December 10, 2007

This text and figure 2 taken from Yang et al. (2006; Journal of Solution Chemistry, Vol. 35, **pp.** 589-590). Text and figure are copyright protected and therefore not included in this notebook.

StreamAnalyzer calculations at 25 C (MSE model) were done to provide quantitative support to the above statements.

1. A stream comprising 10 moles NaCl, 30 moles NaNO3, and 55.5087 moles H2O was used as input. A bubble point calculation was done, and the solid phases that resulted were extracted into a different (solids only) stream. The salt mixture is comprised of 2.79984 moles of NaNO3 and 3.16059 moles of NaCl [NaNO3/(NaNO3+NaCl) ratio of 0.4697). The calculated water activity (equal to the MDRH of the salt mixture) is 66.19 %.

   Then a new stream of H2O only was created and an isothermal calculation was done on the H2O stream.

2. A mixed stream was created comprising the H2O stream added to the 2.79984 moles NaNO3 plus 3.16059 moles NaCl. A ratio survey (isothermal or bubble point give the same results) was conducted, ranging from an H2O ratio of 5e-5 to 1.0 (the ratio is relative to 55.5087 moles H2O). The results are tabulated in the following table:

H2O added moles	Na+1 molal	NO3-1 molal	Cl-1 molal	NO3/Cl ratio	H2O Activity	NO3/(NO3+Cl) aqueous ratio	NaCl(s) mol	NaNO3(s) mol	NO3/(NO3+Cl) solid ratio
2.78E-03	11.04	7.20	3.84	1.88	66.19	0.652	3.1604	2.79948	0.470
0.557834	11.04	7.20	3.84	1.88	66.19	0.652	3.12201	2.72746	0.466
1.11289	11.04	7.20	3.84	1.88	66.19	0.652	3.08361	2.65545	0.463
1.66795	11.04	7.20	3.84	1.88	66.19	0.652	3.04522	2.58343	0.459
2.22301	11.04	7.20	3.84	1.88	66.19	0.652	3.00682	2.51141	0.455
2.77807	11.04	7.20	3.84	1.88	66.19	0.652	2.96843	2.43939	0.451
3.33313	11.04	7.20	3.84	1.88	66.19	0.652	2.93004	2.36737	0.447
3.88819	11.04	7.20	3.84	1.88	66.19	0.652	2.89164	2.29536	0.443
4.44325	11.04	7.20	3.84	1.88	66.19	0.652	2.85325	2.22334	0.438
4.99831	11.04	7.20	3.84	1.88	66.19	0.652	2.81485	2.15132	0.433
5.55337	11.04	7.20	3.84	1.88	66.19	0.652	2.77646	2.0793	0.428
6.10842	11.04	7.20	3.84	1.88	66.19	0.652	2.73806	2.00729	0.423
6.66348	11.04	7.20	3.84	1.88	66.19	0.652	2.69967	1.93527	0.418
7.21854	11.04	7.20	3.84	1.88	66.19	0.652	2.66128	1.86325	0.412
7.7736	11.04	7.20	3.84	1.88	66.19	0.652	2.62288	1.79123	0.406
8.32866	11.04	7.20	3.84	1.88	66.19	0.652	2.58449	1.71921	0.399
8.88372	11.04	7.20	3.84	1.88	66.19	0.652	2.54609	1.6472	0.393
9.43878	11.04	7.20	3.84	1.88	66.19	0.652	2.5077	1.57518	0.386
9.99384	11.04	7.20	3.84	1.88	66.19	0.652	2.46931	1.50316	0.378
10.5489	11.04	7.20	3.84	1.88	66.19	0.652	2.43091	1.43114	0.371
11.104	11.04	7.20	3.84	1.88	66.19	0.652	2.39252	1.35913	0.362
11.659	11.04	7.20	3.84	1.88	66.19	0.652	2.35412	1.28711	0.353
12.2141	11.04	7.20	3.84	1.88	66.19	0.652	2.31573	1.21509	0.344
12.7691	11.04	7.20	3.84	1.88	66.19	0.652	2.27734	1.14307	0.334
13.3242	11.04	7.20	3.84	1.88	66.19	0.652	2.23894	1.07105	0.324
13.8793	11.04	7.20	3.84	1.88	66.19	0.652	2.20055	0.999036	0.312
14.4343	11.04	7.20	3.84	1.88	66.19	0.652	2.16215	0.927018	0.300
14.9894	11.04	7.20	3.84	1.88	66.19	0.652	2.12376	0.855	0.287

15.5444	11.04	7.20	3.84	1.88	66.19	0.652	2.08536	0.782982	0.273
16.0995	11.04	7.20	3.84	1.88	66.19	0.652	2.04697	0.710965	0.258
16.6545	11.04	7.20	3.84	1.88	66.19	0.652	2.00858	0.638947	0.241
17.2096	11.04	7.20	3.84	1.88	66.19	0.652	1.97018	0.566929	0.223
17.7647	11.04	7.20	3.84	1.88	66.19	0.652	1.93179	0.494911	0.204
18.3197	11.04	7.20	3.84	1.88	66.19	0.652	1.89339	0.422893	0.183
18.8748	11.04	7.20	3.84	1.88	66.19	0.652	1.855	0.350875	0.159
19.4298	11.04	7.20	3.84	1.88	66.19	0.652	1.81661	0.278858	0.133
19.9849	11.04	7.20	3.84	1.88	66.19	0.652	1.77821	0.20684	0.104
20.54	11.04	7.20	3.84	1.88	66.19	0.652	1.73982	0.134822	0.072
21.095	11.04	7.20	3.84	1.88	66.19	0.652	1.70142	0.062804	0.036
21.6501	11.02	7.18	3.85	1.87	66.22	0.651	1.66053	0	0.000
22.2051	10.89	7.00	3.89	1.80	66.44	0.642	1.60247	0	0.000
22.7602	10.77	6.83	3.94	1.73	66.66	0.634	1.54427	0	0.000
23.3153	10.65	6.67	3.99	1.67	66.87	0.626	1.48594	0	0.000
23.8703	10.54	6.51	4.03	1.62	67.06	0.618	1.42747	0	0.000
24.4254	10.43	6.36	4.07	1.56	67.25	0.610	1.36889	0	0.000
24.9804	10.33	6.22	4.11	1.51	67.43	0.602	1.3102	0	0.000
25.5355	10.24	6.09	4.15	1.47	67.61	0.595	1.2514	0	0.000
26.0906	10.14	5.96	4.19	1.42	67.77	0.587	1.1925	0	0.000
26.6456	10.06	5.83	4.22	1.38	67.93	0.580	1.13352	0	0.000
27.2007	9.97	5.71	4.26	1.34	68.08	0.573	1.07444	0	0.000
27.7557	9.89	5.60	4.29	1.31	68.23	0.566	1.01529	0	0.000
28.3108	9.81	5.49	4.32	1.27	68.37	0.559	0.956059	0	0.000
28.8658	9.74	5.38	4.35	1.24	68.51	0.553	0.896756	0	0.000
29.4209	9.67	5.28	4.38	1.21	68.64	0.547	0.837384	0	0.000
29.976	9.60	5.18	4.41	1.18	68.77	0.540	0.777947	0	0.000
30.531	9.53	5.09	4.44	1.15	68.89	0.534	0.718449	0	0.000
31.0861	9.47	5.00	4.47	1.12	69.01	0.528	0.658893	0	0.000
31.6411	9.41	4.91	4.49	1.09	69.12	0.522	0.599281	0	0.000
32.1962	9.35	4.83	4.52	1.07	69.23	0.516	0.539616	0	0.000
32.7513	9.29	4.75	4.54	1.04	69.34	0.511	0.479901	0	0.000
33.3063	9.23	4.67	4.57	1.02	69.45	0.505	0.420138	0	0.000
33.8614	9.18	4.59	4.59	1.00	69.55	0.500	0.360329	0	0.000
34.4164	9.13	4.52	4.61	0.98	69.64	0.495	0.300477	0	0.000
34.9715	9.08	4.44	4.63	0.96	69.74	0.489	0.240583	0	0.000
35.5266	9.03	4.37	4.66	0.94	69.83	0.484	0.180649	0	0.000
36.0816	8.98	4.31	4.68	0.92	69.92	0.479	0.120677	0	0.000
36.6367	8.94	4.24	4.70	0.90	70.00	0.475	0.060668	0	0.000
37.1917	8.89	4.18	4.72	0.89	70.09	0.470	6.24E-04	0	0.000
37.7468	8.77	4.12	4.65	0.89	70.53	0.470	0	0	#DIV/0!
38.3018	8.64	4.06	4.58	0.89	70.97	0.470	0	0	#DIV/0!
38.8569	8.51	4.00	4.51	0.89	71.39	0.470	0	0	#DIV/0!
39.412	8.39	3.94	4.45	0.89	71.80	0.470	0	0	#DIV/0!
39.967	8.28	3.89	4.39	0.89	72.21	0.470	0	0	#DIV/0!
40.5221	8.16	3.84	4.33	0.89	72.60	0.470	0	0	#DIV/0!
41.0771	8.05	3.78	4.27	0.89	72.98	0.470	0	0	#DIV/0!
41.6322	7.95	3.73	4.21	0.89	73.35	0.470	0	0	#DIV/0!
42.1873	7.84	3.68	4.16	0.89	73.71	0.470	0	0	#DIV/0!
42.7423	7.74	3.64	4.10	0.89	74.07	0.470	0	0	#DIV/0!

43.2974	7.64	3.59	4.05	0.89	74.41	0.470	0	0	#DIV/0!
43.8524	7.54	3.54	4.00	0.89	74.75	0.470	0	0	#DIV/0!
44.4075	7.45	3.50	3.95	0.89	75.08	0.470	0	0	#DIV/0!
44.9626	7.36	3.46	3.90	0.89	75.40	0.470	0	0	#DIV/0!
45.5176	7.27	3.41	3.85	0.89	75.71	0.470	0	0	#DIV/0!
46.0727	7.18	3.37	3.81	0.89	76.02	0.470	0	0	#DIV/0!
46.6277	7.10	3.33	3.76	0.89	76.32	0.470	0	0	#DIV/0!
47.1828	7.01	3.29	3.72	0.89	76.61	0.470	0	0	#DIV/0!
47.7379	6.93	3.26	3.68	0.89	76.89	0.470	0	0	#DIV/0!
48.2929	6.85	3.22	3.63	0.89	77.17	0.470	0	0	#DIV/0!
48.848	6.77	3.18	3.59	0.89	77.44	0.470	0	0	#DIV/0!
49.403	6.70	3.15	3.55	0.89	77.71	0.470	0	0	#DIV/0!
49.9581	6.62	3.11	3.51	0.89	77.97	0.470	0	0	#DIV/0!
50.5131	6.55	3.08	3.47	0.89	78.22	0.470	0	0	#DIV/0!
51.0682	6.48	3.04	3.44	0.89	78.47	0.470	0	0	#DIV/0!
51.6233	6.41	3.01	3.40	0.89	78.72	0.470	0	0	#DIV/0!
52.1783	6.34	2.98	3.36	0.89	78.95	0.470	0	0	#DIV/0!
52.7334	6.27	2.95	3.33	0.89	79.19	0.470	0	0	#DIV/0!
53.2884	6.21	2.92	3.29	0.89	79.42	0.470	0	0	#DIV/0!
53.8435	6.14	2.89	3.26	0.89	79.64	0.470	0	0	#DIV/0!
54.3986	6.08	2.86	3.23	0.89	79.86	0.470	0	0	#DIV/0!
54.9536	6.02	2.83	3.19	0.89	80.07	0.470	0	0	#DIV/0!
55.5087	5.96	2.80	3.16	0.89	80.28	0.470	0	0	#DIV/0!

