The results for SD-9/94.2-94.4 and UZ-14/1277.7-1278.0 are also included. As shown in the figure, the SD-9/94.2-94.4 and UZ-14/1277.7-1278.0 waters become Ca-Mg-Cl brines after evaporation at 110 C, as expected based on the chemical divide diagram shown on page 11. . The calculated pHs are 5.78 and 6.3 for SD-9/94.2-94.4 and and UZ-14/1277.7-1278.0, respectively



Legend:
○ - Ave. J-13
◇ - NRG-6/244.6-245.0
□ - NRG-6/158.2-158.6
⊕ - SD-9/94.2-94.4
∇ - UZ-14/85.2-85.6
\+ - UZ-14/1277.7-1278.0
Δ - UZ-14/1542.3-1542.8

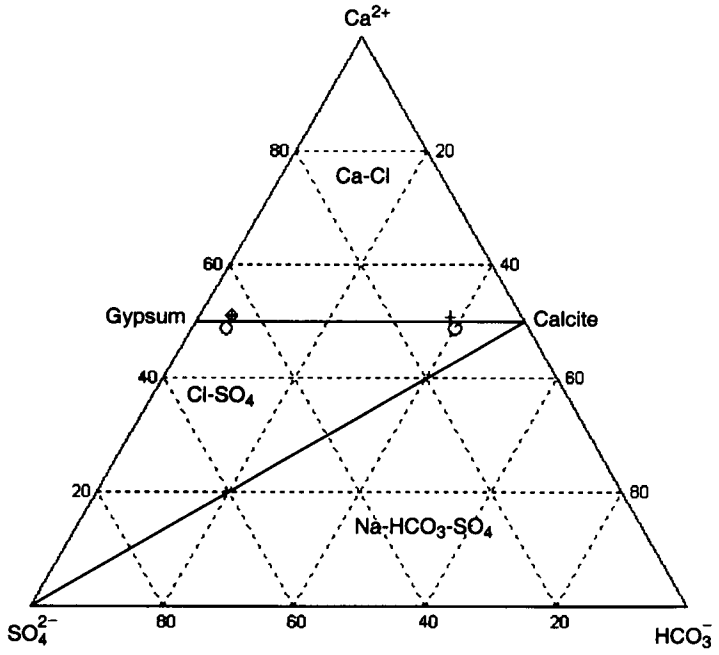
For comparison, the initial YM water compositions are plotted on the next page.



Legend:
○ - Ave. J-13
◇ - NRG-6/244.6-245.0
□ - NRG-6/158.2-158.6
⊕ - SD-9/94.2-94.4
∇ - UZ-14/85.2-85.6
\+ - UZ-14/1277.7-1278.0
Δ - UZ-14/1542.3-1542.8

October 19, 2001

To test the chemical divide approach, two more calculations were done by L. Yang on compositions slightly different from that given for SD-9/94.2-94.4 and UZ-14/1277.7-1278.0. The equivalents of Ca2+ were lowered slightly (and charge balanced with Na+) such that the compositions plot just below the gypsum-calcite line in a ternary Ca-SO4-HCO3 plot, as shown by the two open circles in the figure below:



The initial compositions given to L. Yang for simulation are as follows:

Database: D:\Workdir\Documents\NEARFLD\WP Water Chem\Salt Precipitate Analysis\SALT ANALYSES.HC3

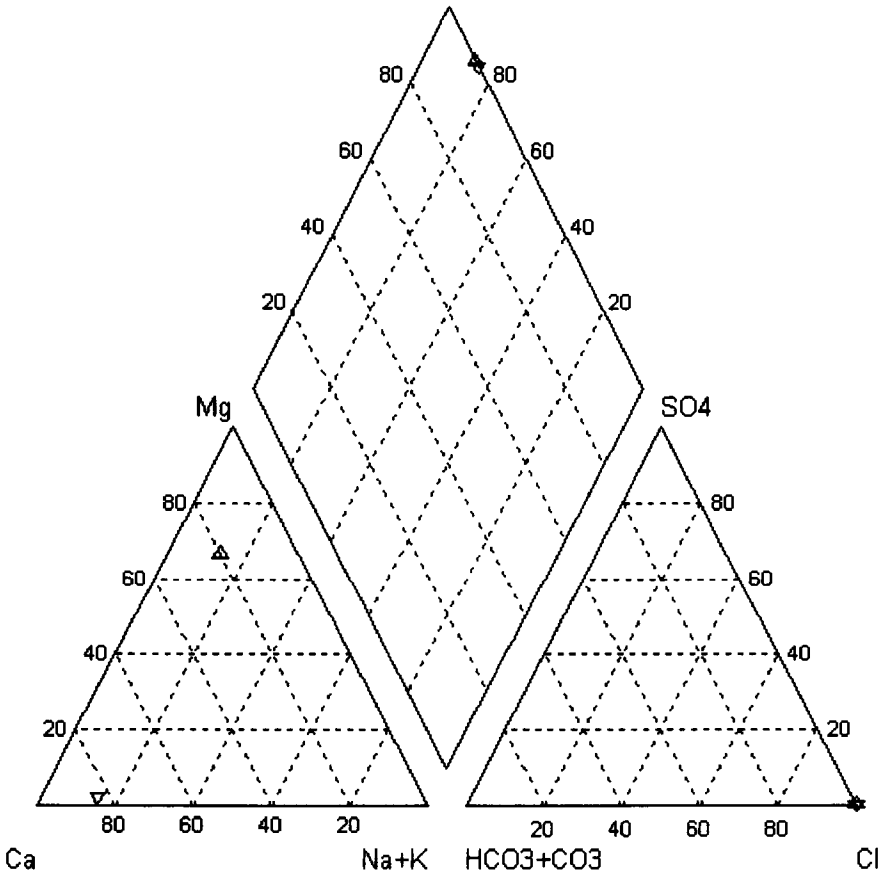
SampleID	SD-9/94.2-94.4 changed	
Water Type	Ca-SO4-Cl	
Ph (Lab)	6.2	
Cations	**(mg/l)**	**(meq/l)**
Na+	5.536E+01	2.408E+00
K+	0.00E+00	0.00E+00
Mg++	2.40E+01	1.97E+00
Ca++	1.142E+02	5.700E+00
Anions	**(mg/l)**	**(meq/l)**
F-	0.00E+00	0.00E+00
Cl-	1.70E+02	4.80E+00
SO4--	2.60E+02	5.41E+00

SampleID	UZ-14/1277.7-1278 changed	
Water Type	Ca-Na-Cl-HCO3	
Ph (Lab)	not avail.	
Cations	**(mg/l)**	**(meq/l)**
Na+	5.173E+01	2.250E+00
K+	0.00E+00	0.00E+00
Mg++	5.10E+00	4.20E-01
Ca++	6.814E+01	3.400E+00
Anions	**(mg/l)**	**(meq/l)**
F-	0.00E+00	0.00E+00
Cl-	1.30E+02	3.67E+00
SO4--	3.80E+01	7.91E-01

NO3-	1.10E+01	1.77E-01	NO3-	1.50E+01	2.42E-01
HCO3-	3.70E+01	6.07E-01	HCO3-	1.70E+02	2.79E+00
CO3--	0.00E+00	0.00E+00	CO3--	0.00E+00	0.00E+00

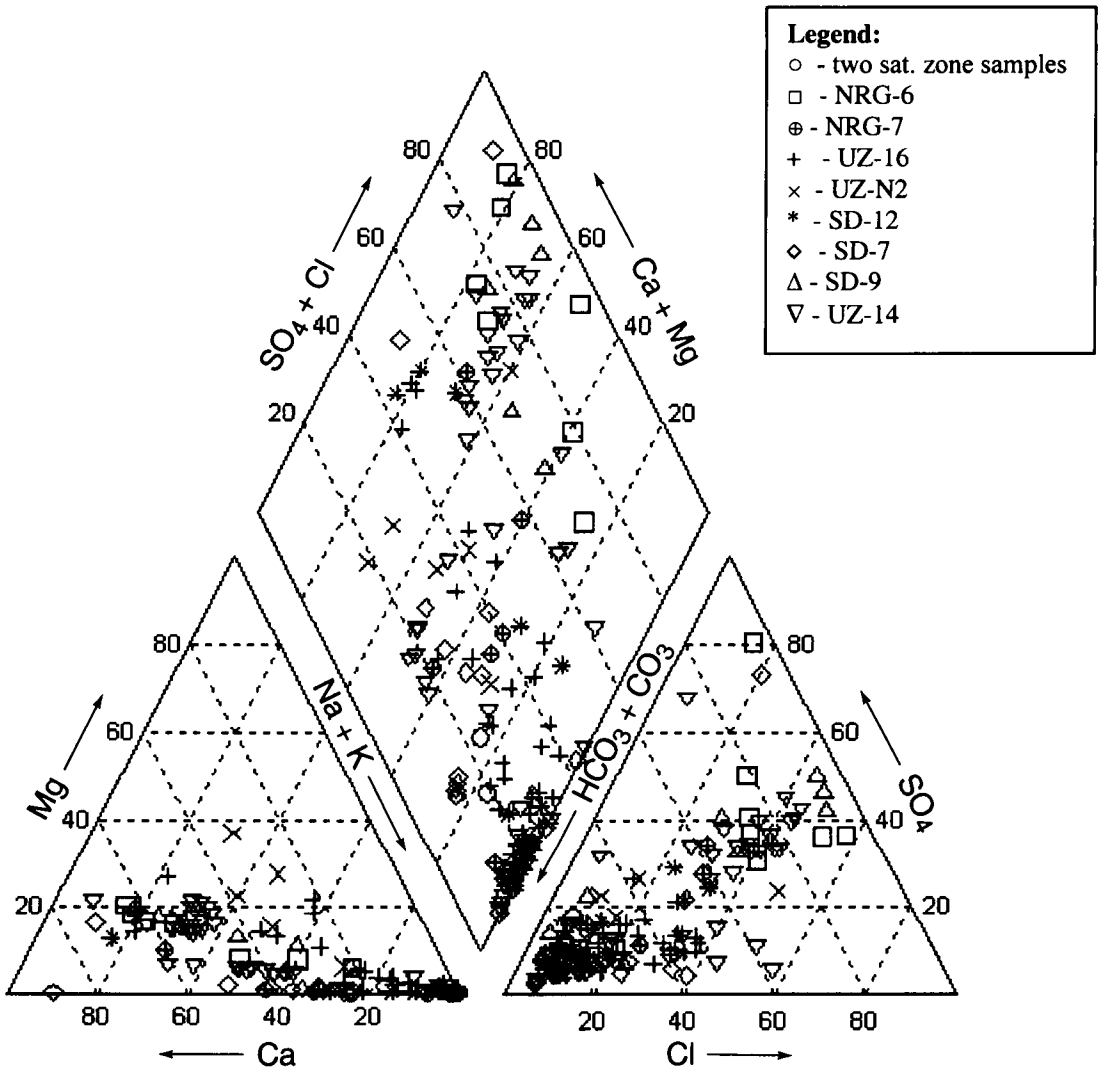
Uncharge d	(mg/l)	Uncharged	(mg/l)
SiO2	74	SiO2	38
Al	0	Al	0

The following figure shows the result of L. Yang's simulation of evaporation using the OLI ESP program (legend: modified SD-9/94.2-94.4, triangle, and modified UZ-14/1277.7-1278.0, inverted triangle). For comparison, see figure on page 13 of this notebook. . The calculated pHs are 5.73 and 6.26 for the evaporated modified SD-9/94.2-94.4 and evaporated modified UZ-14/1277.7-1278.0, respectively

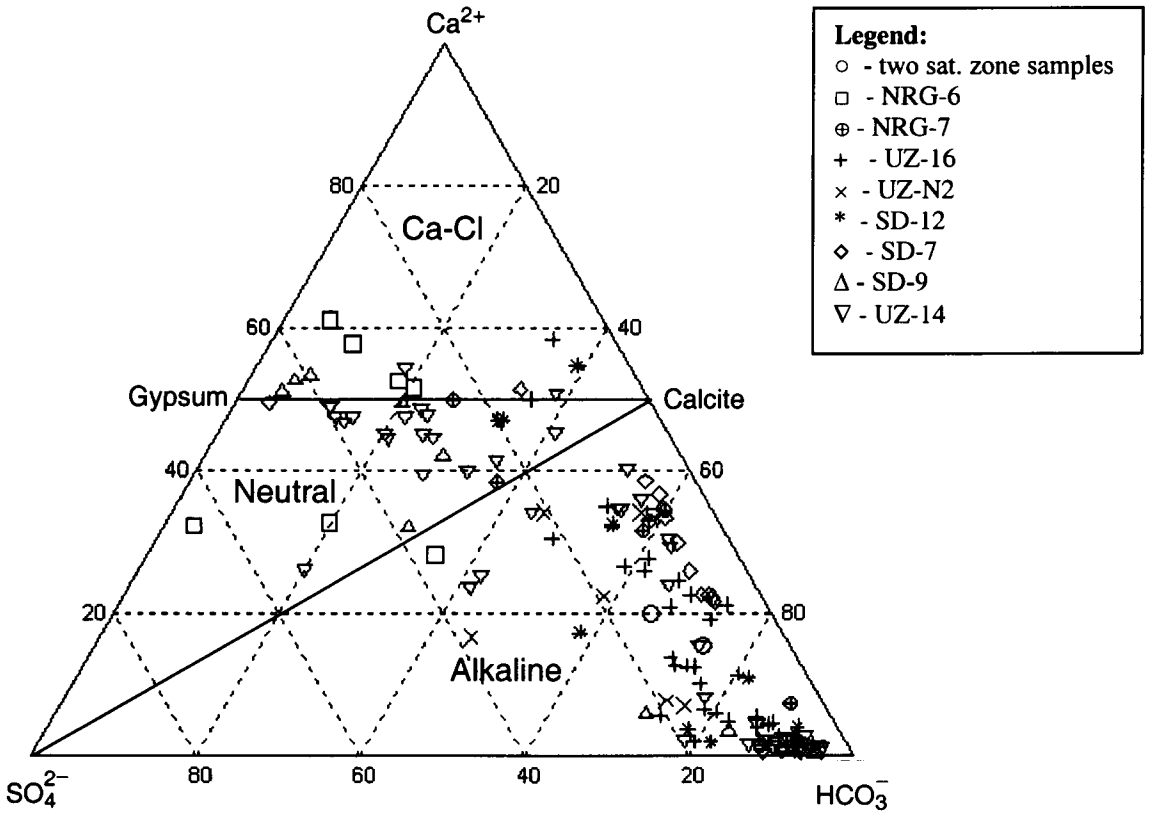


January 21, 2002

Yucca Mountain porewater, perched water, and groundwater data from Yang et al. (1996, 1998) were input into an Excel spreadsheet, imported into an Aquachem datafile, and plotted in a Piper diagram shown below:



The following is a chemical-divide type of plot for the Yang et al. data:



January 22, 2002

The following pages document the results of calculations done to validate the acquired software SOLCALC Version 1.0, per the Software Validation Test Plan for SOLCALC Version 1.0 prepared by R.T. Pabalan.

1. SOLCALC Validation Test Case 1: NaCl(s) solubility as a function of temperature

The following is the "solcalc.out" output file of SOLCALC showing the calculated solubility of NaCl(s) (halite) from 25 to 300 °C. For each calculation, the temperature and pressure are input interactively, and saturation with halite is also specified interactively.

```
      SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

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

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     6

                     EQUATION       LOG K

                        20          1.5810

                     IONIC STRENGTH =   6.1390

                 ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

CATION #  1   0.61729E+01      0.10055E+01        0.61390E+01      0.0009
ANION #   1   0.61729E+01      0.10055E+01        0.61390E+01      0.0009

     SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

                TEMP(C) =   50.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     7

                     EQUATION       LOG K

                        20          1.6132

                     IONIC STRENGTH =   6.2732

                 ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

CATION #  1   0.64061E+01      0.10212E+01        0.62732E+01      0.0009
ANION #   1   0.64061E+01      0.10212E+01        0.62732E+01      0.0009

     SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

                TEMP(C) =   75.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     8

                     EQUATION       LOG K
```

```
                    20          1.6074

                IONIC STRENGTH =   6.4479

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.63637E+01       0.98694E+00         0.64479E+01       0.0009
ANION #   1   0.63637E+01       0.98694E+00         0.64479E+01       0.0009

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =  100.00     PRESS(BARS) =     1.02

  NUMBER CORRESPONDING TO SATURATED SOLID      20

           THE NUMBER OF ITERATIONS IS     9

                EQUATION       LOG K

                   20          1.5731

                IONIC STRENGTH =   6.6601

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.61172E+01       0.91849E+00         0.66601E+01       0.0009
ANION #   1   0.61172E+01       0.91849E+00         0.66601E+01       0.0009

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =  125.00     PRESS(BARS) =     2.33

  NUMBER CORRESPONDING TO SATURATED SOLID      20

           THE NUMBER OF ITERATIONS IS    11

                EQUATION       LOG K

                   20          1.5149

                IONIC STRENGTH =   6.9099

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.57206E+01       0.82788E+00         0.69099E+01       0.0004
ANION #   1   0.57206E+01       0.82788E+00         0.69099E+01       0.0004

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =  150.00     PRESS(BARS) =     4.77

  NUMBER CORRESPONDING TO SATURATED SOLID      20

           THE NUMBER OF ITERATIONS IS    12

                EQUATION       LOG K

                   20          1.4343

                IONIC STRENGTH =   7.2007

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.52135E+01       0.72403E+00         0.72007E+01       0.0007
ANION #   1   0.52135E+01       0.72403E+00         0.72007E+01       0.0007
```

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 175.00 PRESS(BARS) = 8.93

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.3312

IONIC STRENGTH = 7.5419

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.46304E+01	0.61395E+00	0.75419E+01	0.0006
ANION #	1	0.46304E+01	0.61395E+00	0.75419E+01	0.0006

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 200.00 PRESS(BARS) = 15.55

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 16

EQUATION	LOG K
20	1.2045

IONIC STRENGTH = 7.9500

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.40017E+01	0.50336E+00	0.79500E+01	0.0007
ANION #	1	0.40017E+01	0.50336E+00	0.79500E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 225.00 PRESS(BARS) = 25.49

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 19

EQUATION	LOG K
20	1.0512

IONIC STRENGTH = 8.4480

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.33544E+01	0.39707E+00	0.84480E+01	0.0007
ANION #	1	0.33544E+01	0.39707E+00	0.84480E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 250.00 PRESS(BARS) = 39.75

NUMBER CORRESPONDING TO SATURATED SOLID 20

```
            THE NUMBER OF ITERATIONS IS    23

                EQUATION       LOG K

                   20          0.8666

                IONIC STRENGTH =   9.0622

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.27119E+01       0.29926E+00         0.90622E+01       0.0006
ANION #   1   0.27119E+01       0.29926E+00         0.90622E+01       0.0006

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =  275.00     PRESS(BARS) =    59.44

  NUMBER CORRESPONDING TO SATURATED SOLID      20

            THE NUMBER OF ITERATIONS IS    27

                EQUATION       LOG K

                   20          0.6416

                IONIC STRENGTH =   9.7972

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.20932E+01       0.21366E+00         0.97972E+01       0.0010
ANION #   1   0.20932E+01       0.21366E+00         0.97972E+01       0.0010

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =  300.00     PRESS(BARS) =    85.84

  NUMBER CORRESPONDING TO SATURATED SOLID      20

            THE NUMBER OF ITERATIONS IS    32

                EQUATION       LOG K

                   20          0.3591

                IONIC STRENGTH =  10.5346

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.15119E+01       0.14352E+00         0.10535E+02       0.0008
ANION #   1   0.15119E+01       0.14352E+00         0.10535E+02       0.0008
```

2. SOLCALC Validation Test Case 2: NaCl(s) and/or KCl(s) solubility in mixed NaCl+KCl solutions

The following is the "solcalc.out" output file of SOLCALC showing the calculated solubility of NaCl(s) (halite) and/or KCl(s) (sylvite) in mixed NaCl+KCl solutions. For each calculation, the temperature and pressure are input interactively. When calculating the solubility of NaCl, the concentration of K^+ is fixed at the experimentally measured value (listed in the output file) and saturation with halite is specified interactively. When calculating the solubility of KCl, the concentration of Na^+ is fixed at the experimentally measured value (listed in the output file) and saturation with sylvite is specified interactively. When calculating the solubility when the two solids are saturated, saturation with halite and sylvite is specified interactively.

a) Solubility of two solids, NaCl + KCl:

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

              TEMP(C) =   40.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

     NUMBER CORRESPONDING TO SATURATED SOLID      53

              THE NUMBER OF ITERATIONS IS    18


                   EQUATION       LOG K

                      20          1.6058
                      53          1.0420

                   IONIC STRENGTH =   7.6121

               ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

  CATION #  1   0.54722E+01       0.11013E+01         0.49691E+01       -.0002
  CATION #  2   0.14940E+01       0.56527E+00         0.26430E+01       0.0006
  ANION #   1   0.73727E+01       0.96854E+00         0.76121E+01       -.0002

    SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS


              TEMP(C) =  100.00     PRESS(BARS) =     1.02

    NUMBER CORRESPONDING TO SATURATED SOLID      20

    NUMBER CORRESPONDING TO SATURATED SOLID      53

              THE NUMBER OF ITERATIONS IS    17


                   EQUATION       LOG K

                      20          1.5731
                      53          1.3272

                   IONIC STRENGTH =   9.4399

               ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

  CATION #  1   0.46882E+01       0.10043E+01         0.46683E+01       -.0003
  CATION #  2   0.26612E+01       0.55771E+00         0.47716E+01       0.0007
  ANION #   1   0.79820E+01       0.84556E+00         0.94399E+01       -.0003

    SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS


              TEMP(C) =  150.00     PRESS(BARS) =     4.77

    NUMBER CORRESPONDING TO SATURATED SOLID      20

    NUMBER CORRESPONDING TO SATURATED SOLID      53

              THE NUMBER OF ITERATIONS IS    20


                   EQUATION       LOG K

                      20          1.4343
                      53          1.3524
```

IONIC STRENGTH = 11.4302

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.36768E+01	0.75567E+00	0.48656E+01	0.0001
CATION #	2	0.30454E+01	0.46392E+00	0.65646E+01	0.0009
ANION #	1	0.73924E+01	0.64674E+00	0.11430E+02	0.0001

b) NaCl solubility:

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 7

EQUATION LOG K

20 1.6058

IONIC STRENGTH = 6.2139

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.63517E+01	0.10222E+01	0.62139E+01	0.0005
ANION #	1	0.63517E+01	0.10222E+01	0.62139E+01	0.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION LOG K

20 1.6058

CATION # TOTAL

2 0.8700

IONIC STRENGTH = 6.6563

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.60543E+01	0.10463E+01	0.57863E+01	-.0005
CATION #	2	0.46351E+00	0.53277E+00	0.87000E+00	0.0000
ANION #	1	0.66639E+01	0.10011E+01	0.66563E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	1.4070

IONIC STRENGTH = 6.9380

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.58744E+01	0.10621E+01	0.55310E+01	0.0006
CATION #	2	0.76311E+00	0.54236E+00	0.14070E+01	0.0000
ANION #	1	0.68678E+01	0.98989E+00	0.69380E+01	0.0006

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	1.7330

IONIC STRENGTH = 7.1122

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.57667E+01	0.10720E+01	0.53792E+01	0.0009
CATION #	2	0.95020E+00	0.54830E+00	0.17330E+01	0.0000
ANION #	1	0.69960E+01	0.98366E+00	0.71122E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	2.5660

IONIC STRENGTH = 7.5690

ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR

CATION #	1	0.54968E+01	0.10987E+01	0.50030E+01	-.0003
CATION #	2	0.14467E+01	0.56381E+00	0.25660E+01	0.0000
ANION #	1	0.73397E+01	0.96970E+00	0.75690E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 9

EQUATION	LOG K
20	1.5731

IONIC STRENGTH = 6.6601

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009
ANION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 9

EQUATION	LOG K
20	1.5731

CATION #	TOTAL
2	2.0460

IONIC STRENGTH = 7.7679

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.54608E+01	0.95436E+00	0.57219E+01	-.0005
CATION #	2	0.10746E+01	0.52523E+00	0.20460E+01	0.0000
ANION #	1	0.68528E+01	0.88219E+00	0.77679E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION	LOG K
20	1.5731

CATION #	TOTAL

2 4.0240

IONIC STRENGTH = 8.9574

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.48878E+01	0.99074E+00	0.49334E+01	-.0007
CATION #	2	0.22114E+01	0.54954E+00	0.40240E+01	0.0000
ANION #	1	0.76562E+01	0.85473E+00	0.89574E+01	-.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION LOG K

20 1.5731

CATION # TOTAL

2 4.0860

IONIC STRENGTH = 8.9967

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.48708E+01	0.99187E+00	0.49107E+01	-.0007
CATION #	2	0.22483E+01	0.55025E+00	0.40860E+01	0.0000
ANION #	1	0.76828E+01	0.85396E+00	0.89967E+01	-.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 12

EQUATION LOG K

20 1.4343

IONIC STRENGTH = 7.2007

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007
ANION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

```
          THE NUMBER OF ITERATIONS IS    12

              EQUATION       LOG K

                 20          1.4343

              CATION #       TOTAL

                  2          4.0240

              IONIC STRENGTH =   9.5997

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.41787E+01       0.74945E+00         0.55757E+01       -.0007
CATION #  2   0.18438E+01       0.45820E+00         0.40240E+01        0.0000
ANION #   1   0.65047E+01       0.67759E+00         0.95997E+01       -.0007

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =  150.00     PRESS(BARS) =     4.77

  NUMBER CORRESPONDING TO SATURATED SOLID      20

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      2

          THE NUMBER OF ITERATIONS IS    13

              EQUATION       LOG K

                 20          1.4343

              CATION #       TOTAL

                  2          5.3650

              IONIC STRENGTH =  10.5313

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.38983E+01       0.75455E+00         0.51663E+01        0.0005
CATION #  2   0.24841E+01       0.46303E+00         0.53650E+01        0.0000
ANION #   1   0.69724E+01       0.66207E+00         0.10531E+02        0.0005
```

c) KCl solubility:

```
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   40.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

          THE NUMBER OF ITERATIONS IS    13

              EQUATION       LOG K

                 53          1.0420

              IONIC STRENGTH =   5.3909

           ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  2   0.33189E+01       0.61564E+00         0.53909E+01        0.0008
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ANION #   1   0.33189E+01      0.61564E+00        0.53909E+01      0.0008

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =   40.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

           THE NUMBER OF ITERATIONS IS    17

               EQUATION       LOG K

                  53          1.0420

               CATION #       TOTAL

                   1          1.7480

               IONIC STRENGTH =   6.0490

            ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

CATION #  1   0.15105E+01      0.86412E+00        0.17480E+01      0.0000
CATION #  2   0.25588E+01      0.59492E+00        0.43010E+01      0.0005
ANION #   1   0.43048E+01      0.71165E+00        0.60490E+01      0.0000

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =   40.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

           THE NUMBER OF ITERATIONS IS    13

               EQUATION       LOG K

                  53          1.0420

               CATION #       TOTAL

                   1          1.8270

               IONIC STRENGTH =   6.0817

            ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

CATION #  1   0.15869E+01      0.86859E+00        0.18270E+01      0.0000
CATION #  2   0.25275E+01      0.59406E+00        0.42547E+01      0.0005
ANION #   1   0.43580E+01      0.71658E+00        0.60817E+01      0.0000

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =   40.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

           THE NUMBER OF ITERATIONS IS    14

               EQUATION       LOG K
```

```
                    53          1.0420

                CATION #        TOTAL

                    1           3.4860

                IONIC STRENGTH =   6.8308

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.34044E+01       0.97659E+00         0.34860E+01       0.0000
CATION #  2   0.19322E+01       0.57766E+00         0.33448E+01       0.0008
ANION #   1   0.57009E+01       0.83459E+00         0.68308E+01       0.0000

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =   40.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      1

           THE NUMBER OF ITERATIONS IS    14

                EQUATION        LOG K

                    53          1.0420

                CATION #        TOTAL

                    1           3.5920

                IONIC STRENGTH =   6.8830

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.35364E+01       0.98452E+00         0.35920E+01       0.0000
CATION #  2   0.18980E+01       0.57671E+00         0.32910E+01       0.0009
ANION #   1   0.58036E+01       0.84318E+00         0.68830E+01       0.0000


  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =  100.00     PRESS(BARS) =     1.02

  NUMBER CORRESPONDING TO SATURATED SOLID      53

           THE NUMBER OF ITERATIONS IS    17

                EQUATION        LOG K

                    53          1.3272

                IONIC STRENGTH =   7.4256

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  2   0.46088E+01       0.62067E+00         0.74256E+01       0.0008
ANION #   1   0.46088E+01       0.62067E+00         0.74256E+01       0.0008

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =  100.00     PRESS(BARS) =     1.02
```

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION LOG K

53 1.3272

CATION # TOTAL

1 1.7170

IONIC STRENGTH = 8.0612

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.14993E+01	0.87323E+00	0.17170E+01	0.0000
CATION #	2	0.37902E+01	0.59743E+00	0.63442E+01	0.0006
ANION #	1	0.56043E+01	0.69522E+00	0.80612E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION LOG K

53 1.3272

CATION # TOTAL

1 1.7440

IONIC STRENGTH = 8.0721

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.15248E+01	0.87431E+00	0.17440E+01	0.0000
CATION #	2	0.37783E+01	0.59706E+00	0.63281E+01	0.0006
ANION #	1	0.56219E+01	0.69646E+00	0.80721E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 12

EQUATION LOG K

53 1.3272

CATION # TOTAL

1 2.5670

IONIC STRENGTH = 8.4187

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.23313E+01	0.90817E+00	0.25670E+01	0.0000
CATION #	2	0.34297E+01	0.58610E+00	0.58517E+01	0.0009
ANION #	1	0.61934E+01	0.73567E+00	0.84187E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	3.4220

IONIC STRENGTH = 8.8096

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.32359E+01	0.94561E+00	0.34220E+01	0.0000
CATION #	2	0.30962E+01	0.57469E+00	0.53876E+01	0.0010
ANION #	1	0.68604E+01	0.77874E+00	0.88096E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	3.4780

IONIC STRENGTH = 8.8364

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.32976E+01	0.94814E+00	0.34780E+01	0.0000
CATION #	2	0.30754E+01	0.57394E+00	0.53584E+01	0.0010
ANION #	1	0.69069E+01	0.78164E+00	0.88364E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 16

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	4.2780

IONIC STRENGTH = 9.2346

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.42155E+01	0.98539E+00	0.42780E+01	0.0000
CATION #	2	0.27910E+01	0.56309E+00	0.49566E+01	0.0006
ANION #	1	0.76107E+01	0.82415E+00	0.92346E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 10

EQUATION	LOG K
53	1.3524

IONIC STRENGTH = 8.9531

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	2	0.47449E+01	0.52997E+00	0.89531E+01	-.0009
ANION #	1	0.47449E+01	0.52997E+00	0.89531E+01	-.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	1.7110

IONIC STRENGTH = 9.6823

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.12096E+01	0.70698E+00	0.17110E+01	0.0000
CATION #	2	0.40507E+01	0.50816E+00	0.79713E+01	-.0007
ANION #	1	0.55579E+01	0.57403E+00	0.96823E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	2.5670

IONIC STRENGTH = 10.1005

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.18525E+01	0.72167E+00	0.25670E+01	0.0000
CATION #	2	0.37433E+01	0.49689E+00	0.75335E+01	-.0009
ANION #	1	0.60143E+01	0.59545E+00	0.10100E+02	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 15

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	3.4220

IONIC STRENGTH = 10.5576

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.25170E+01	0.73552E+00	0.34220E+01	0.0000
CATION #	2	0.34622E+01	0.48520E+00	0.71356E+01	0.0010
ANION #	1	0.65025E+01	0.61590E+00	0.10558E+02	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K

```
                    53          1.3524

                CATION #        TOTAL

                    1           4.2780

                IONIC STRENGTH =  11.0590

              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.32004E+01       0.74811E+00         0.42780E+01       0.0000
CATION #  2   0.32065E+01       0.47286E+00         0.67810E+01       -.0009
ANION #   1   0.70213E+01       0.63490E+00         0.11059E+02       0.0000
```

3. SOLCALC Validation Test Case 3: Solubility in the NaCl-KCl-$MgCl_2$ system

The following is the "solcalc.out" output file of SOLCALC for solubility calculations in the NaCl-KCl-$MgCl_2$ system [two solids saturated: NaCl(s) (halite) and KCl(s) (sylvite) in an aqueous solution containing K^+, Na^+, Mg^{2+}, and Cl^- ions]. For each calculation, the temperature, pressure, and experimentally measured Mg^{2+} concentration (listed in the output file) are input interactively, and saturation with both halite and sylvite are also specified interactively.

```
  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   90.00     PRESS(BARS) =     0.71

  NUMBER CORRESPONDING TO SATURATED SOLID      20

  NUMBER CORRESPONDING TO SATURATED SOLID      53

            THE NUMBER OF ITERATIONS IS    15

                EQUATION       LOG K

                   20          1.5899
                   53          1.3018

                IONIC STRENGTH =   9.0981

              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.48702E+01       0.10400E+01         0.46829E+01       -.0003
CATION #  2   0.25087E+01       0.56820E+00         0.44152E+01       0.0008
ANION #   1   0.79856E+01       0.87773E+00         0.90981E+01       -.0003

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =   90.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      20