The results show deliquescence occurs at a RH of 66.19% after addition of a small amount of H2O (2.78E-3 moles, the minimum value in the simulation). As more water is added, the RH remains constant because both salts are saturated, but the ratio of NaNO3 to total salts decreases until NaNO3 is completely dissolved, leaving only NaCl solid. At a value of added H2O equal to 21.65 moles, only NaCl solid is present and as more water is added, the aqueous solution becomes richer in Cl relative to NO3 as more NaCl is dissolved. After adding 37.7468 moles H2O (and an RH value of 70.09 %), NaCl is completely dissolved and the aqueous composition has changed from X_{MDRH} = 3.84 molal NaCl + 7.30 molal NaNO3 to X = 4.65 molal NaCl + 4.12 molal NaNO3. Adding more water (or raising the RH further) dilutes the aqueous solution.

3. Another calculation was done using a composition corresponding to the eutonic composition, X_C, of an NaCl-NaNO3 mixture. The value of X_C was derived by separating the liquid stream from step (1) and evaporating it (by reducing the total pressure from 0.0313849 atm to 3.13849e-005 atm. **The value of X_C is 3.83941 moles NaCl + 7.20016 moles NaNO3 [ratio NaNO3/(NaNO3+NaCl) equal to 0.6522].** The solids that precipitated were separated into a separate stream, then H2O stream was added using a ratio survey (isothermal). The results are tabulated in the following table. The results of the ratio survey (see table) show that the relative humidity (or water activity) remains constant as both NaCl and NaNO3 dissolve. The aqueous concentrations as well as the relative amounts of NO3 and Cl in both the solid and the aqueous phases remain constant, until NaNO3 and NaCl both dissolve completely (after addition of

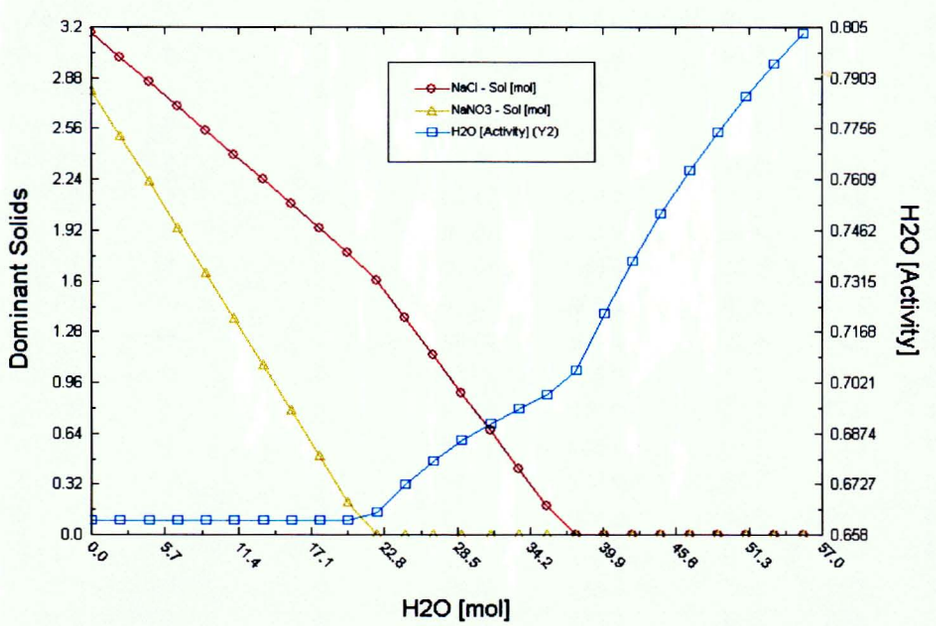
1.0008 moles H2O). With further addition of H2O, the relative humidity rises (to > 90 % RH, although the tabulated values were truncated).

Ratio	H2O added	Na+1	Cl-1	NO3-1	NO3/(NO3 + Cl) aqueous ratio	H2O	NaCl(s)	NaNO3(s)	NaNO3/(NaNO3 + NaCl)
---	moles	molal	molal	molal		Activity	mol	mol	solid ratio
1.00E-03	0.0555087	11.04	3.84	7.20	0.652	66.19	3.83557	7.19296	0.652
0.05099	2.83039	11.04	3.84	7.20	0.652	66.19	3.64363	6.83292	0.652
0.10098	5.60527	11.04	3.84	7.20	0.652	66.19	3.45168	6.47289	0.652
0.15097	8.38015	11.04	3.84	7.20	0.652	66.19	3.25974	6.11285	0.652
0.20096	11.155	11.04	3.84	7.20	0.652	66.19	3.0678	5.75282	0.652
0.25095	13.9299	11.04	3.84	7.20	0.652	66.19	2.87586	5.39278	0.652
0.30094	16.7048	11.04	3.84	7.20	0.652	66.19	2.68392	5.03274	0.652
0.35093	19.4797	11.04	3.84	7.20	0.652	66.19	2.49198	4.67271	0.652
0.40092	22.2545	11.04	3.84	7.20	0.652	66.19	2.30003	4.31267	0.652
0.45091	25.0294	11.04	3.84	7.20	0.652	66.19	2.10809	3.95264	0.652
0.5009	27.8043	11.04	3.84	7.20	0.652	66.19	1.91615	3.5926	0.652
0.55089	30.5792	11.04	3.84	7.20	0.652	66.19	1.72421	3.23257	0.652
0.60088	33.3541	11.04	3.84	7.20	0.652	66.19	1.53227	2.87253	0.652
0.65087	36.1289	11.04	3.84	7.20	0.652	66.19	1.34032	2.5125	0.652
0.70086	38.9038	11.04	3.84	7.20	0.652	66.19	1.14838	2.15246	0.652
0.75085	41.6787	11.04	3.84	7.20	0.652	66.19	0.956441	1.79243	0.652
0.80084	44.4536	11.04	3.84	7.20	0.652	66.19	0.764499	1.43239	0.652
0.85083	47.2285	11.04	3.84	7.20	0.652	66.19	0.572557	1.07236	0.652
0.90082	50.0033	11.04	3.84	7.20	0.652	66.19	0.380615	0.712323	0.652
0.95081	52.7782	11.04	3.84	7.20	0.652	66.19	0.188673	0.352288	0.651
1.0008	55.5531	11.03	3.84	7.19	0.652	66.22	0	0	#DIV/0!
1.05079	58.328	10.51	3.65	6.85	0.652	67.76	0	0	#DIV/0!
1.10078	61.1028	10.03	3.49	6.54	0.652	69.17	0	0	#DIV/0!
1.15077	63.8777	9.59	3.34	6.26	0.652	70.48	0	0	#DIV/0!
1.20076	66.6526	9.19	3.20	6.00	0.652	71.68	0	0	#DIV/0!
1.25075	69.4275	8.83	3.07	5.76	0.652	72.80	0	0	#DIV/0!
1.30074	72.2024	8.49	2.95	5.54	0.652	73.84	0	0	#DIV/0!
1.35073	74.9772	8.17	2.84	5.33	0.652	74.80	0	0	#DIV/0!
1.40072	77.7521	7.88	2.74	5.14	0.652	75.70	0	0	#DIV/0!
1.45071	80.527	7.61	2.65	4.96	0.652	76.54	0	0	#DIV/0!
1.5007	83.3019	7.36	2.56	4.80	0.652	77.33	0	0	#DIV/0!
1.55069	86.0768	7.12	2.48	4.64	0.652	78.06	0	0	#DIV/0!
1.60068	88.8516	6.90	2.40	4.50	0.652	78.76	0	0	#DIV/0!
1.65067	91.6265	6.69	2.33	4.36	0.652	79.40	0	0	#DIV/0!
1.70066	94.4014	6.49	2.26	4.23	0.652	80.02	0	0	#DIV/0!
1.75065	97.1763	6.31	2.19	4.11	0.652	80.59	0	0	#DIV/0!
1.80064	99.9511	6.13	2.13	4.00	0.652	81.14	0	0	#DIV/0!
1.85063	102.726	5.97	2.07	3.89	0.652	81.65	0	0	#DIV/0!
1.90062	105.501	5.81	2.02	3.79	0.652	82.14	0	0	#DIV/0!
1.95061	108.276	5.66	1.97	3.69	0.652	82.61	0	0	#DIV/0!
2.0006	111.051	5.52	1.92	3.60	0.652	83.04	0	0	#DIV/0!
2.05059	113.826	5.38	1.87	3.51	0.652	83.46	0	0	#DIV/0!
2.10058	116.6	5.26	1.83	3.43	0.652	83.86	0	0	#DIV/0!
2.15057	119.375	5.13	1.79	3.35	0.652	84.24	0	0	#DIV/0!

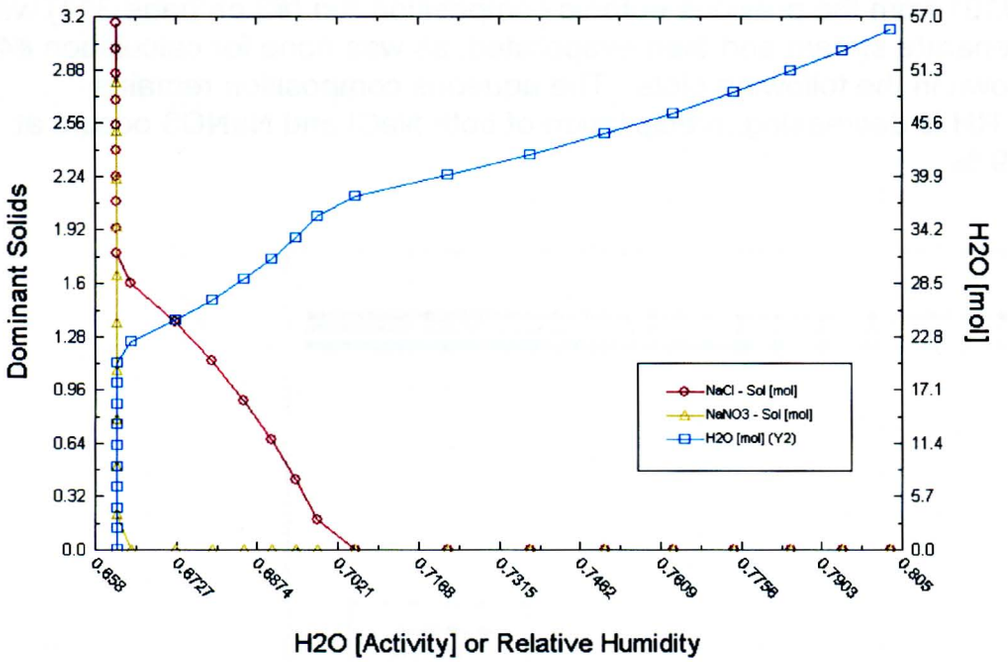
2.20056	122.15	5.02	1.74	3.27	0.652	84.60	0	0	#DIV/0!
2.25055	124.925	4.91	1.71	3.20	0.652	84.95	0	0	#DIV/0!
2.30054	127.7	4.80	1.67	3.13	0.652	85.28	0	0	#DIV/0!
2.35053	130.475	4.70	1.63	3.06	0.652	85.59	0	0	#DIV/0!
2.40052	133.25	4.60	1.60	3.00	0.652	85.89	0	0	#DIV/0!
2.45051	136.025	4.50	1.57	2.94	0.652	86.18	0	0	#DIV/0!
2.5005	138.799	4.41	1.54	2.88	0.652	86.46	0	0	#DIV/0!
2.55049	141.574	4.33	1.51	2.82	0.652	86.73	0	0	#DIV/0!
2.60048	144.349	4.25	1.48	2.77	0.652	86.98	0	0	#DIV/0!
2.65047	147.124	4.17	1.45	2.72	0.652	87.23	0	0	#DIV/0!
2.70046	149.899	4.09	1.42	2.67	0.652	87.47	0	0	#DIV/0!
2.75045	152.674	4.01	1.40	2.62	0.652	87.70	0	0	#DIV/0!
2.80044	155.449	3.94	1.37	2.57	0.652	87.92	0	0	#DIV/0!
2.85043	158.224	3.87	1.35	2.53	0.652	88.13	0	0	#DIV/0!
2.90042	160.998	3.81	1.32	2.48	0.652	88.33	0	0	#DIV/0!
2.95041	163.773	3.74	1.30	2.44	0.652	88.53	0	0	#DIV/0!
3.0004	166.548	3.68	1.28	2.40	0.652	88.72	0	0	#DIV/0!