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

            THE NUMBER OF ITERATIONS IS    13

                EQUATION       LOG K
```

20	1.5899
53	1.3018

CATION #	TOTAL
3	0.1300

IONIC STRENGTH = 9.2405

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.46471E+01	0.10319E+01	0.45034E+01	-.0004
CATION #	2	0.23935E+01	0.55060E+00	0.43471E+01	0.0010
CATION #	3	0.13625E+00	0.10481E+01	0.13000E+00	0.0000
ANION #	1	0.83699E+01	0.91871E+00	0.91105E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.4000

IONIC STRENGTH = 9.5389

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.42092E+01	0.10169E+01	0.41393E+01	-.0003
CATION #	2	0.21680E+01	0.51625E+00	0.41996E+01	0.0007
CATION #	3	0.40956E+00	0.10239E+01	0.40000E+00	0.0000
ANION #	1	0.92404E+01	0.10111E+01	0.91389E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.6600

IONIC STRENGTH = 9.8300

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.38188E+01	0.10048E+01	0.38005E+01	-.0004
CATION #	2	0.19669E+01	0.48572E+00	0.40495E+01	0.0009
CATION #	3	0.66427E+00	0.10065E+01	0.66000E+00	0.0000
ANION #	1	0.10185E+02	0.11107E+01	0.91700E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 15

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.9200

IONIC STRENGTH = 10.1259

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.34564E+01	0.99488E+00	0.34742E+01	-.0003
CATION #	2	0.17803E+01	0.45745E+00	0.38917E+01	0.0006
CATION #	3	0.91527E+00	0.99486E+00	0.92000E+00	0.0000
ANION #	1	0.11253E+02	0.12224E+01	0.92059E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.1800

IONIC STRENGTH = 10.4277

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.31201E+01	0.98712E+00	0.31608E+01	-.0003
CATION #	2	0.16071E+01	0.43121E+00	0.37268E+01	0.0006
CATION #	3	0.11674E+01	0.98932E+00	0.11800E+01	0.0000

ANION # 1 0.12466E+02 0.13480E+01 0.92477E+01 -.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.4400

IONIC STRENGTH = 10.7366

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.28082E+01	0.98150E+00	0.28611E+01	-.0003
CATION #	2	0.14464E+01	0.40681E+00	0.35555E+01	0.0007
CATION #	3	0.14260E+01	0.99027E+00	0.14400E+01	0.0000
ANION #	1	0.13851E+02	0.14899E+01	0.92966E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.6700

IONIC STRENGTH = 11.0170

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.25513E+01	0.97833E+00	0.26079E+01	-.0004
CATION #	2	0.13141E+01	0.38660E+00	0.33991E+01	0.0007
CATION #	3	0.16650E+01	0.99703E+00	0.16700E+01	0.0000
ANION #	1	0.15245E+02	0.16310E+01	0.93470E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

```
 NUMBER CORRESPONDING TO SATURATED SOLID      20

 NUMBER CORRESPONDING TO SATURATED SOLID      53

 NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

          THE NUMBER OF ITERATIONS IS    18


               EQUATION       LOG K

                  20          1.5899
                  53          1.3018

               CATION #       TOTAL

                   3          1.9300

               IONIC STRENGTH =  11.3433

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.22814E+01       0.97682E+00         0.23356E+01       -.0003
CATION #  2   0.11751E+01       0.36519E+00         0.32178E+01       0.0007
CATION #  3   0.19535E+01       0.10122E+01         0.19300E+01       0.0000
ANION #   1   0.17049E+02       0.18111E+01         0.94133E+01       -.0003

 SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS


          TEMP(C) =   90.00     PRESS(BARS) =     1.00

 NUMBER CORRESPONDING TO SATURATED SOLID      20

 NUMBER CORRESPONDING TO SATURATED SOLID      53

 NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

          THE NUMBER OF ITERATIONS IS    19


               EQUATION       LOG K

                  20          1.5899
                  53          1.3018

               CATION #       TOTAL

                   3          2.1800

               IONIC STRENGTH =  11.6681

            ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.20414E+01       0.97750E+00         0.20884E+01       -.0004
CATION #  2   0.10514E+01       0.34590E+00         0.30397E+01       0.0008
CATION #  3   0.22569E+01       0.10353E+01         0.21800E+01       0.0000
ANION #   1   0.19053E+02       0.20081E+01         0.94881E+01       -.0004

 SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS


          TEMP(C) =   90.00     PRESS(BARS) =     1.00

 NUMBER CORRESPONDING TO SATURATED SOLID      20

 NUMBER CORRESPONDING TO SATURATED SOLID      53

 NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3
```

THE NUMBER OF ITERATIONS IS 19

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.4300

IONIC STRENGTH = 12.0052

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.18195E+01	0.98036E+00	0.18560E+01	-.0004
CATION #	2	0.93716E+00	0.32776E+00	0.28593E+01	0.0008
CATION #	3	0.25956E+01	0.10682E+01	0.24300E+01	0.0000
ANION #	1	0.21377E+02	0.22325E+01	0.95752E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 17

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.6700

IONIC STRENGTH = 12.3421

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.16229E+01	0.98523E+00	0.16472E+01	-.0005
CATION #	2	0.83589E+00	0.31133E+00	0.26849E+01	0.0010
CATION #	3	0.29655E+01	0.11107E+01	0.26700E+01	0.0000
ANION #	1	0.23967E+02	0.24779E+01	0.96721E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.9000

IONIC STRENGTH = 12.6785

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.14489E+01	0.99194E+00	0.14607E+01	-.0005
CATION #	2	0.74630E+00	0.29641E+00	0.25178E+01	0.0009
CATION #	3	0.33739E+01	0.11634E+01	0.29000E+01	0.0000
ANION #	1	0.26844E+02	0.27452E+01	0.97785E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.1200

IONIC STRENGTH = 13.0140

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.12954E+01	0.10003E+01	0.12950E+01	-.0004
CATION #	2	0.66719E+00	0.28282E+00	0.23590E+01	0.0008
CATION #	3	0.38283E+01	0.12270E+01	0.31200E+01	0.0000
ANION #	1	0.30027E+02	0.30349E+01	0.98940E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.3900

IONIC STRENGTH = 13.4458

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.11233E+01	0.10133E+01	0.11086E+01	-.0004
CATION #	2	0.57857E+00	0.26696E+00	0.21672E+01	0.0007
CATION #	3	0.44975E+01	0.13267E+01	0.33900E+01	0.0000
ANION #	1	0.34626E+02	0.34434E+01	0.10056E+02	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.6400

IONIC STRENGTH = 13.8670

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.97950E+00	0.10280E+01	0.95279E+00	-.0004
CATION #	2	0.50451E+00	0.25299E+00	0.19942E+01	0.0007
CATION #	3	0.52612E+01	0.14454E+01	0.36400E+01	0.0000
ANION #	1	0.39709E+02	0.38828E+01	0.10227E+02	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.8800

IONIC STRENGTH = 14.2919

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.85489E+00	0.10448E+01	0.81827E+00	-.0004
CATION #	2	0.44033E+00	0.24014E+00	0.18336E+01	0.0008

```
CATION #  3   0.61668E+01      0.15894E+01        0.38800E+01      0.0000
ANION #   1   0.45497E+02      0.43697E+01        0.10412E+02      -.0004

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   90.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      20

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

          THE NUMBER OF ITERATIONS IS    20

              EQUATION       LOG K

                 20          1.5899
                 53          1.3018

              CATION #       TOTAL

                 3           4.1600

              IONIC STRENGTH =  14.8143

            ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

CATION #  1   0.72533E+00      0.10674E+01        0.67951E+00      -.0004
CATION #  2   0.37359E+00      0.22576E+00        0.16548E+01      0.0009
CATION #  3   0.75088E+01      0.18050E+01        0.41600E+01      0.0000
ANION #   1   0.53624E+02      0.50331E+01        0.10654E+02      -.0004
```

4. SOLCALC Validation Test Case 4: Vapor pressure of KCl solutions as a function of concentration

The following is the "vpcalc.out" output file of SOLCALC showing the results of calculating the vapor pressure (VP) of KCl solutions at 300 °C as a function of concentration. For each calculation, the temperature, pressure, and K^+ and Cl^- concentrations are input interactively. The following concentrations of K^+ and Cl^- are used (note: m_{K+} is equal to m_{Cl-}): 0.549, 0.966, 1.392, 1.904, 2.954, 3.388, 4.283, and 4.528. These concentration values are used because experimental vapor pressure data are available at these concentrations from Zarembo et al. (1976).

TEMP(C)	TOTMOL	OSMO	**VP bar**	P0-VP bar	VP/P0	(P0-VP) mm Hg
300.00	1.0980	0.7224	**84.01**	1.82	0.97875	1368.11
300.00	1.9320	0.6957	**82.78**	3.06	0.96440	2291.88
300.00	2.7840	0.6815	**81.57**	4.26	0.95034	3196.84
300.00	3.8080	0.6732	**80.16**	5.68	0.93388	4256.99
300.00	5.9080	0.6715	**77.30**	8.53	0.90066	6395.72
300.00	6.7760	0.6743	**76.13**	9.70	0.88699	7275.27
300.00	8.5660	0.6832	**73.72**	12.11	0.85887	9085.76
300.00	9.0560	0.6861	**73.06**	12.77	0.85121	9579.23

5. SOLCALC Validation Test Case 5: Vapor pressure of mixed NaCl-KCl-$MgCl_2$ solutions as a function of total concentration and temperature

The following is the "vpcalc.out" output file of SOLCALC showing the results of calculating the vapor pressure of mixed NaCl-KCl-$MgCl_2$ solutions as a function of total concentration and temperature. For each calculation, the temperature, pressure, and Na^+, Mg^{2+}, Cl^-, and SO_4^- concentrations are input interactively. The ion concentrations were calculated from the (i) simulated seawater composition and (ii) concentrate multiple of seawater composition given by Liu and Lindsay (1971). The ion concentrations used as input are as follows:

Temp (°C)	Concentrate multiple	m_{Na}	m_{Mg}	m_{Cl}	m_{SO4}
75	2.8476	1.384361	0.19153	1.597931	0.084745
75	5.8158	2.827351	0.391171	3.263536	0.173078
100	1.4884	0.723586	0.10011	0.835216	0.044295
100	2.8528	1.386889	0.191879	1.600849	0.084899
100	5.8377	2.837998	0.392644	3.275825	0.17373
106	1.4888	0.72378	0.100137	0.83544	0.044307
125	1.4907	0.724704	0.100264	0.836506	0.044363
125	2.863	1.391847	0.192565	1.606572	0.085203
125	5.8811	2.859097	0.395563	3.300179	0.175022
150	1.4949	0.726746	0.100547	0.838863	0.044488
150	2.8813	1.400744	0.193796	1.616841	0.085747
150	5.9597	2.897308	0.400849	3.344286	0.177361
175	1.5018	0.7301	0.101011	0.842735	0.044694
175	2.9128	1.416058	0.195915	1.634518	0.086685
175	6.1004	2.965709	0.410313	3.423239	0.181548
200	1.5126	0.73535	0.101737	0.848795	0.045015
200	2.963	1.440462	0.199291	1.662687	0.088179
200	6.3279	3.076309	0.425615	3.550901	0.188318
225	1.5291	0.743372	0.102847	0.858054	0.045506
225	3.0415	1.478625	0.204571	1.706738	0.090515
225	6.698	3.256233	0.450507	3.758583	0.199332
250	3.1648	1.538568	0.212864	1.775928	0.094184
250	7.3078	3.552687	0.491523	4.100772	0.21748
275	3.3622	1.634534	0.226142	1.886699	0.100059
275	8.3482	4.058477	0.5615	4.684592	0.248442
300	3.6957	1.796665	0.248573	2.073842	0.109984
300	10.2027	4.960043	0.686234	5.725245	0.303632

TEMP(C)	TOTMOL	OSMO	VP bar	P0-VP bar	VP/P0	**(P0-VP) mm Hg**
75.00	3.2586	0.9629	0.36	0.02	0.94452	**16.05**
75.00	6.6551	1.0979	0.34	0.05	0.87569	**35.96**
100.00	1.7032	0.9021	0.99	0.03	0.97221	**21.12**
100.00	3.2645	0.9493	0.96	0.06	0.94482	**41.94**
100.00	6.6802	1.0753	0.89	0.12	0.87685	**93.60**
106.00	1.7037	0.8990	1.22	0.03	0.97224	**26.03**
125.00	1.7058	0.8878	2.26	0.06	0.97231	**48.19**
125.00	3.2762	0.9302	2.19	0.13	0.94510	**95.54**

125.00	6.7299	1.0460	2.04	0.28	0.87788	**212.53**
150.00	1.7106	0.8698	4.63	0.13	0.97231	**98.80**
150.00	3.2971	0.9064	4.50	0.26	0.94522	**195.48**
150.00	6.8198	1.0114	4.18	0.58	0.87826	**434.37**
175.00	1.7185	0.8482	8.67	0.25	0.97218	**186.07**
175.00	3.3332	0.8780	8.43	0.49	0.94500	**367.90**
175.00	6.9808	0.9725	7.82	1.09	0.87736	**820.34**
200.00	1.7309	0.8226	15.10	0.44	0.97188	**327.64**
200.00	3.3906	0.8447	14.67	0.86	0.94435	**648.53**
200.00	7.2411	0.9289	13.59	1.95	0.87471	**1460.07**
225.00	1.7498	0.7921	24.75	0.73	0.97136	**547.41**
225.00	3.4804	0.8057	24.03	1.45	0.94304	**1088.52**
225.00	7.6647	0.8802	22.15	3.33	0.86930	**2497.72**
250.00	3.6215	0.7594	37.38	2.35	0.94080	**1764.35**
250.00	8.3625	0.8257	34.15	5.58	0.85955	**4186.03**
275.00	3.8474	0.7026	55.70	3.73	0.93720	**2799.49**
275.00	9.5530	0.7636	50.07	9.36	0.84255	**7018.41**
300.00	4.2291	0.6287	79.96	5.87	0.93156	**4406.32**
300.00	11.6752	0.6883	69.87	15.96	0.81405	**11971.52**

January 24, 2002

The following is an alternative approach to the chemical divide analysis shown on page 9 of this notebook. See the discussion of the chemical divide approach in Spencer (2000; Reviews in Mineralogy **40**, p. 175). Two of the waters evolve into an alkaline brine, two from neutral brines, and one evolves into a Ca-Cl brine.

SampleID	**Ave-J13 Harrar**		**NRG-6/158.2-158.6**		**NRG-6/244.6**		**UZ-14/1542.3**		**UZ-14-85.2-85.6**	
Water Type	Na-Ca-HCO3		Ca-Mg-Cl-SO4		Na-Ca-SO4-Cl		Na-HCO3		Ca-Na-HCO3-Cl-SO4	
Reference	Harrar et al. 1990		Yang et al. 1998		Yang et al. 1998		Yang et al. 1996		Yang et al. 1996	
Ph (Lab)	7.41		6.8		7.2		8.6		6.9	
Cations	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)
Na+	4.58E+01	1.99E+00	3.56E+01	1.55E+00	7.20E+01	3.13E+00	2.07E+02	9.00E+00	4.35E+01	1.89E+00
K+	5.04E+00	1.29E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mg++	2.01E+00	1.65E-01	2.33E+01	1.92E+00	4.90E+00	4.03E-01	5.00E-01	4.11E-02	1.32E+01	1.09E+00
Ca++	1.30E+01	6.49E-01	1.22E+02	6.09E+00	3.30E+01	1.65E+00	3.60E+00	1.80E-01	4.99E+01	2.49E+00
Anions	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)	(mg/l)	(meq/l)
F-	2.18E+00	1.15E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cl-	7.14E+00	2.01E-01	1.85E+02	5.22E+00	4.90E+01	1.38E+00	2.00E+01	5.64E-01	6.00E+01	1.69E+00
SO4--	1.84E+01	3.83E-01	1.59E+02	3.31E+00	1.15E+02	2.39E+00	2.80E+01	5.83E-01	6.60E+01	1.37E+00
NO3-	8.78E+00	1.42E-01	3.20E+01	5.16E-01	4.00E+01	6.45E-01	4.00E+00	6.45E-02	2.20E+01	3.55E-01
HCO3-	1.29E+02	2.11E+00	3.40E+01	5.57E-01	6.10E+01	1.00E+00	3.84E+02	6.29E+00	1.31E+02	2.15E+00
CO3--	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.60E+01	1.53E+00	0.00E+00	0.00E+00
Chemical divide analysis:										
alkalinity =		2.11E+00		5.57E-01		1.00E+00		7.83E+00		2.15E+00
Is Ca2+>alk?		no		yes		yes		no		yes
		Alkaline water						Alkaline water		
If yes (i.e., Ca>alk), then is Ca > (SO4+alkalinity)?				3.87E+00		3.39E+00				3.52E+00
				Ca-Cl brine		Neutral brine				Neutral brine

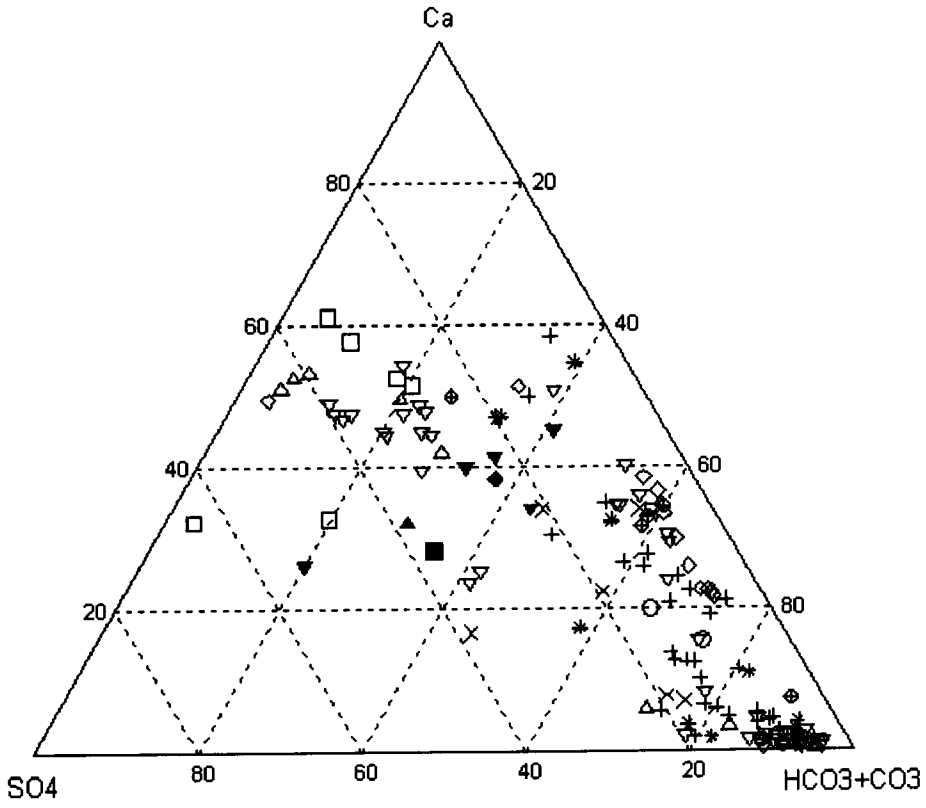
A similar chemical divide shown in the previous table was done on the Yang et al. (1996, 1998) YM water data, which are plotted on page 18. The analysis show that of the total 152 analyses, 12 compositions resulted in Ca-Cl brines, 27 formed neutral brines, and 113 formed alkaline brines. Thus, approximately 25 % of the YM water compositions reported by Yang et al. (1996, 1998) could result in brines rich in Mg and/or Ca. The brines, if evaporated completely, could form salt mixtures with low deliquescence points.

The following is a table of YM water compositions from Yang et al. that are close to the dividing line between the alkaline waters and the neutral waters (see page 18 of this notebook). The compositions will be provided to Lietai Yang, who will do the OLI ESP simulation of evaporation. Units in millimoles/liter.

SampleID	pHLab	Na	K	Mg	Ca	F	Cl	SO4
UE-25 NRG-6	7.4	4.31927	0	0.172768	0.606287	n.a.	2.17189	0.801616
UE-25 NRG-7a	8.3	3.566768	0	0.152201	1.072854	n.a.	1.511861	0.681894
UE-25 UZ-N2	0	1.091779	0	0.160428	0.359281	n.a.	0.282064	0.218623
USW SD-9	7.5	4.132232	0	0.390786	1.072854	n.a.	1.805207	1.290914
USW UZ-14-a	0	2.131361	0	0.185109	1.546906	n.a.	2.453953	0.468477
USW UZ-14-b	6.9	1.892127	0	0.542987	1.24501	n.a.	1.692382	0.687099
USW UZ-14-c	0	1.739887	0.161125	0.12752	0.923154	n.a.	0.203086	0.596527
USW UZ-14-d	7	1.796433	0	0.567668	1.27495	n.a.	1.24108	0.864079
USW UZ-14-e	8.3	3.827751	0.148338	0.168655	1.122754	n.a.	0.437199	2.321563

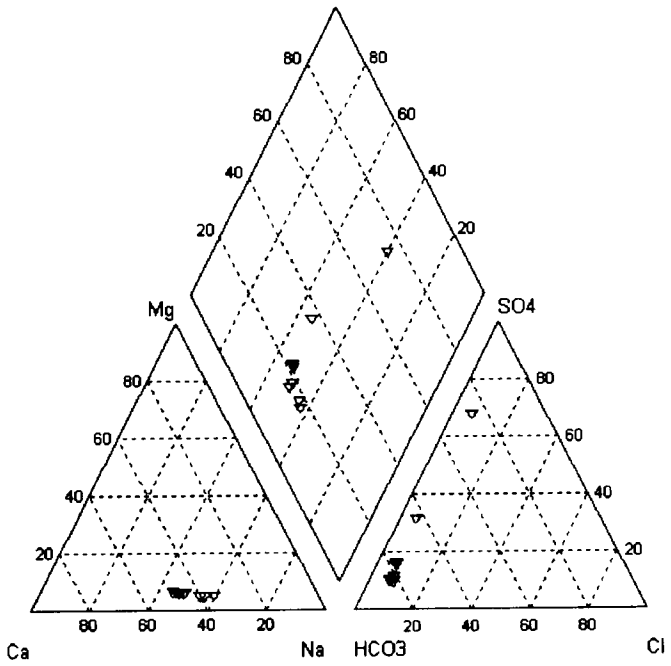
SampleID	NO3	HCO3	CO3	SIO2	Al
UE-25 NRG-6	0.7579423	1.507999	0	1.021801	3.71E-02
UE-25 NRG-7a	0.7047251	2.098085	0	1.146613	3.71E-02
UE-25 UZ-N2	0.4402516	0.953973	0	9.65E-02	0
USW SD-9	3.06E-02	1.999738	0	0.97354	0
USW UZ-14-a	0.2741493	2.78652	0	0.732235	0
USW UZ-14-b	0.3547815	2.147259	0	1.494425	1.11E-02
USW UZ-14-c	0.2048057	2.360346	0	0.356133	0
USW UZ-14-d	0.3709079	2.098085	0	1.527709	0
USW UZ-14-e	0	1.739116	0	0.128141	0

In the following page, the compositions listed in the above table is plotted in a chemical-divide type of ternary plot (as solid symbols).


Ca
80
20
60
40
40
60
20
80
SO4
80
60
40
20
HCO3+CO3

February 13, 2002

In preparation for conducting water-rock experiments to determine the potential thermal-chemical effects on the hydraulic properties of Calico Hills vitric tuffs, the database of Yucca Mountain groundwater compositions presented by Yang et al. (1996, 1998) was evaluated. The perched waters in well USW UZ-14 were selected as the most appropriate. A Piper diagram of their chemical compositions is shown below. The solid triangle represents the composition selected for the water-rock experiment.



Thermodynamic calculations were done using Geochemist's Workbench to determine the mineral saturation for the selected composition. The calculation is necessary because the UZ-14 samples were exposed to a higher pCO2, and precipitation of minerals like calcite is expected when exposed to atmospheric pCO2 conditions. The GWB calculations are documented as follows:

1) UZ-14 perched water; log pCO2 = -2.5 atm (value at depth)

React> show

Temperature is 25 C
Thermo dataset: D:\Gwb\Gtdata\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 H+)	fugacity = .00316227766
Na+	total mg/l = 35
K+	total mg/l = 4.1
Ca++	total mg/l = 31
Mg++	total mg/l = 2.5

Cl- total mg/l = 7
SO4-- total mg/l = 24.2
HCO3- total mg/l = 146.4 (charge balance)
NO3- (swapped for NH3(aq)) total mg/l = 17.1
SiO2(aq) total mg/l = 40.7

No reactants specified.

React> go

Solving for initial system.
...suppressed loading of: Dolomite
...suppressed loading of: Dolomite-ord
...suppressed loading of: Quartz
...suppressed loading of: Talc

Loaded: 321 aqueous species,
124 minerals,
22 gases,
0 surface species,
11 elements,
7 oxides.

N-R converged in 12 its., resmax = 4.09e-015, Xi = 0.0000
Charge balance: HCO3- molality adjusted from .002399 to .002403

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

Removing CO2(g) from basis vector
Swapping CO2(aq) in for CO2(g)
4 supersaturated phases, most = Tridymite
Swapping Tridymite in for SiO2(aq)
N-R converged in 9 its., resmax = 1.25e-014, Xi = 0.0000

No reaction path specified.