4. What happens if a droplet of brine with composition X_A drops from the drift wall onto the waste package surface that is at a lower relative humidity?

To answer this question, StreamAnalyzer was used to evaporate the NaCl+NaNO3 solution that resulted from calculation #2 discussed on page 309 (the solution composition is the last datapoint of the table on page 311. The input composition was derived by extracting into a separate stream the survey point #101 for that calculation. The evaporation was simulated by doing a composition survey (H2O was varied from 55.5087 moles to 5E-5 moles at constant temperature (25 C). The plot of solids present and water activity as a function of amount of H2O is shown below:

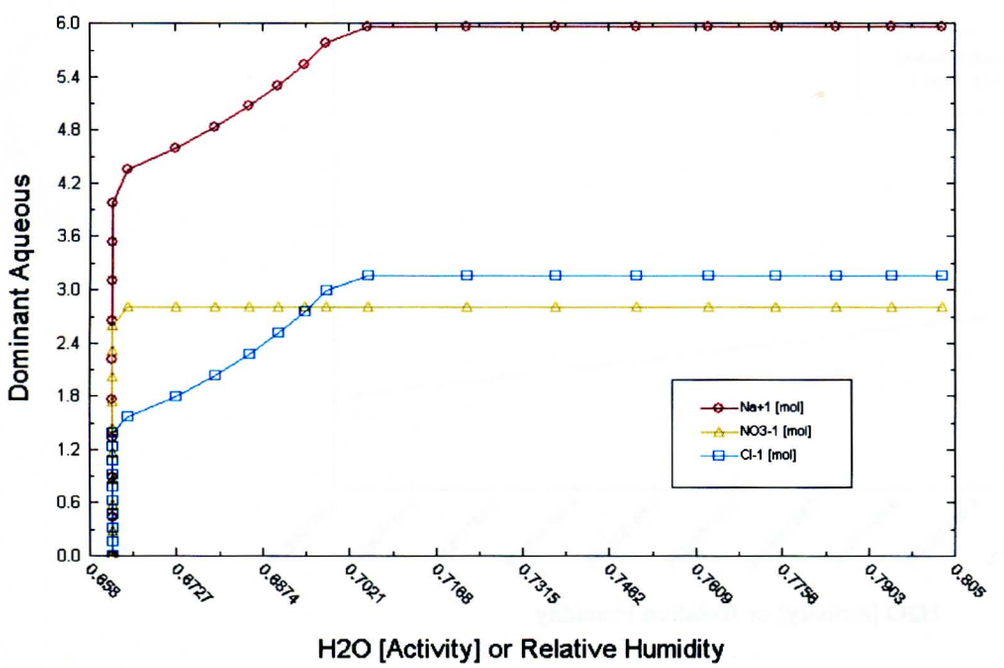


The following is a plot of solids present and of amount of H2O as a function of relative humidity:



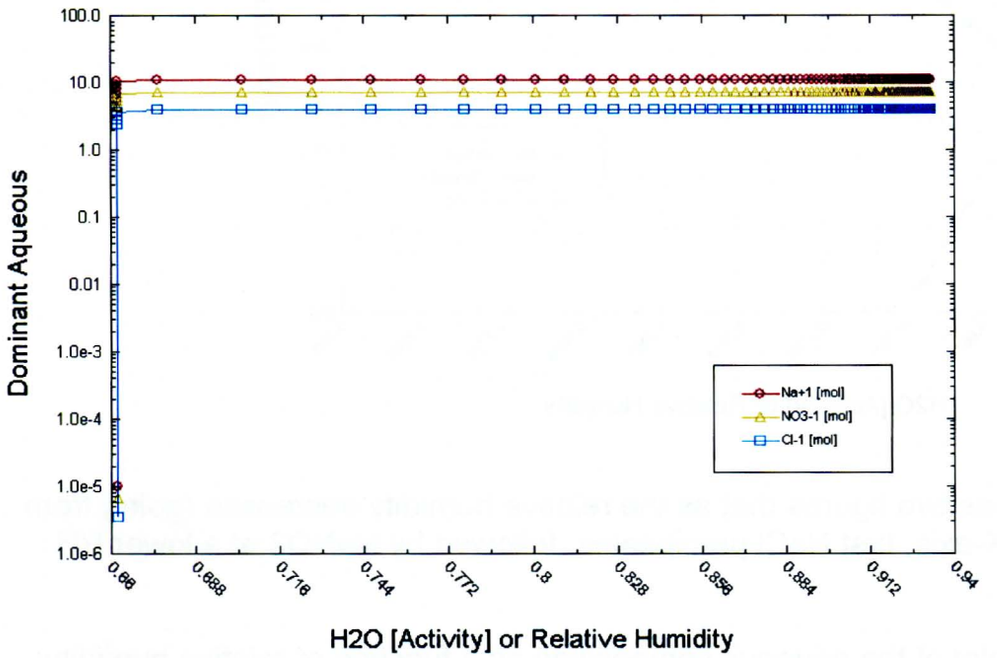
One can see in these two figures that as the relative humidity decreases (going from right to left on the X-axis, first NaCl precipitates, followed by NaNO3 at a lower RH value.

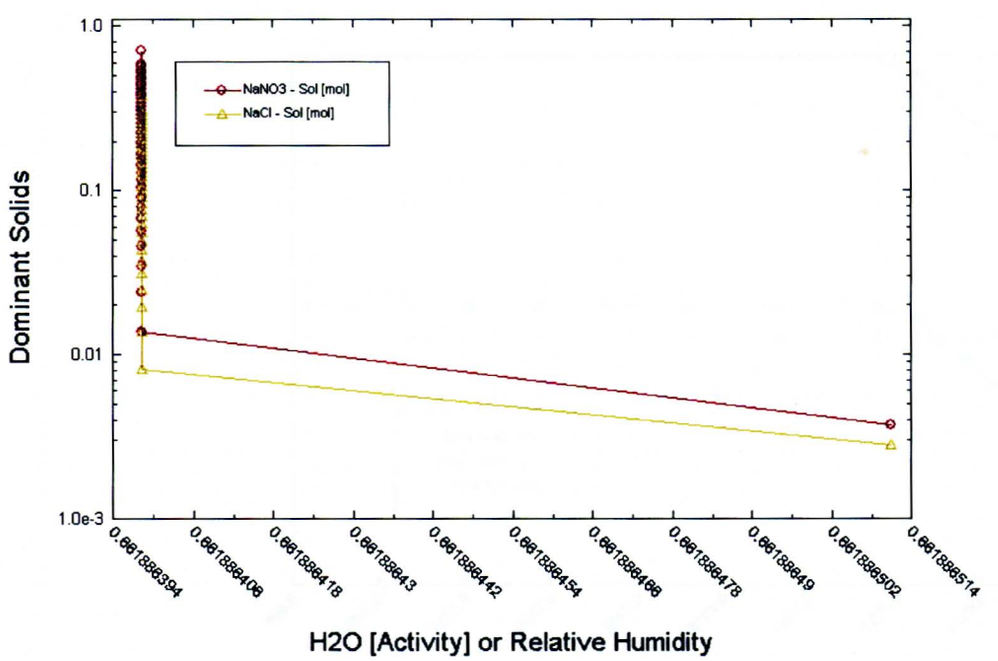
The following is a plot of the aqueous composition as a function of relative humidity:



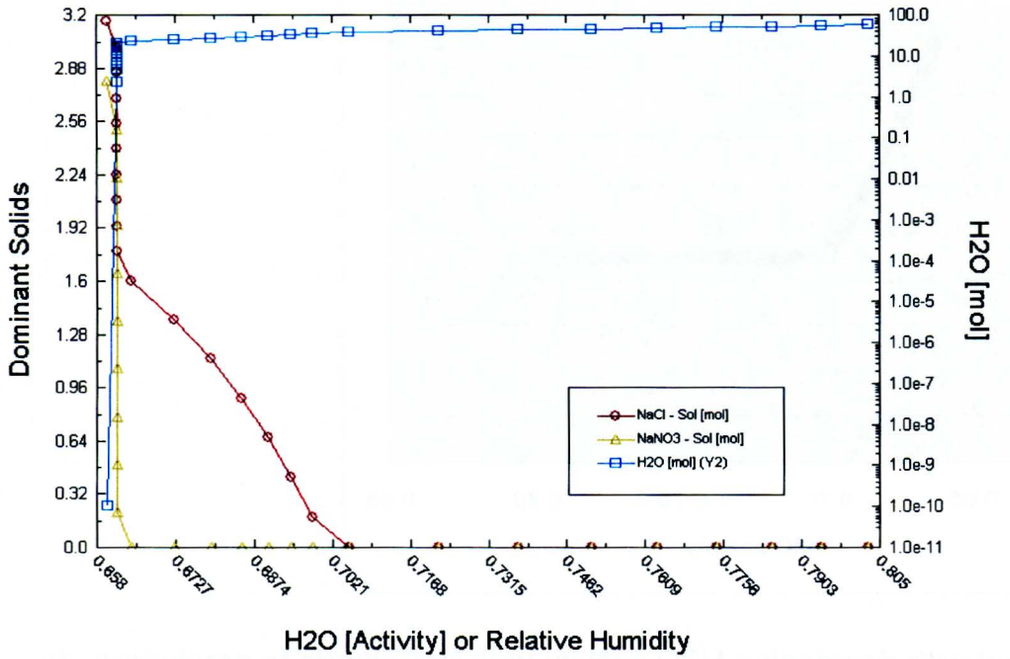
5. **What if the composition of the solution corresponds to the eutonic composition of the salt mixture?**

The survey point #101 from the previous eutonic composition run (#3 on page 311) was separated into a separate stream and then evaporated, as was done for calculation #4. The results are shown in the following plots. The aqueous composition remains constant while the RH is decreasing; precipitation of both NaCl and NaNO3 occurs at the MDRH of 66.19 %.