```
Step #     0              Xi = 0.0000
Temperature =  25.0 C     Pressure =  1.013 bars
pH =  7.654               log fO2 =   -0.699
Eh =   0.7659 volts       pe =  12.9473
Ionic strength      =     0.004389
Activity of water   =     0.999993
Solvent mass        =     1.000000 kg
Solution mass       =     1.000326 kg
Solution density    =     1.013    g/cm3
Chlorinity          =     0.000197 molal
Dissolved solids    =          326 mg/kg sol'n
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002353	143.6	0.9311	-2.6593
Na+	0.001516	34.84	0.9311	-2.8503

Ca++	0.0007397	29.64	0.7591	-3.2506
SiO2(aq)	0.0006735	40.46	1.0000	-3.1716
NO3-	0.0002750	17.05	0.9298	-3.5923
O2(aq)	0.0002528	8.086	1.0000	-3.5973
SO4--	0.0002339	22.46	0.7508	-3.7554
Cl-	0.0001974	6.995	0.9298	-3.7363
CO2(aq)	0.0001074	4.726	1.0000	-3.9689
K+	0.0001047	4.093	0.9298	-4.0116
Mg++	9.723e-005	2.363	0.7670	-4.1274
CaHCO3+	1.472e-005	1.487	0.9311	-4.8632
CaSO4(aq)	1.274e-005	1.733	1.0000	-4.8950
CO3--	6.159e-006	0.3695	0.7529	-5.3337
CaCO3(aq)	5.530e-006	0.5533	1.0000	-5.2573
NaHCO3(aq)	4.411e-006	0.3704	1.0000	-5.3555
HSiO3-	3.641e-006	0.2806	0.9311	-5.4698
MgSO4(aq)	3.379e-006	0.4066	1.0000	-5.4712
MgHCO3+	1.905e-006	0.1625	0.9311	-5.7510
NaSO4-	1.759e-006	0.2093	0.9311	-5.7857
CaNO3+	7.729e-007	0.07887	0.9311	-6.1429
OH-	4.904e-007	0.008337	0.9305	-6.3408
MgCO3(aq)	3.294e-007	0.02777	1.0000	-6.4823
NaHSiO3(aq)	2.130e-007	0.02131	1.0000	-6.6716
KSO4-	1.392e-007	0.01881	0.9311	-6.8874
NaCl(aq)	4.329e-008	0.002529	1.0000	-7.3636
H+	2.365e-008	2.383e-005	0.9372	-7.6543
NaCO3-	2.298e-008	0.001907	0.9311	-7.6696
CaCl+	2.231e-008	0.001684	0.9311	-7.6826
MgCl+	1.077e-008	0.0006436	0.9311	-7.9987

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.8277s/sat	Cristobalite(bet	-0.1663
Tridymite	0.6562s/sat	Aragonite	-0.2487
Chalcedony	0.5565s/sat	Talc	-0.2811
Cristobalite(alp	0.2772s/sat	SiO2(am)	-0.4580
Dolomite	0.0986s/sat	Monohydrocalcite	-0.9380
Dolomite-ord	0.0986s/sat	Magnesite	-1.4260
Coesite	0.0177s/sat	Dolomite-dis	-1.4458
Calcite	-0.1043	Gypsum	-2.5238
Ice	-0.1387	Anhydrite	-2.6997

(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)	0.003162	-2.500
HCl(g)	2.013e-018	-17.696
N2(g)	8.853e-019	-18.053
NO2(g)	1.929e-019	-18.715
NO(g)	2.892e-025	-24.539
Cl2(g)	2.628e-028	-27.580
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-048	-47.208
SO2(g)	1.013e-055	-54.994

NH3(g)	1.125e-068	-67.949
Na(g)	6.908e-076	-75.161
K(g)	9.132e-078	-77.039
Mg(g)	5.376e-130	-129.270
H2S(g)	6.158e-143	-142.211
CH4(g)	3.890e-145	-144.410
Ca(g)	6.010e-152	-151.221
C(g)	3.246e-189	-188.489
Si(g)	2.984e-220	-219.525
S2(g)	2.154e-228	-227.667
C2H4(g)	7.603e-237	-236.119

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Ca++	0.0007735	0.0007735	30.99		
Cl-	0.0001974	0.0001974	6.998		
H+	-0.0001847	-0.0001847	-0.1861		
H2O	55.51	55.51	9.997e+005		
HCO3-	0.002494	0.002494	152.1		
K+	0.0001049	0.0001049	4.099		
Mg++	0.0001029	0.0001029	2.499		
NH3(aq)	0.0002758	0.0002758	4.695		
Na+	0.001522	0.001522	34.99		
O2(aq)	0.0008043	0.0008043	25.73		
SO4--	0.0002519	0.0002519	24.19		
SiO2(aq)	0.0006774	0.0006774	40.69		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.0007735	0.0007735	30.99		
Carbon	0.002494	0.002494	29.95		
Chlorine	0.0001974	0.0001974	6.998		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001029	0.0001029	2.499		
Nitrogen	0.0002758	0.0002758	3.862		
Oxygen	55.52	55.52	8.880e+005		
Potassium	0.0001049	0.0001049	4.099		
Silicon	0.0006774	0.0006774	19.02		
Sodium	0.001522	0.001522	34.99		
Sulfur	0.0002519	0.0002519	8.075		

Step #	0	Xi	= 0.0000
Temperature =	25.0 C	Pressure =	1.013 bars
pH =	7.666	log fO2 =	-0.699
Eh =	0.7652 volts	pe =	12.9361
Ionic strength	=	0.004389	
Activity of water	=	0.999993	
Solvent mass	=	1.000000 kg	
Solution mass	=	1.000294 kg	
Solution density	=	1.013 g/cm3	
Chlorinity	=	0.000197 molal	
Dissolved solids	=	294 mg/kg sol'n	

Minerals in system	moles	log moles	grams	volume (cm3)
Tridymite	0.0005278	-3.277	0.03172	
(total)			0.03172	0.0000*

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002356	143.7	0.9311	-2.6589
Na+	0.001516	34.85	0.9311	-2.8502
Ca++	0.0007396	29.63	0.7591	-3.2507
NO3-	0.0002750	17.05	0.9298	-3.5923
O2(aq)	0.0002528	8.086	1.0000	-3.5973
SO4--	0.0002339	22.46	0.7508	-3.7554
Cl-	0.0001974	6.995	0.9298	-3.7363
SiO2(aq)	0.0001487	8.930	1.0000	-3.8278
CO2(aq)	0.0001048	4.610	1.0000	-3.9797
K+	0.0001047	4.093	0.9298	-4.0116
Mg++	9.722e-005	2.362	0.7670	-4.1275
CaHCO3+	1.473e-005	1.488	0.9311	-4.8629
CaSO4(aq)	1.273e-005	1.733	1.0000	-4.8950
CO3--	6.326e-006	0.3795	0.7529	-5.3221
CaCO3(aq)	5.679e-006	0.5683	1.0000	-5.2457
NaHCO3(aq)	4.416e-006	0.3708	1.0000	-5.3550
MgSO4(aq)	3.379e-006	0.4066	1.0000	-5.4712
MgHCO3+	1.907e-006	0.1627	0.9311	-5.7506
NaSO4-	1.759e-006	0.2094	0.9311	-5.7857
HSiO3-	8.246e-007	0.06355	0.9311	-6.1147
CaNO3+	7.727e-007	0.07886	0.9311	-6.1430
OH-	5.032e-007	0.008556	0.9305	-6.3295
MgCO3(aq)	3.383e-007	0.02852	1.0000	-6.4706
KSO4-	1.392e-007	0.01881	0.9311	-6.8874
NaHSiO3(aq)	4.825e-008	0.004828	1.0000	-7.3165
NaCl(aq)	4.329e-008	0.002529	1.0000	-7.3636
NaCO3-	2.361e-008	0.001959	0.9311	-7.6579
H+	2.305e-008	2.322e-005	0.9372	-7.6656
CaCl+	2.230e-008	0.001684	0.9311	-7.6826
MgCl+	1.077e-008	0.0006435	0.9311	-7.9987

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.1715s/sat	Coesite	-0.6385
Dolomite-ord	0.1218s/sat	Cristobalite(bet	-0.8225
Dolomite	0.1218s/sat	Monohydrocalcite	-0.9264
Tridymite	0.0000 sat	SiO2(am)	-1.1142
Calcite	-0.0927	Magnesite	-1.4143
Chalcedony	-0.0997	Dolomite-dis	-1.4226
Ice	-0.1387	Gypsum	-2.5238
Aragonite	-0.2371	Anhydrite	-2.6997
Cristobalite(alp	-0.3790	Talc	-2.8385

(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)	0.003085	-2.511
HCl(g)	1.962e-018	-17.707
N2(g)	8.406e-019	-18.075
NO2(g)	1.880e-019	-18.726
NO(g)	2.818e-025	-24.550
Cl2(g)	2.496e-028	-27.603
H2(g)	6.267e-042	-41.203
CO(g)	6.037e-048	-47.219
SO2(g)	9.622e-056	-55.017
NH3(g)	1.096e-068	-67.960
Na(g)	7.090e-076	-75.149
K(g)	9.371e-078	-77.028
Mg(g)	5.661e-130	-129.247
H2S(g)	5.848e-143	-142.233
CH4(g)	3.794e-145	-144.421
Ca(g)	6.328e-152	-151.199
C(g)	3.166e-189	-188.499
Si(g)	6.585e-221	-220.181
S2(g)	1.942e-228	-227.712
C2H4(g)	7.234e-237	-236.141

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Ca++	0.0007735	0.0007735	30.99		
Cl-	0.0001974	0.0001974	6.998		
H+	-0.0001847	-0.0001847	-0.1861		
H2O	55.51	55.51	9.997e+005		
HCO3-	0.002494	0.002494	152.1		
K+	0.0001049	0.0001049	4.099		
Mg++	0.0001029	0.0001029	2.499		
NH3(aq)	0.0002758	0.0002758	4.695		
Na+	0.001522	0.001522	34.99		
O2(aq)	0.0008043	0.0008043	25.73		
SO4--	0.0002519	0.0002519	24.19		
SiO2(aq)	0.0006774	0.0001495	8.982		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.0007735	0.0007735	30.99		
Carbon	0.002494	0.002494	29.95		
Chlorine	0.0001974	0.0001974	6.998		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001029	0.0001029	2.499		
Nitrogen	0.0002758	0.0002758	3.862		
Oxygen	55.52	55.52	8.880e+005		
Potassium	0.0001049	0.0001049	4.099		
Silicon	0.0006774	0.0001495	4.199		
Sodium	0.001522	0.001522	34.99		
Sulfur	0.0002519	0.0002519	8.076		

2) UZ-14 perched water; log pCO2 = -3.5 atm (atmospheric value)

React> log f CO2(g) = -3.5
React> go

Solving for initial system.
...suppressed loading of: Dolomite
...suppressed loading of: Dolomite-ord
...suppressed loading of: Quartz
...suppressed loading of: Talc

Loaded: 321 aqueous species,
124 minerals,
22 gases,
0 surface species,
11 elements,
7 oxides.

N-R converged in 12 its., resmax = 1.78e-014, Xi = 0.0000
Charge balance: HCO3- molality adjusted from .002399 to .002403

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

Removing CO2(g) from basis vector
Swapping CO3-- in for CO2(g)
10 supersaturated phases, most = Antigorite
Swapping Antigorite in for CO3--
N-R converged in 10 its., resmax = 8.64e-015, Xi = 0.0000
6 supersaturated phases, most = Tremolite
Swapping Tremolite in for Mg++
N-R converged in 11 its., resmax = 5.29e-014, Xi = 0.0000
Antigorite is undersaturated
Swapping Mg++ in for Antigorite
N-R converged in 10 its., resmax = 9.84e-014, Xi = 0.0000
5 supersaturated phases, most = Tridymite
Swapping Tridymite in for SiO2(aq)
N-R converged in 10 its., resmax = 1.07e-013, Xi = 0.0000
4 supersaturated phases, most = Antigorite
Swapping Antigorite in for Mg++
N-R converged in 11 its., resmax = 3.43e-014, Xi = 0.0000
Tremolite is undersaturated
Swapping CO3-- in for Tremolite
N-R converged in 9 its., resmax = 9.91e-013, Xi = 0.0000
2 supersaturated phases, most = Calcite
Swapping Calcite in for CO3--
N-R converged in 17 its., resmax = 7.7e-013, Xi = 0.0000
Antigorite is undersaturated
Swapping Mg++ in for Antigorite
N-R converged in 12 its., resmax = 1.74e-013, Xi = 0.0000

No reaction path specified.

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

pH = 8.615 log fO2 = -0.699
Eh = 0.7091 volts pe = 11.9864
Ionic strength = 0.004317
Activity of water = 0.999993
Solvent mass = 1.000000 kg
Solution mass = 1.000315 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.000197 molal
Dissolved solids = 314 mg/kg sol'n

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002150	131.1	0.9316	-2.6984
Na+	0.001515	34.81	0.9316	-2.8505
Ca++	0.0007037	28.19	0.7607	-3.2714
SiO2(aq)	0.0006437	38.67	1.0000	-3.1913
NO3-	0.0002750	17.05	0.9303	-3.5920
O2(aq)	0.0002528	8.086	1.0000	-3.5973
SO4--	0.0002345	22.52	0.7524	-3.7534
Cl-	0.0001974	6.995	0.9303	-3.7361
K+	0.0001047	4.093	0.9303	-4.0113
Mg++	9.512e-005	2.311	0.7684	-4.1362
CO3--	5.133e-005	3.079	0.7545	-4.4119
CaCO3(aq)	4.403e-005	4.405	1.0000	-4.3563
HSiO3-	3.178e-005	2.449	0.9316	-4.5286
CaHCO3+	1.281e-005	1.295	0.9316	-4.9231
CaSO4(aq)	1.220e-005	1.660	1.0000	-4.9138
CO2(aq)	1.074e-005	0.4726	1.0000	-4.9689
OH-	4.479e-006	0.07615	0.9310	-5.3799
NaHCO3(aq)	4.030e-006	0.3384	1.0000	-5.3947
MgSO4(aq)	3.328e-006	0.4004	1.0000	-5.4779
MgCO3(aq)	2.697e-006	0.2273	1.0000	-5.5692
NaHSiO3(aq)	1.860e-006	0.1861	1.0000	-5.7305
NaSO4-	1.765e-006	0.2101	0.9316	-5.7839
MgHCO3+	1.706e-006	0.1455	0.9316	-5.7988
CaNO3+	7.368e-007	0.07519	0.9316	-6.1634
NaCO3-	1.918e-007	0.01591	0.9316	-6.7480
KSO4-	1.398e-007	0.01889	0.9316	-6.8851
NaCl(aq)	4.329e-008	0.002529	1.0000	-7.3636
CaOH+	3.346e-008	0.001910	0.9316	-7.5062
CaCl+	2.126e-008	0.001605	0.9316	-7.7031
MgCl+	1.056e-008	0.0006308	0.9316	-8.0071

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	42.8287s/sat	Coesite	-0.0020
Tremolite	6.6226s/sat	Monohydrocalcite	-0.0370
Talc	5.3795s/sat	Ice	-0.1387
Sepiolite	2.7856s/sat	Cristobalite(bet	-0.1860
Dolomite	1.9126s/sat	Diopside	-0.2935
Dolomite-ord	1.9126s/sat	SiO2(am)	-0.4777
Chrysotile	1.7749s/sat	Magnesite	-0.5129
Quartz	0.8080s/sat	Anthophyllite	-0.6667

Calcite	0.7967s/sat	Enstatite	-1.4239
Aragonite	0.6523s/sat	Huntite	-2.3134
Tridymite	0.6365s/sat	Gypsum	-2.5426
Chalcedony	0.5368s/sat	Anhydrite	-2.7185
Dolomite-dis	0.3682s/sat	Okenite	-2.8052
Cristobalite(alp	0.2575s/sat	Wollastonite	-2.9928

(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
HCl(g)	2.204e-019	-18.657
NO2(g)	2.113e-020	-19.675
N2(g)	1.061e-020	-19.974
NO(g)	3.166e-026	-25.499
Cl2(g)	3.150e-030	-29.502
H2(g)	6.267e-042	-41.203
CO(g)	6.189e-049	-48.208
SO2(g)	1.219e-057	-56.914
NH3(g)	1.232e-069	-68.909
Na(g)	6.311e-075	-74.200
K(g)	8.351e-077	-76.078
Mg(g)	4.401e-128	-127.356
H2S(g)	7.408e-145	-144.130
CH4(g)	3.890e-146	-145.410
Ca(g)	4.785e-150	-149.320
C(g)	3.246e-190	-189.489
Si(g)	2.852e-220	-219.545
S2(g)	3.116e-232	-231.506
C2H4(g)	7.603e-239	-238.119

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Ca++	0.0007735	0.0007735	30.99		
Cl-	0.0001974	0.0001974	6.998		
H+	-0.0004014	-0.0004014	-0.4045		
H2O	55.51	55.51	9.997e+005		
HCO3-	0.002277	0.002277	138.9		
K+	0.0001049	0.0001049	4.099		
Mg++	0.0001029	0.0001029	2.499		
NH3(aq)	0.0002758	0.0002758	4.695		
Na+	0.001522	0.001522	34.99		
O2(aq)	0.0008043	0.0008043	25.73		
SO4--	0.0002519	0.0002519	24.19		
SiO2(aq)	0.0006774	0.0006774	40.69		

		In fluid		Sorbed	
Elemental composition	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.0007735	0.0007735	30.99		
Carbon	0.002277	0.002277	27.34		
Chlorine	0.0001974	0.0001974	6.998		

Hydrogen	111.0	111.0	1.119e+005
Magnesium	0.0001029	0.0001029	2.499
Nitrogen	0.0002758	0.0002758	3.862
Oxygen	55.52	55.52	8.880e+005
Potassium	0.0001049	0.0001049	4.099
Silicon	0.0006774	0.0006774	19.02
Sodium	0.001522	0.001522	34.99
Sulfur	0.0002519	0.0002519	8.075

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.914 log fO2 = -0.699
Eh = 0.7505 volts pe = 12.6874
Ionic strength = 0.003934
Activity of water = 0.999993
Solvent mass = 1.000001 kg
Solution mass = 1.000267 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.000197 molal
Dissolved solids = 266 mg/kg sol'n

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0001573	-3.803	0.01574	0.005810
Tridymite	0.0005272	-3.278	0.03168	
(total)			0.04742	0.005810*

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002036	124.2	0.9344	-2.7207
Na+	0.001517	34.86	0.9344	-2.8486
Ca++	0.0005878	23.55	0.7691	-3.3448
NO3-	0.0002752	17.06	0.9332	-3.5905
O2(aq)	0.0002528	8.086	1.0000	-3.5973
SO4--	0.0002360	22.66	0.7614	-3.7455
Cl-	0.0001974	6.996	0.9332	-3.7348
SiO2(aq)	0.0001487	8.930	1.0000	-3.8278
K+	0.0001047	4.093	0.9332	-4.0100
Mg++	9.716e-005	2.361	0.7763	-4.1225
CO2(aq)	5.125e-005	2.255	1.0000	-4.2903
CaSO4(aq)	1.049e-005	1.428	1.0000	-4.9792
CaHCO3+	1.025e-005	1.036	0.9344	-5.0189
CO3--	9.593e-006	0.5755	0.7634	-5.1353
CaCO3(aq)	7.031e-006	0.7035	1.0000	-5.1530
NaHCO3(aq)	3.844e-006	0.3228	1.0000	-5.4152
MgSO4(aq)	3.497e-006	0.4208	1.0000	-5.4563
NaSO4-	1.800e-006	0.2143	0.9344	-5.7741
MgHCO3+	1.667e-006	0.1422	0.9344	-5.8075
HSiO3-	1.457e-006	0.1123	0.9344	-5.8660
OH-	8.890e-007	0.01512	0.9338	-6.0808
CaNO3+	6.226e-007	0.06354	0.9344	-6.2353
MgCO3(aq)	5.262e-007	0.04435	1.0000	-6.2789
KSO4-	1.424e-007	0.01924	0.9344	-6.8759
NaHSiO3(aq)	8.587e-008	0.008592	1.0000	-7.0661
NaCl(aq)	4.362e-008	0.002548	1.0000	-7.3604

NaCO3-	3.631e-008	0.003013	0.9344	-7.4695
CaCl+	1.796e-008	0.001356	0.9344	-7.7752
H+	1.296e-008	1.306e-005	0.9400	-7.9143
MgCl+	1.090e-008	0.0006510	0.9344	-7.9922

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	0.4062s/sat	Coesite	-0.6385
Dolomite	0.4062s/sat	Cristobalite(bet	-0.8225
Quartz	0.1715s/sat	Monohydrocalcite	-0.8337
Tridymite	0.0000 sat	SiO2(am)	-1.1142
Calcite	0.0000 sat	Dolomite-dis	-1.1382
Chalcedony	-0.0997	Magnesite	-1.2226
Ice	-0.1387	Talc	-1.3315
Aragonite	-0.1444	Gypsum	-2.6080
Cristobalite(alp	-0.3790	Anhydrite	-2.7839

(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)	0.001509	-2.821
HCl(g)	1.110e-018	-17.955
N2(g)	2.697e-019	-18.569
NO2(g)	1.065e-019	-18.973
NO(g)	1.596e-025	-24.797
Cl2(g)	7.997e-029	-28.097
H2(g)	6.267e-042	-41.203
CO(g)	2.953e-048	-47.530
SO2(g)	3.132e-056	-55.504
NH3(g)	6.210e-069	-68.207
Na(g)	1.262e-075	-74.899
K(g)	1.667e-077	-76.778
Mg(g)	1.800e-129	-128.745
H2S(g)	1.904e-143	-142.720
CH4(g)	1.856e-145	-144.731
Ca(g)	1.601e-151	-150.795
C(g)	1.549e-189	-188.810
Si(g)	6.585e-221	-220.181
S2(g)	2.058e-229	-228.687
C2H4(g)	1.731e-237	-236.762