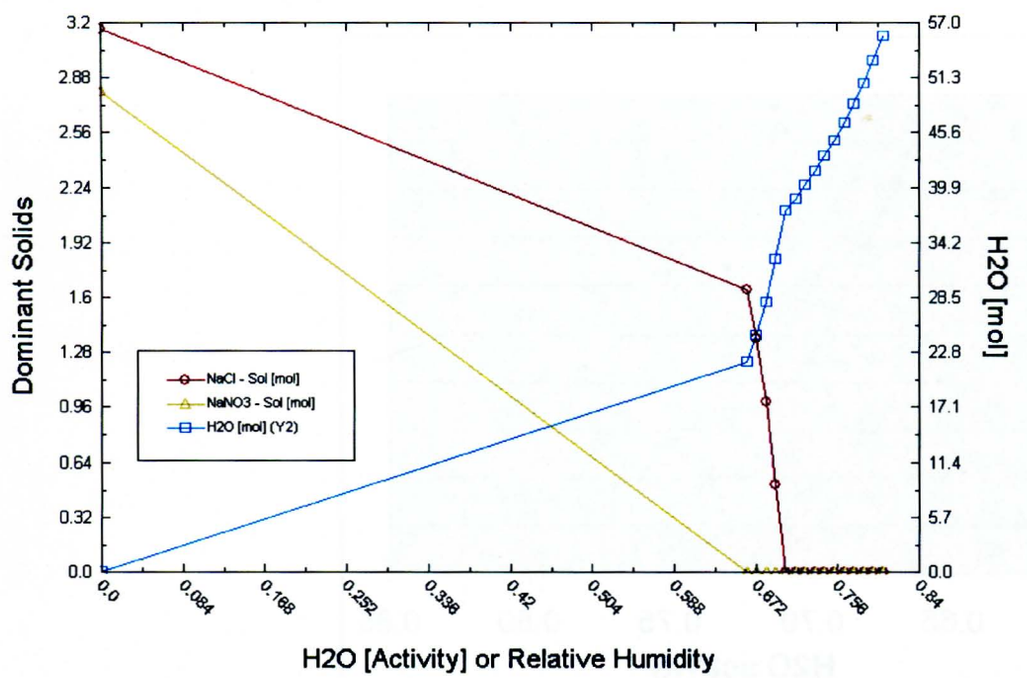




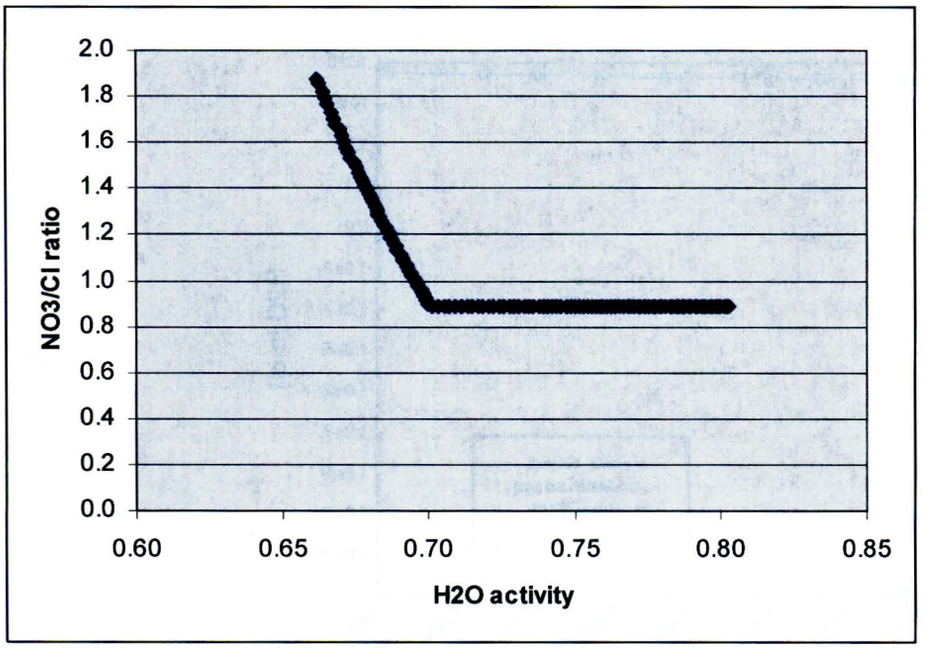
The following figure is similar to that on the top of page 314 and shows the dominant solids versus relative humidity, but for this calculation the minimum moles of H2O was specified to be 1.0E-10, versus 5E-5 in the previous calculation. Note that Y-2 axis in this figure is in log scale.



The previous calculations evaporated the NaCl-NaNO3 solution by decreasing the amount of H2O in the system. The calculations also could have been done by specifying a pressure survey and varying the total pressure from 3.13849e-2 to 3.13849e-5 atm. The value of 3.13849e-2 is the vapor pressure of pure water at 25 C. This latter type of calculation will cause a dryout to occur as liquid water goes into the vapor phase. A typical result is shown below:

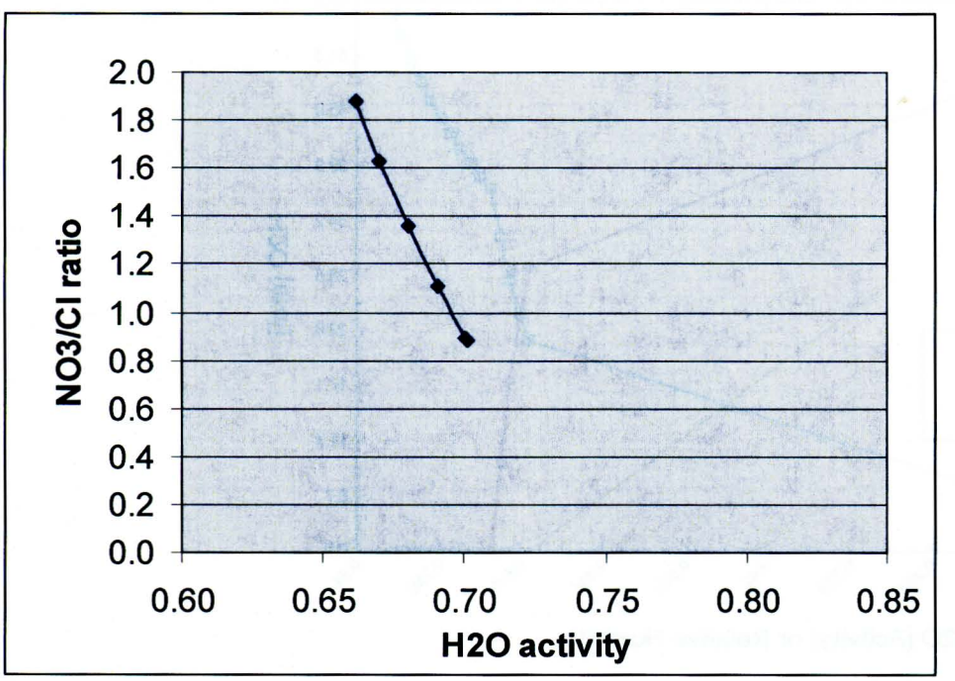


The following is a plot of $NO3^-/Cl^-$ for the evaporation simulations documented on page 314.



The ratio is constant with decreasing H2O activity until NaCl starts to precipitate. In these calculations, no separation of precipitates from the aqueous phase was assumed.

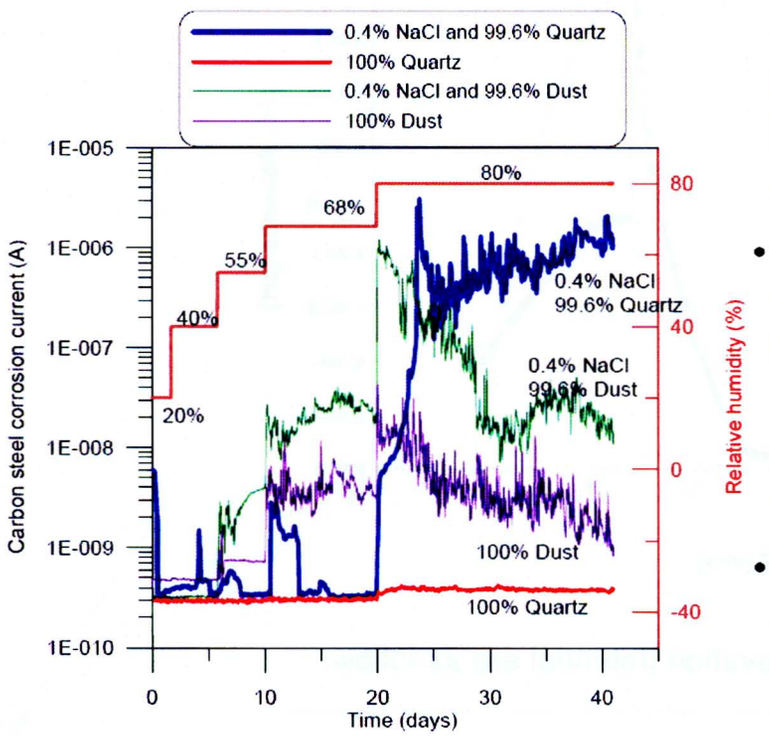
The following is a similar plot from StreamAnalyzer runs in which the precipitated salt was assumed to separate out and not able to react with the aqueous phase. The calculation was done by separating the solids into a separate stream (at intervals of 0.01 water activity). The results look the same as in the figure above.



December 12, 2007

The following is slide #13 of Xihua He's noontime seminar presented today, titled: "Effect of Capillary Retention by Dusts on the Corrosivity of Deliquescence Brines" (coauthored with R. Pabalan and L. Yang):

Results–Test 3: NaCl/Quartz and NaCl/Dust Mixtures



- In 100% quartz test (no NaCl), no deliquescence brine was formed, however, in 100% rock dust test, brine was formed
- Deliquescence brine formed at lower relative humidity (55% RH) in NaCl/dust mixture compared to NaCl/quartz mixture (RH 68%)
- Dust reduced the corrosion current, but did not prevent brine from contacting the metal surface

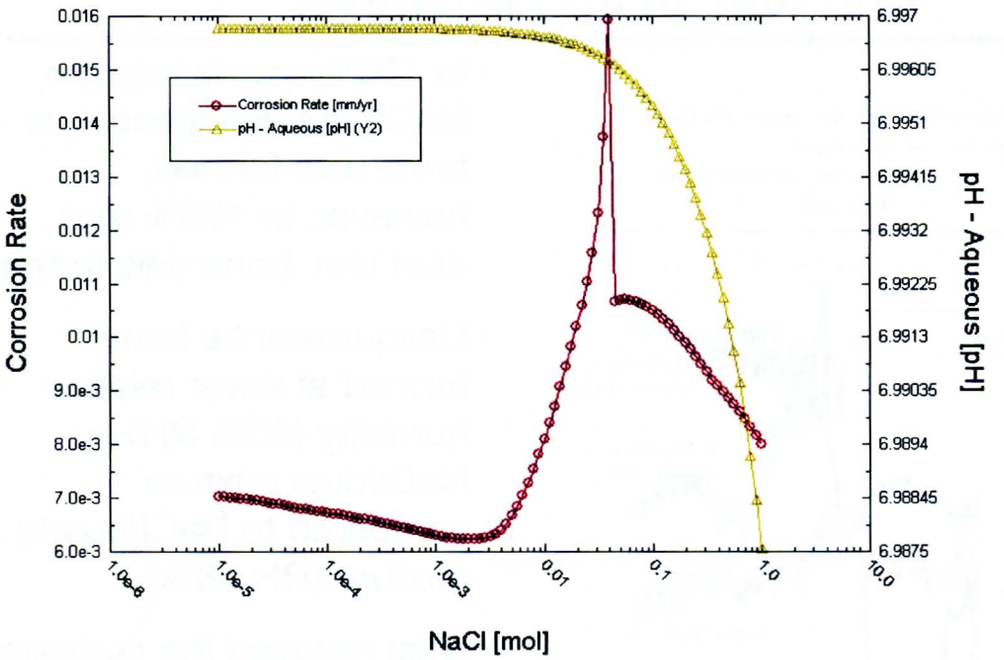
13

Someone asked why the 0.4%NaCl–99.6%Dust and the 100%Dust sample showed decreasing corrosion current with time, whereas the 0.4%NaCl–99.6%Quartz sample showed a continued increase in corrosion current. There was speculation that corrosion inhibitors were being leached from the dust particles and increasing in concentration with time.

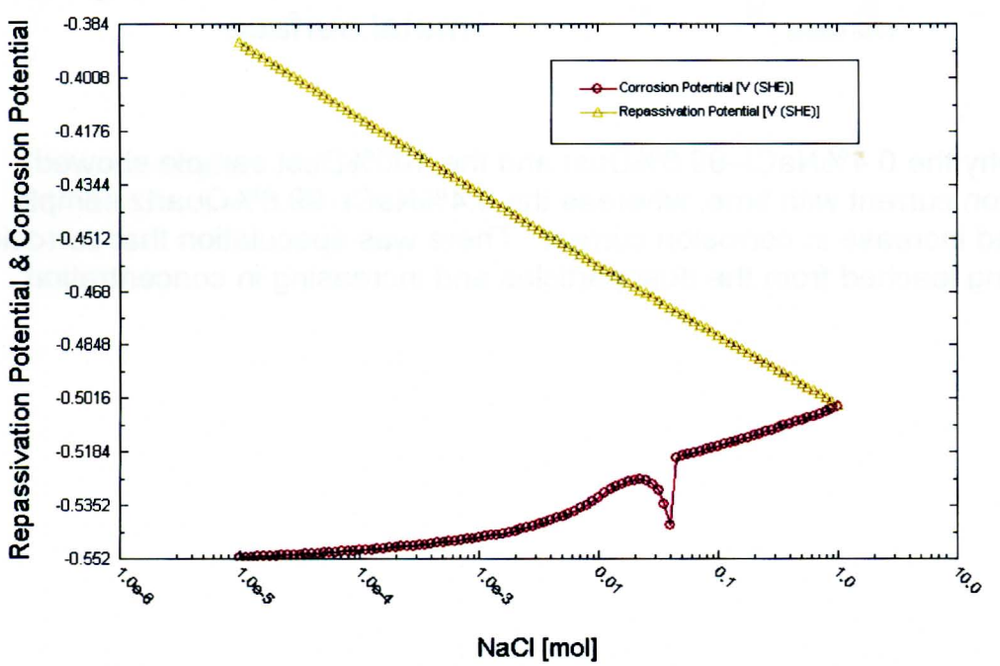
December 14, 2007

Use CorrosionAnalyzer to calculate the corrosion rate of carbon steel (G10100) in salt solutions.