		In fluid		Sorbed	
Original basis	total moles	moles	mg/kg	moles	mg/kg
Ca++	0.0007735	0.0006162	24.69		
Cl-	0.0001974	0.0001974	6.998		
H+	-0.0004014	-0.0002441	-0.2460		
H2O	55.51	55.51	9.997e+005		
HCO3-	0.002277	0.002120	129.3		
K+	0.0001049	0.0001049	4.099		
Mg++	0.0001029	0.0001029	2.499		
NH3(aq)	0.0002758	0.0002758	4.696		

Na+	0.001522	0.001522	34.99
O2(aq)	0.0008043	0.0008043	25.73
SO4--	0.0002519	0.0002519	24.19
SiO2(aq)	0.0006774	0.0001502	9.023

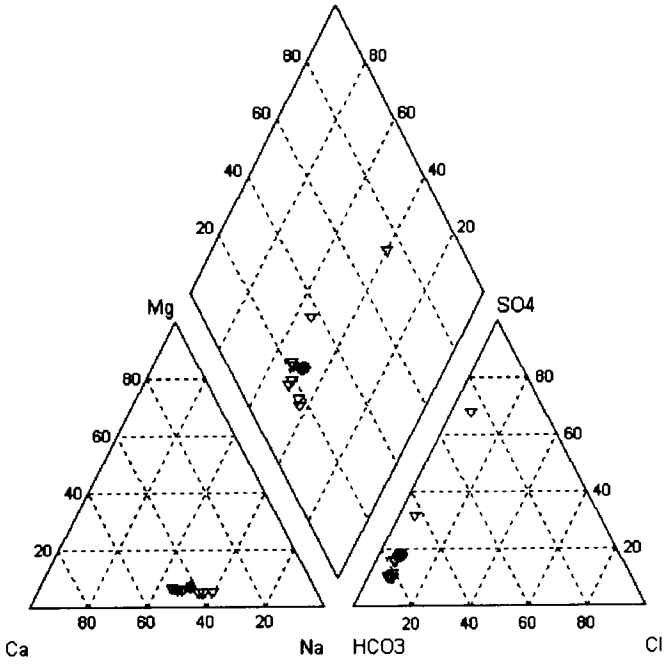
Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.0007735	0.0006162	24.69		
Carbon	0.002277	0.002120	25.46		
Chlorine	0.0001974	0.0001974	6.998		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001029	0.0001029	2.499		
Nitrogen	0.0002758	0.0002758	3.862		
Oxygen	55.52	55.52	8.880e+005		
Potassium	0.0001049	0.0001049	4.099		
Silicon	0.0006774	0.0001502	4.217		
Sodium	0.001522	0.001522	34.99		
Sulfur	0.0002519	0.0002519	8.076		

The output from #2 (moles in fluid phase) were used to design a procedure for preparing the synthetic UZ-14 water. The following is the procedure:

> To prepare one liter of Simulated UZ-14 Perched Water, add reagent grade CaSO4.2H2O and CaCO3, in the amounts shown in the table, to 900 mL of high purity water at room temperature in a beaker and stir until dissolved. Then add the other reagents, in the amounts shown in the table, to the solution and stir until dissolved completely. Care should be taken to weigh/add MgCl2.6H2O amd Ca(NO3)2.4H2O quickly since those are hygroscopic and can cause inaccuracies in weight measurement. Transfer the solution into a 1-L volumetric flask and adjust the volume to 1-L with high purity water.

Ingredient	**millimolar concentration**	**formula wt. of reagent**	**grams reagent per Liter solution**
NaHCO3	1.522	84	0.127848
KNO3	0.105	101.11	0.010617
MgCl2.6H2O	0.103	203.31	0.020941
CaSO4.2H2O	0.252	172.17	0.043387
Ca(NO3)2.4H2O	0.0855	236.15	0.020191
CaCO3	0.2785	100.09	0.027875

A Piper plot of composition calculated from the reagent mass is given in the following page (solid circles):


Mg
SO4
Ca
Na
HCO3
Cl
80
60
40
20

February 28, 2002

On page 47, the compositions of some Yucca Mountain groundwaters taken from the tabulation of Yang et al. (1996, 1998) are listed. It was planned to use these compositions in simulating the evolution of the chemistry as evaporation occurs, using the OLI ESP software. At the present time, only two of these compositions have been used in the simulation, conducted by Lietai Yang. The samples are UE-25 NRG-6 and USW SD-9. These samples were selected because they are close to the chemical divide line Calcite—SO_4^{2-}. Their compositions are (millimoles/kg H_2O):

SampleID	pHLab	Na	K	Mg	Ca	F	Cl	SO4
UE-25 NRG-6	7.4	4.31927	0	0.172768	0.606287	n.a.	2.17189	0.801616
USW SD-9	7.5	4.132232	0	0.390786	1.072854	n.a.	1.805207	1.290914

SampleID	NO3	HCO3	CO3	SIO2	Al
UE-25 NRG-6	0.7579423	1.507999	0	1.021801	3.71E-02
USW SD-9	3.06E-02	1.999738	0	0.97354	0

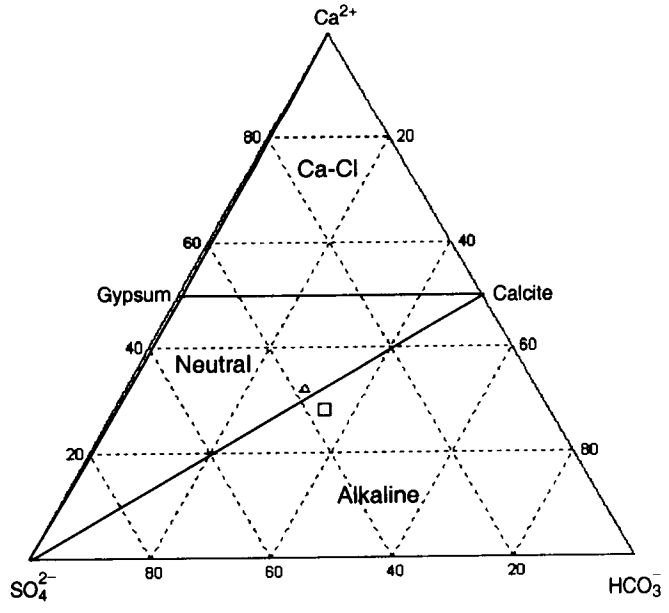
The aqueous speciation of NRG-6 and SD-9 after evaporation simulation (T = 110 °C; concentration factors of 3235 and 1246, respectively) are:

Molals(>1e-7)	NRG-6'	SD-9
H2F2		
CO2	5.717E-08	2.616E-07
H2SO4		
HCL	1.416E-12	3.224E-13
HNO3	2.928E-09	3.157E-11
CASO4	0.0003085	0.0007215
ALOH3	1.234E-08	
KCL		
MGCO3	1.737E-08	6.861E-08
MGH2SIO4	3.94E-07	8.892E-07
MGSO4	5.711E-06	2.338E-05
NAF		
NAHCO3	1.124E-05	4.277E-05
NAHSIO3	0.0084808	0.0141954
NANO3	0.0235675	0.0002321
CACO3	1.114E-06	2.514E-06
SIO2	0.0027822	0.0051067
CAH2SIO4	7.983E-07	1.028E-06
OHION	4.043E-05	0.0001855
ALION		
ALOH2ION	4.05E-12	
ALOH4ION	2.871E-05	
ALOHION	1.186E-16	
ALSO42ION	2.833E-22	
ALSO4ION	1.366E-20	
CAFION		

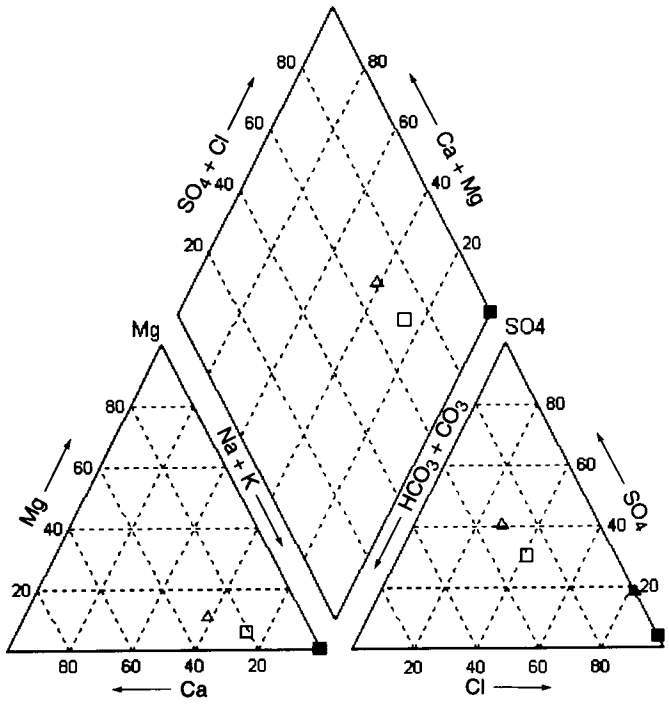
Na+ ion	8.1346755	2.7975658
K+ ion	0	0
Ca2+ ion	0.0159288	0.0047685
Mg2+ ion	0.0001575	0.0002886
Silica ions	0.0036759	0.0106922
Al-OH ions	2.872E-05	0
Cl- ion	6.0043163	2.2503829
NO3- ion	2.1811114	0.037618
SO42- ion	0.1140903	0.2514538
CO32- ion	4.368E-07	5.019E-06
HCO3- ion	5.404E-06	3.996E-05
F- ion	0	0
Charge bal.	-0.246766	0.0167215

CAHCO3ION	2.195E-06	1.167E-06
CAHSIO3ION	0.0005058	8.076E-05
CAION	0.0159288	0.0047685
CANO3ION	0.2493269	0.000296
CAOHION	6.26E-05	1.908E-05
CLION	6.0043163	2.2503829
CO3ION	4.368E-07	5.019E-06
FION		
H2SIO4ION	9.518E-08	6.256E-07
H3SIO4ION	0.0008936	0.0055849
HCO3ION	5.404E-06	3.996E-05
HION	7.672E-09	7.931E-09
HSO4ION	3.678E-09	4.303E-08
KION		
KSO4ION		
MGFION		
MGHCO3ION	9.628E-08	8.967E-08
MGHSIO3ION	3.176E-05	8.885E-06
MGION	0.0001575	0.0002886
MGOHION	1.647E-05	8.795E-06
NA2FION		
NACO3ION	1.047E-07	6.519E-07
NAION	8.1346755	2.7975658
NASO4ION	0.0022368	0.0113701
NO3ION	2.1811114	0.037618
SO4ION	0.1140903	0.2514538

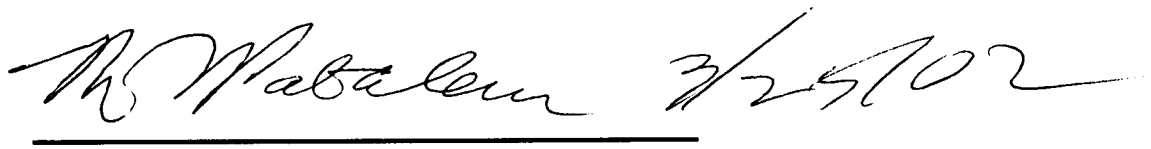
The following is a plot of the original composition (SD-9 triangle; NRG-6 square):



The following is a Piper diagram of the initial (open symbols) and final (closed symbols) compositions of NRG-6 (square) and SD-9 (triangle):



Entries into Scientific Notebook No. 185 for the period September 14, 2001, to March 17, 2002, have been made by



Roberto T. Pabalan / Date

No original entry into this Scientific Notebook has been removed.

Roberto T. Pabalan / Date