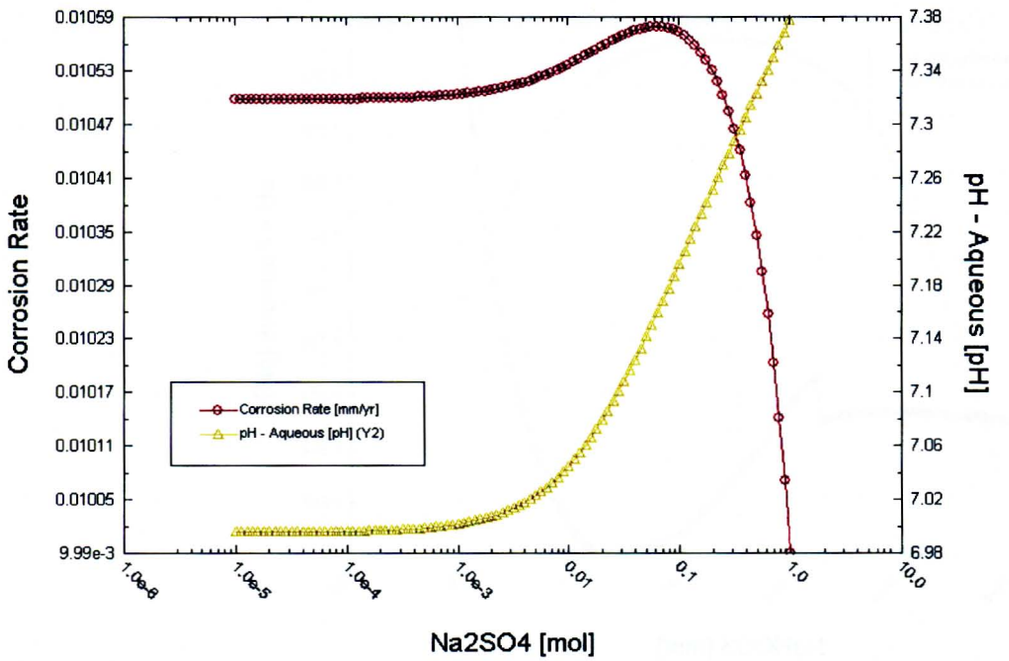
The following is the calculated general corrosion rate (and calculated pH) at 25 °C as a function of NaCl concentration (from 0.00001 to 1.0 molal):



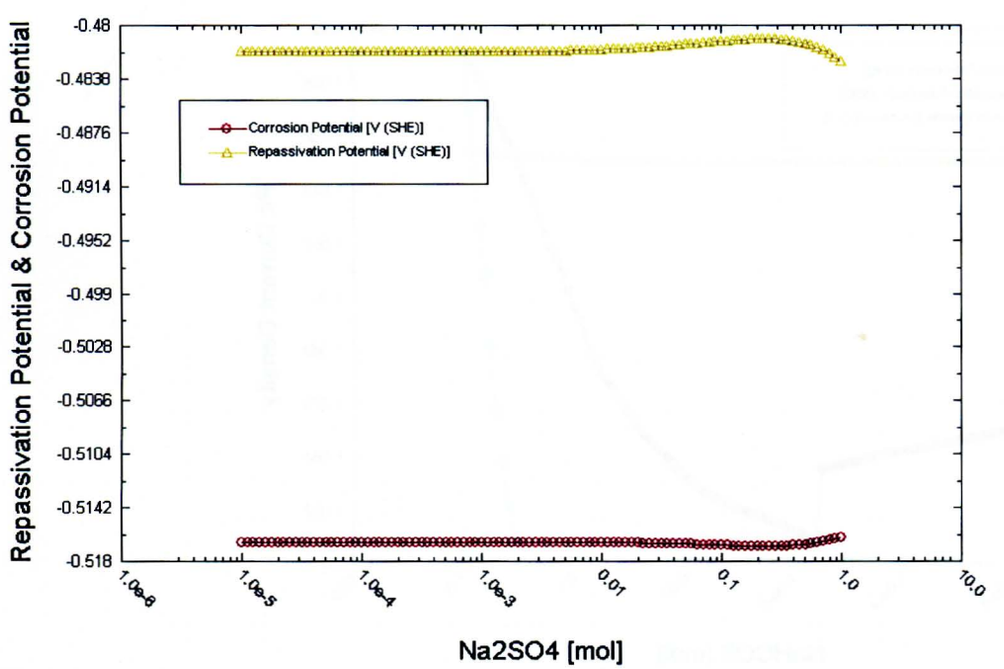
The corrosion potential and repassivation potential are as follow:



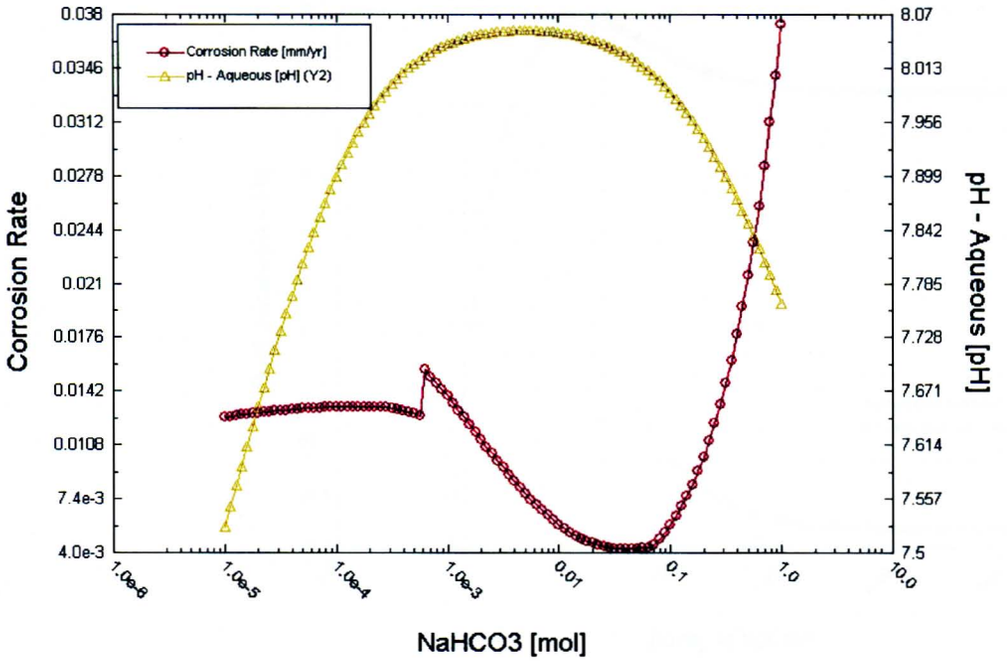
The general corrosion rate and pH in a 0.1 m NaCl solution as a function of Na2SO4 concentration is as follows:



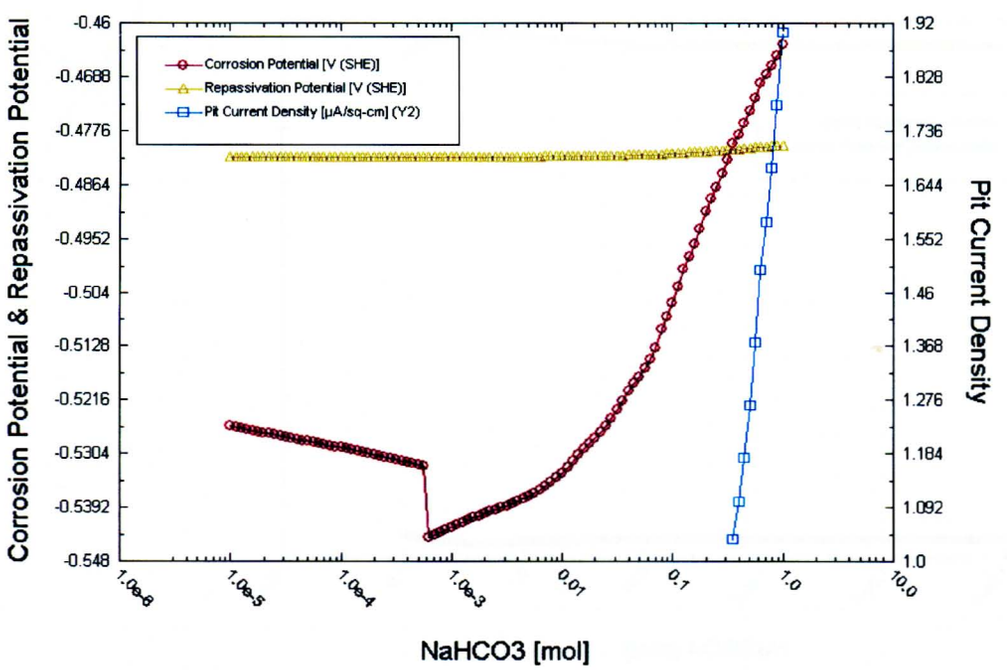
The corrosion potential and repassivation potential are shown below:



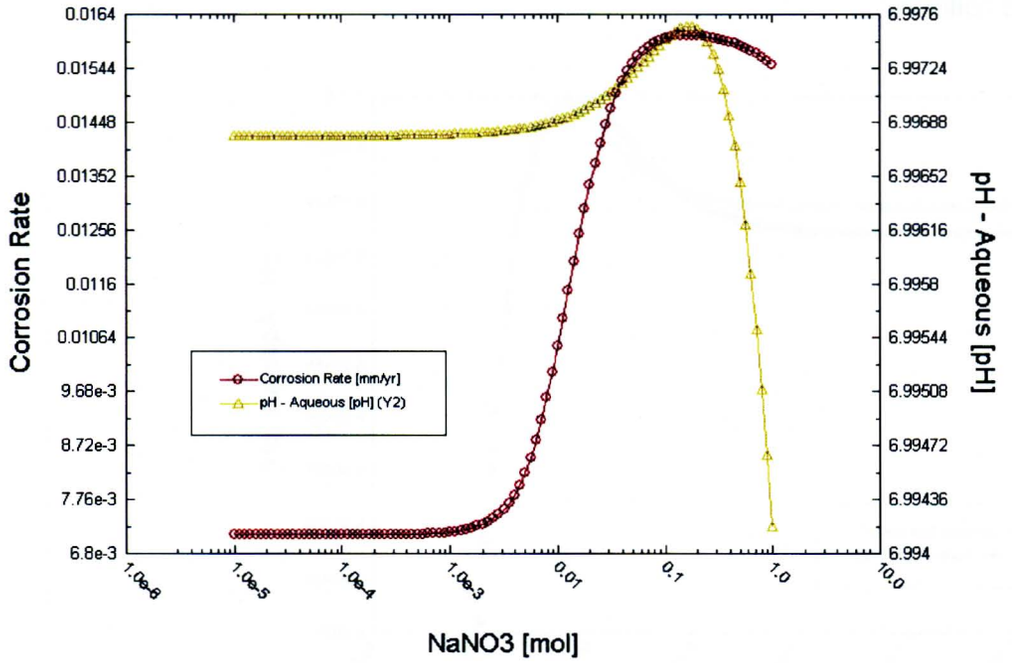
The general corrosion rate in 0.1 m NaCl as a function of NaHCO3 concentration is as follows:



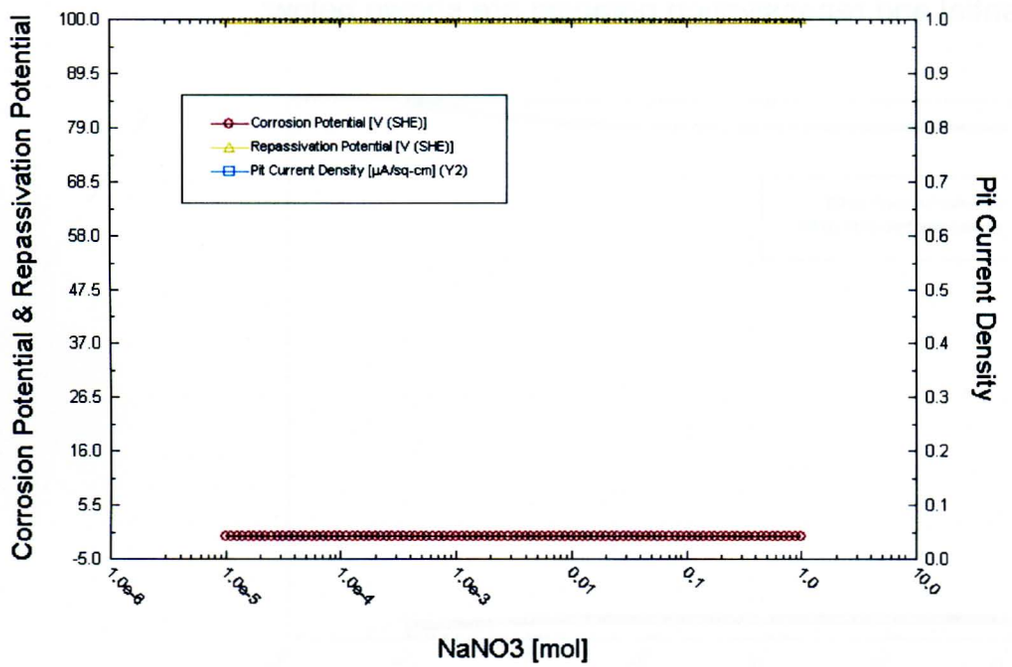
The corrosion potential, repassivation potential, and pit current density are shown below:



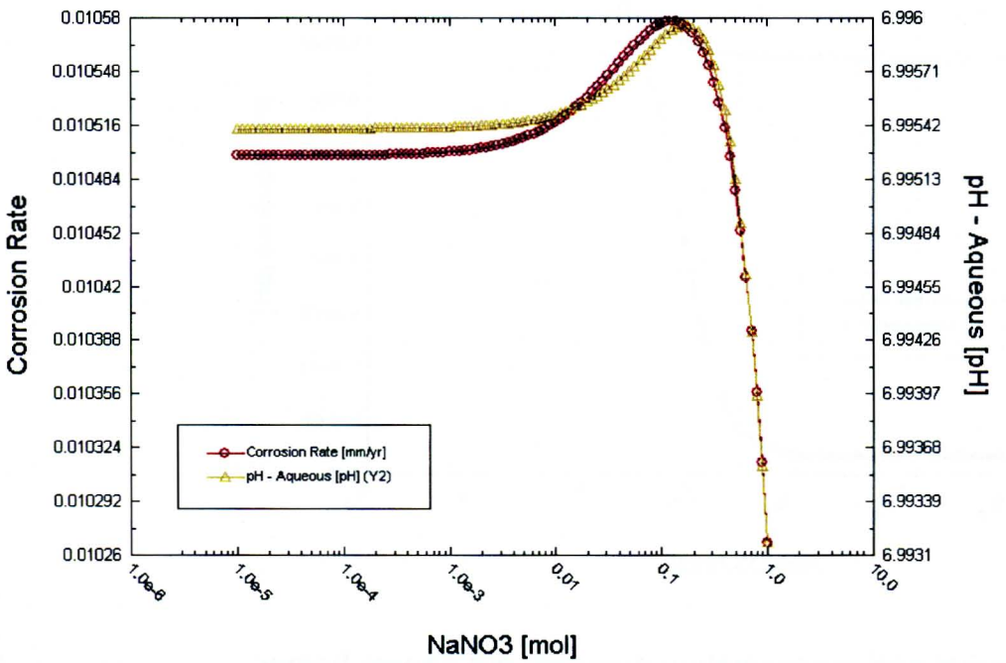
The general corrosion rate in NaNO3 solutions is shown below:



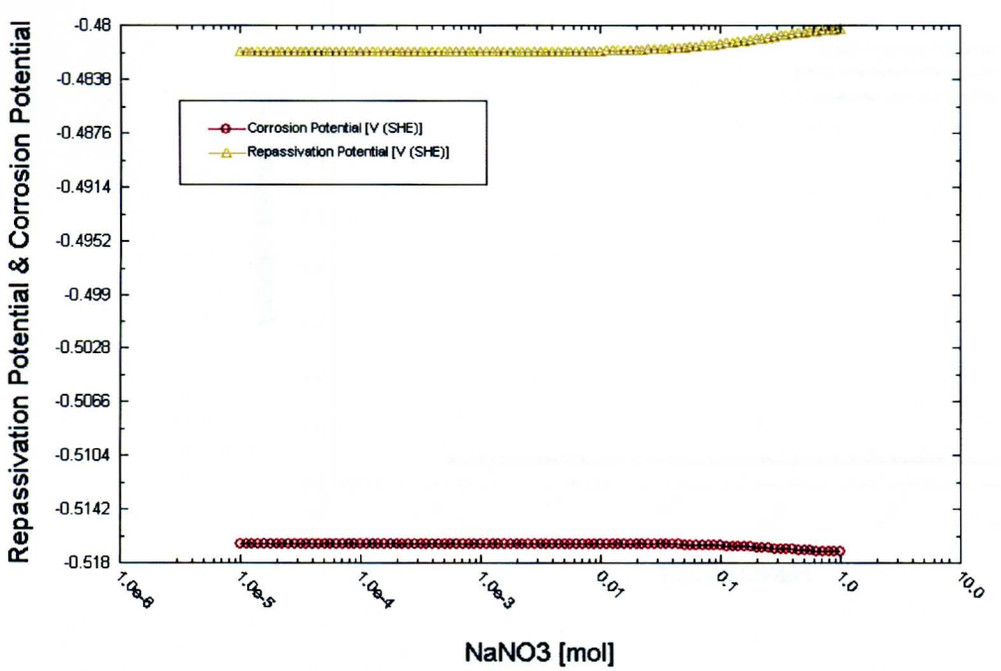
The corrosion potential and repassivation potential are shown below:



The general corrosion rate in a 0.1 m NaCl solution as a function of NaNO3 concentration is as follows:

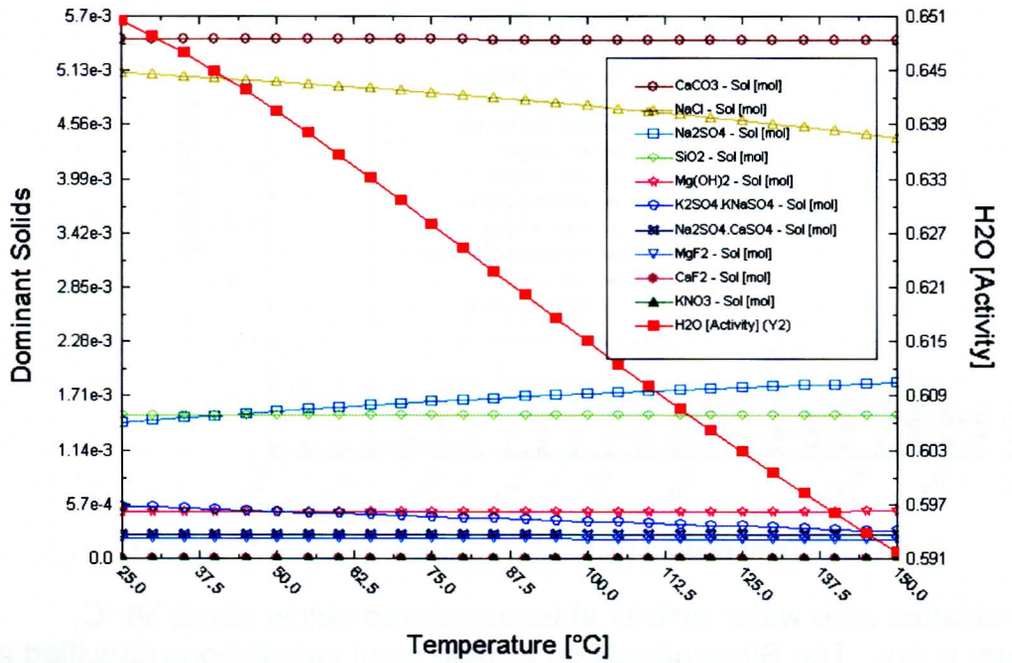


The corrosion potential and repassivation potential are shown below:



January 30, 2008

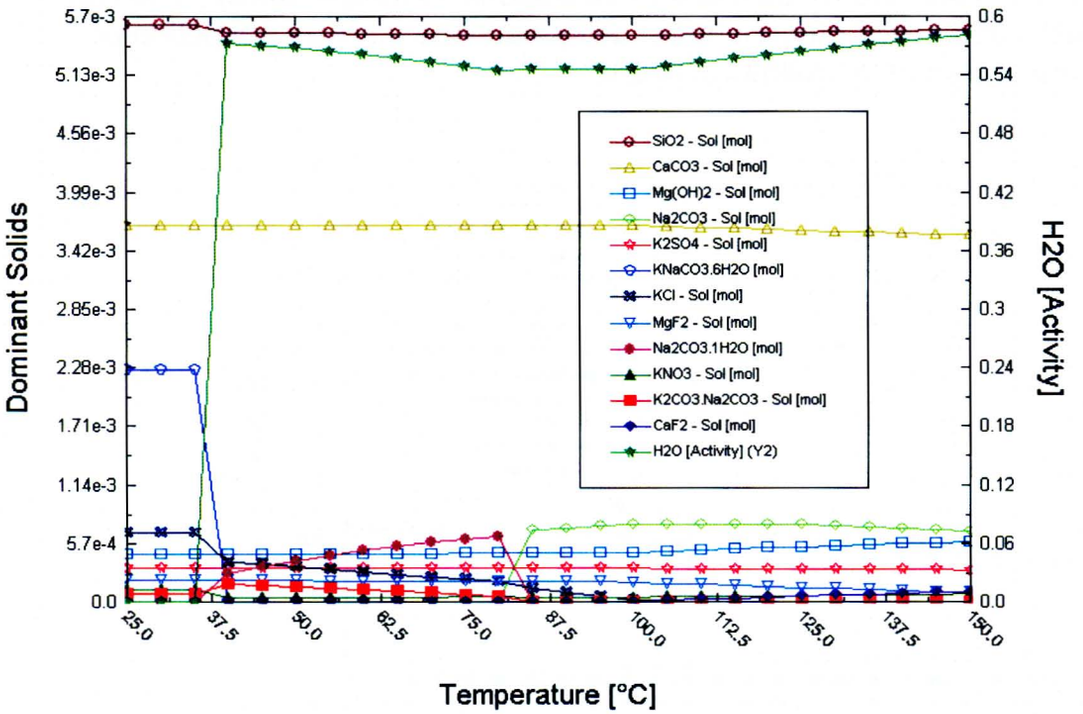
Similar to calculations presented on page 271 of this notebook, the MDRH of salts present in sample C-186101 (salt assemblage NaCl+KNO_3) was calculated using StreamAnalyzer Version 2.0 (bubble point calculations vs temperature). The water activity (=MDRH) and solids present at the deliquescence point as a function of temperature are shown in the following figure:



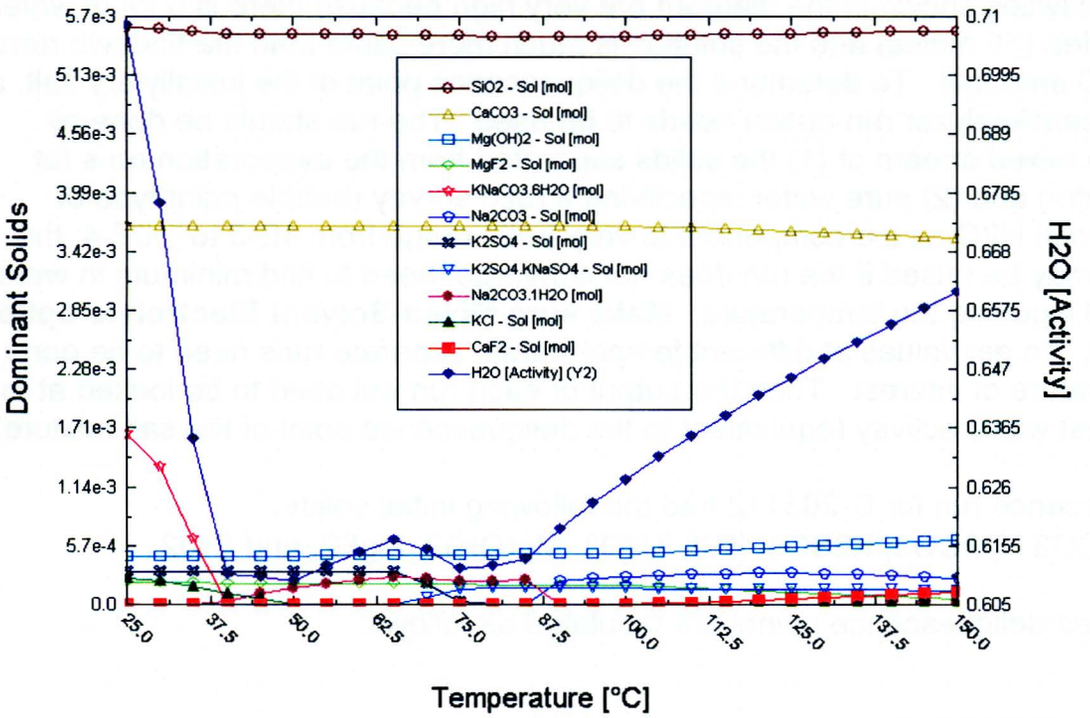
The MDRH values for C-186101 (salt assemblage NaCl+KNO_3) are tabulated below:

Temp, C	MDRH	Temp, C	MDRH
25	65.05	105	61.24
30	64.87	110	61.00
35	64.69	115	60.75
40	64.49	120	60.51
45	64.27	125	60.28
50	64.05	130	60.05
55	63.81	135	59.82
60	63.56	140	59.60
65	63.31	145	59.38
70	63.05	150	59.17
75	62.79		
80	62.53		
85	62.27		
90	62.01		
95	61.75		
100	61.50		

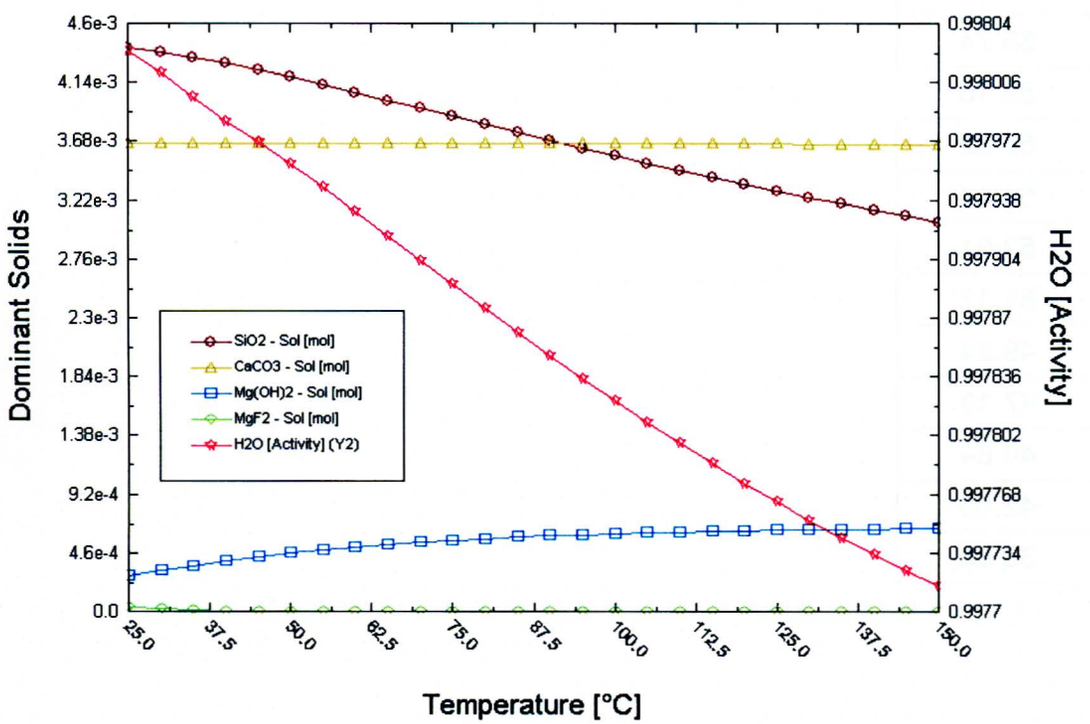
For sample C-203112 (salt assemblage KCl+KNO_3), the calculated water activity and solids present at the deliquescence point as a function of temperature are shown in the following figure.



The above figure indicates zero water activity at temperatures below about 38 °C, indicating the system is dry. The StreamAnalyzer bubble point calculations specified a water amount of 0.0135362 moles, which apparently is not enough water for the system because some of the solids take up water as waters of hydration (at higher temperatures, these hydration waters are released). A separate isothermal (25 °C), bubble point StreamAnalyzer run was done, which indicated that at least 0.04005 moles in needed to assure deliquescence is achieved at 25 °C. Thus, at least this amount of water was specified in the bubble point vs temperature run. The results using a value of 0.201 moles are shown in the following figure:



The above figure has a minimum in the water activity between 37 and 87 °C. This minimum is likely a result of insufficient water in the system. Another run was done using 5.15364 moles of H2O as input. The results are shown below:



The water activities shown in the diagram are very high because there is a lot of water that was added (>5 moles) and the solution is much more dilute than the first two runs at lower H2O amounts. To determine the deliquescence point of the initially dry salt, a different StreamAnalyzer run option needs to be used. The run should be done by generating a mixed stream of (1) the solids separated from the evaporation runs (at P=3.14E-5 atm) and (2) pure water; specifying a ratio survey (bubble point type of calculation) with H2O as the component to vary (ratio range from 1E-5 to 1.0E-4; the lower value may be raised if the run does not converge; need to find minimum in water activity), and inputting the temperature. **Make sure Mixed-Solvent Electrolyte option is specified.** To get values at different temperatures, separate runs need to be done at each temperature of interest. Then the output of each run will need to be looked at to find the lowest water activity (equivalent to the deliquescence point of the salt mixture).

The deliquescence run for C-203112 had the following initial solids:
CaCO3, K2CO3·Na2CO3, K2SO4, KCl, KNO3, Mg(OH)2, MgF2, and SiO2.

The calculated deliquescence points are tabulated as follows:

Temp, C	MDRH(%)
25	70.60
30	67.39
40	57.18
50	56.74
60	56.10
70	55.32
80	54.44
90	52.91
100	51.17
110	49.24
120	47.13
130	44.84
140	42.40
150	39.80

Sample C-186098 was rerun to determine the MDRH for the following initial solids: $2Na_2SO_4 \cdot Na_2CO_3$, $CaCO_3$, KNO_3, $Mg(OH)_2$, Na_2SO_4, $Na_2SO_4 \cdot NaF$, NaCl, $NaNO_3$, and SiO_2. The MDRH values are listed below. These values are somewhat different from those on page 272 because of the different calculation types used (for comparison, the previous values are listed in column–3. The newer values are more representative of the MDRH for the solid assemblage listed in this paragraph.

Temp, C	MDRH(%)	MDRH(%) (previous run, p. 422)
25	64.43	64.43
30	63.16	63.16
40	59.97	59.97
50	55.86	55.86
60	51.28	51.28
70	47.58	48.18
80	43.68	45.92
90	39.63	41.45
100	35.44	36.80
110	31.12	32.00
120	26.69	27.71
130	22.31	27.26
140	18.30	26.78
150	17.32	26.30

Sample C-186101 was rerun to determine the MDRH for the following initial solids: $CaCO_3$, $K_2SO_4 \cdot KNaSO_4$, KNO_3, $Mg(OH)_2$, MgF_2, Na_2SO_4, $Na_2SO_4.CaSO_4$, NaCl, and SiO_2. The calculated MDRHs are tabulated in the second column; the third column lists the values derived previously (page 324). The differences arise from the higher water amount in the previous run.

Temp, C	MDRH(%)	MDRH(%) (previous run, p. 474)
25	65.05	65.05
30	63.82	64.87
40	61.01	64.49
50	57.78	64.05
60	54.16	63.56
70	50.19	63.05
80	45.94	62.53
90	41.46	62.01
100	36.80	61.50
110	31.98	61.00
120	27.04	60.51
130	22.28	60.05
140	18.25	59.60
150	17.22	59.17

Sample C-186088 was rerun to determine the MDRH for the following initial solids: $CaCO_3$, $K_2SO_4 \cdot KNaSO_4$, KCl , KNO_3, $Mg(OH)_2$, Na2CO3, $Na_2SO_4 \cdot NaF_2$, NaCl and SiO_2. The calculated MDRHs are compared with the previous values (p. 427) in the table below. The newer values better represent the MDRH of the mineral assemblage listed in this paragraph.

Temp, C	MDRH(%)	MDRH(%) (previous run, p. 427)
25	65.02	65.02
30	64.68	64.68
40	63.54	63.54
50	61.66	61.66
60	59.20	59.19
70	56.30	56.46
80	53.11	54.21

90	49.68	53.74
100	46.02	51.99
110	42.15	50.92
120	38.11	49.87
130	33.90	48.85
140	29.54	47.87
150	25.01	47.04

The following values for sample C-203120 were taken from page 284. The solid assemblage comprises $Ca(NO_3)_2$, $Ca(NO_3)_2{\cdot}4KNO_3$, $CaCO_3$, $CaSO_4$, $Mg(OH)_2$, NaCl, $NaNO_3$, and SiO_2. Additional calculations indicate deliquescence can occur at lower values, depending on the amount of water in the system.

Temp, C	MDRH(%)
25	4.50
30	5.11
40	6.40
50	7.73
60	9.02
70	10.17
80	11.08
90	11.73
100	12.10
110	12.23
120	12.38
130	12.52
140	12.46
150	12.20

Sample C-203117 was rerun to determine the MDRH for the following initial solids: $Ca(NO_3)_2 \cdot 4KNO_3$, $CaCO_3$, $CaSO_4$, KNO_3, $Mg(OH)_2$, MgF_2, NaCl, $NaNO_3$, and SiO_2

Temp, C	MDRH(%)
25	37.45
30	38.16
40	39.08
50	39.28
60	38.77
70	37.57
80	35.75
90	33.41
100	30.62
110	27.44
120	23.91
130	20.00
140	16.37
150	15.66

February 1, 2008

The potential of deliquescence brines to initiate localized corrosion of Alloy 22 depends on the relative concentrations of chloride ions to corrosion inhibitors like nitrate, sulfate, carbonate, and bicarbonate. pH is an important factor for generalized corrosion. StreamAnalyzer Version 2.0 was used to calculate the concentration ratios of chloride to nitrate at the deliquescence point of the representative leachate samples. The values are listed in the following table. pH values at selected temperatures are also listed.

Calculated Concentration Ratios of Chloride to Nitrate Ions as a Function of Temperature of Six Samples Representing Six Key Salt Assemblages. Listed in Brackets are Calculated pHs at 25, 50, 100, and 150 °C.*

	Sample Number					
Temp (°C)	**C-186098**	**C-186101**	**C-203112**	**C-186088**	**C-203120 (from page 284)**	**C-203117**
25	0.56 [10.98]	0.60 [9.70]	0.15 (0.48)‡ [11.6]	2.1 [11.5]	2.59E-04 [9.35]	0.042 [7.98]
30	0.45	0.50	3.4 (0.37)	1.9	3.24E-04	0.040
40	0.28	0.34	4.2 (0.15)	1.3	4.82E-04	0.036
50	0.17 [10.43]	0.24 [9.13]	4.8 (0.19) [11.6]	0.85 [10.9]	6.77E-04 [9.29]	0.032 [7.49]
60	0.11	0.16	5.5 (0.22)	0.59	9.13E-04	0.028
70	0.081	0.12	6.4 (0.25)	0.44	1.19E-03	0.025
80	0.063	0.084	7.7 (0.28)	0.33	1.53E-03	0.022
90	0.051	0.063	9.7 (0.28)	0.26	1.94E-03	0.021
100	0.042 [9.65]	0.049 [8.33]	13 (0.28) [11.1]	0.20 [10.3]	2.44E-03 [8.21]	0.020 [6.96]
110	0.036	0.039	18 (0.27)	0.16	3.07E-03	0.020
120	0.031	0.032	0.18 (0.18)	0.13	3.87E-03	0.021
130	0.028	0.028	0.16 (0.15)	0.11	4.89E-03	0.022
140	0.027	0.027	0.14 (0.14)	0.097	6.17E-03	0.023
150	0.032 [9.30]	0.033 [8.00]	0.13 (0.13) [10.8]	0.088 [9.86]	7.75E-03 [7.55]	0.028 [6.72]

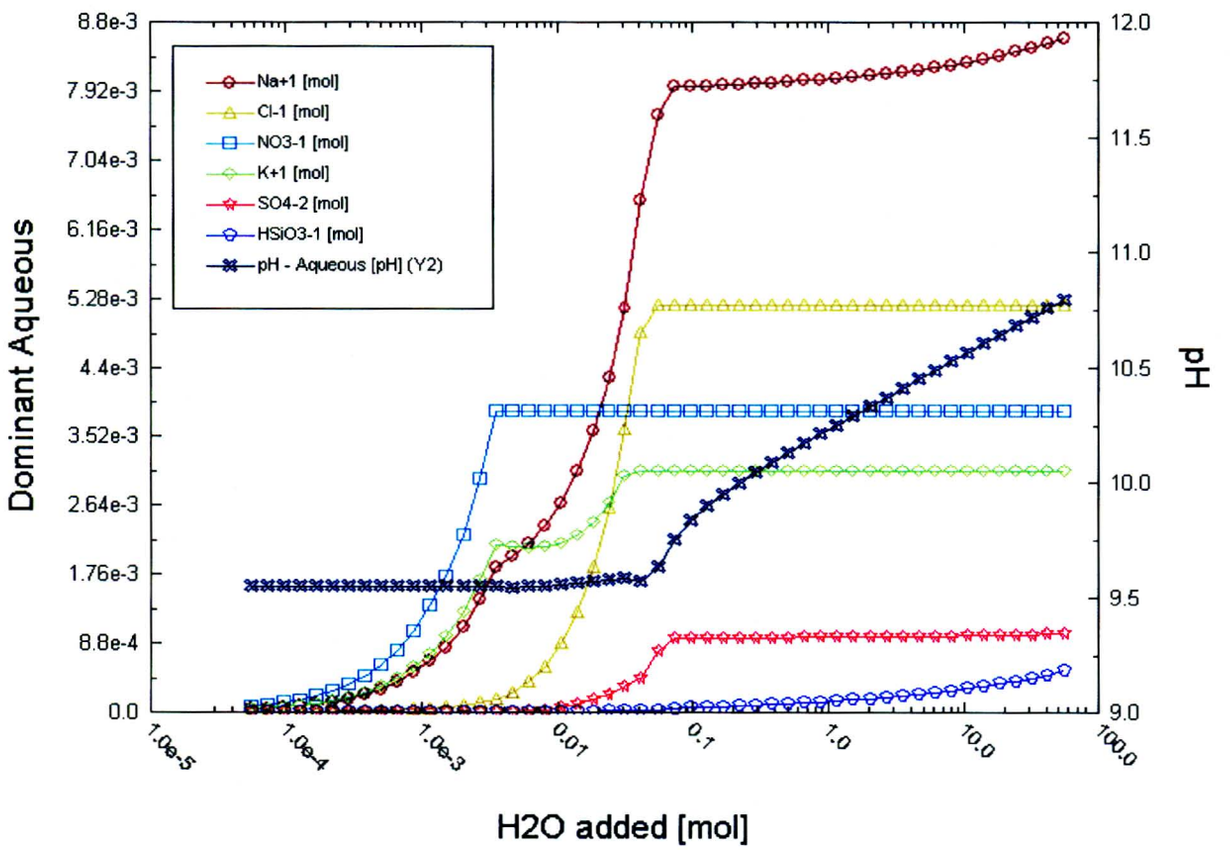
*Each sample number represents a key salt assemblage, as in:
C-186098: $NaCl+NaNO_3+KNO_3$; C-186101: $NaCl+KNO_3$;
C-203112: $KCl+KNO_3$; C-186088: $NaCl+KCl+KNO_3$
C-203120: $NaCl+NaNO_3+Ca(NO_3)_2+ Ca(NO_3)_2{\cdot}4KNO_3$
C-203117: $NaCl+NaNO_3+KNO_3+ Ca(NO_3)_2{\cdot}4KNO_3$
‡Values in parentheses are the concentration ratios of $Cl^-/(NO_3^-+SO_4^{2-}+HCO_3^-+CO_3^{2-})$

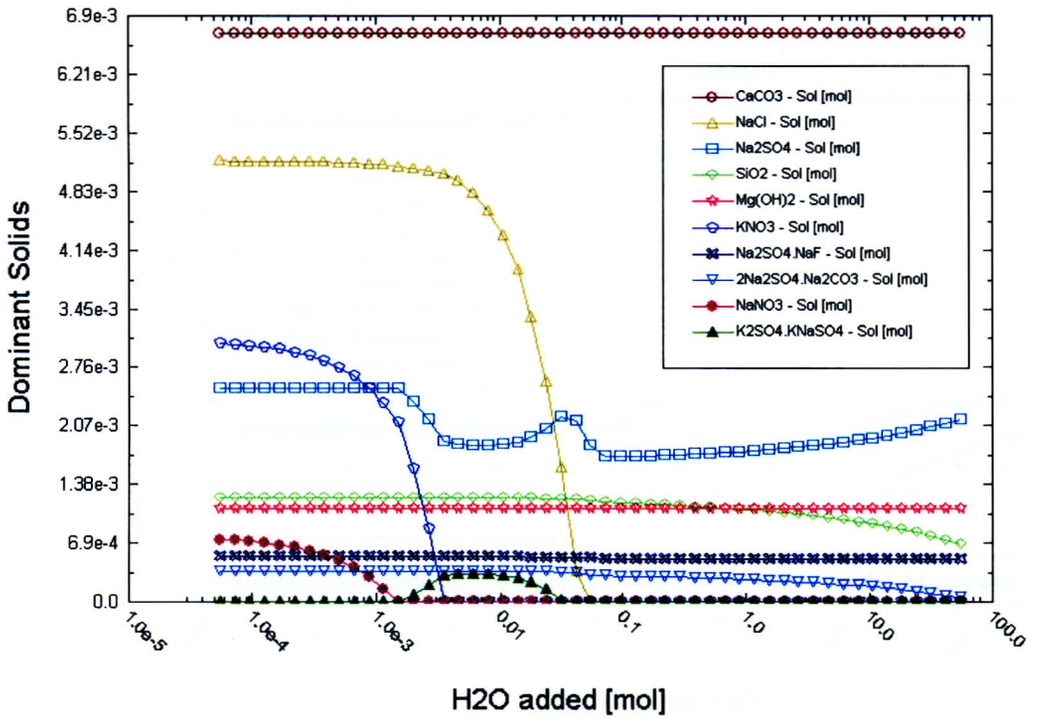
The values tabulated in the above table indicates the chloride to nitrate ratios of the deliquescence brines mostly are low (less than 10). Where the ratios are greater than 10 (for sample C-203112), the ratio of chloride to the sum of the corrosion inhibitors (nitrate+sulfate+bicarbonate+carbonate) are very low. The pHs are neutral to alkaline, ranging from 6.7 to 11.6, which are unlikely to cause generalized corrosion of Alloy 22 at high temperature.

February 4, 2008

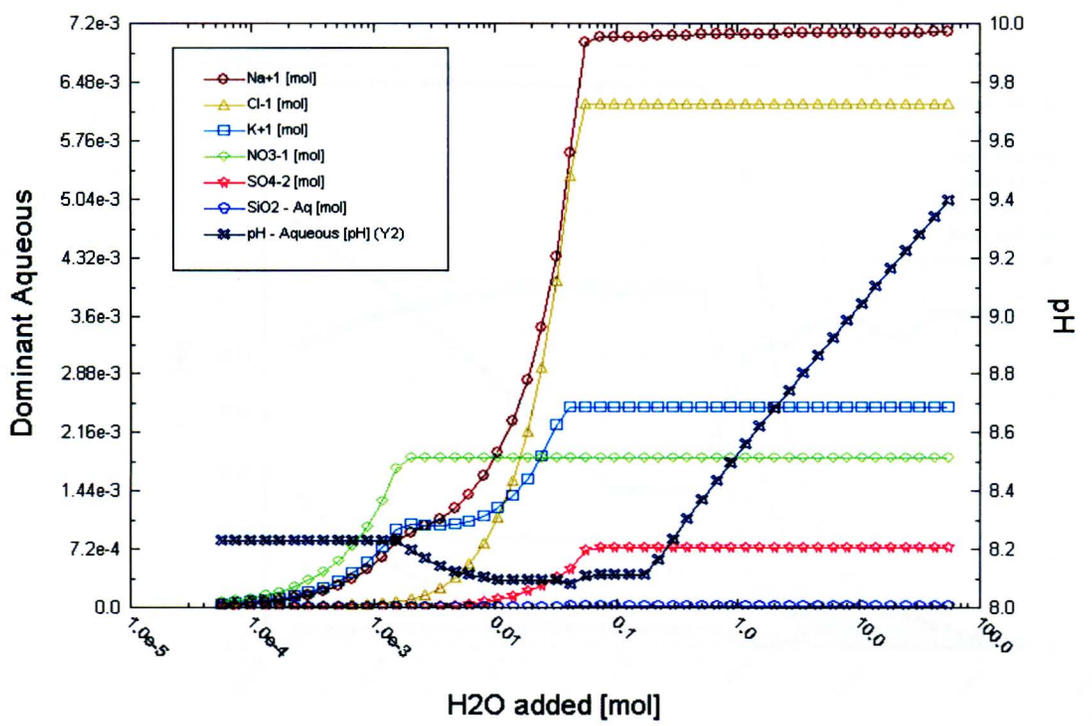
StreamAnalyzer Version 2.0 was used to calculate the evolution of the chemistry of the aqueous and solid phases of an initially dry solid mixture as water is added. (isothermal, mixed stream calculations).

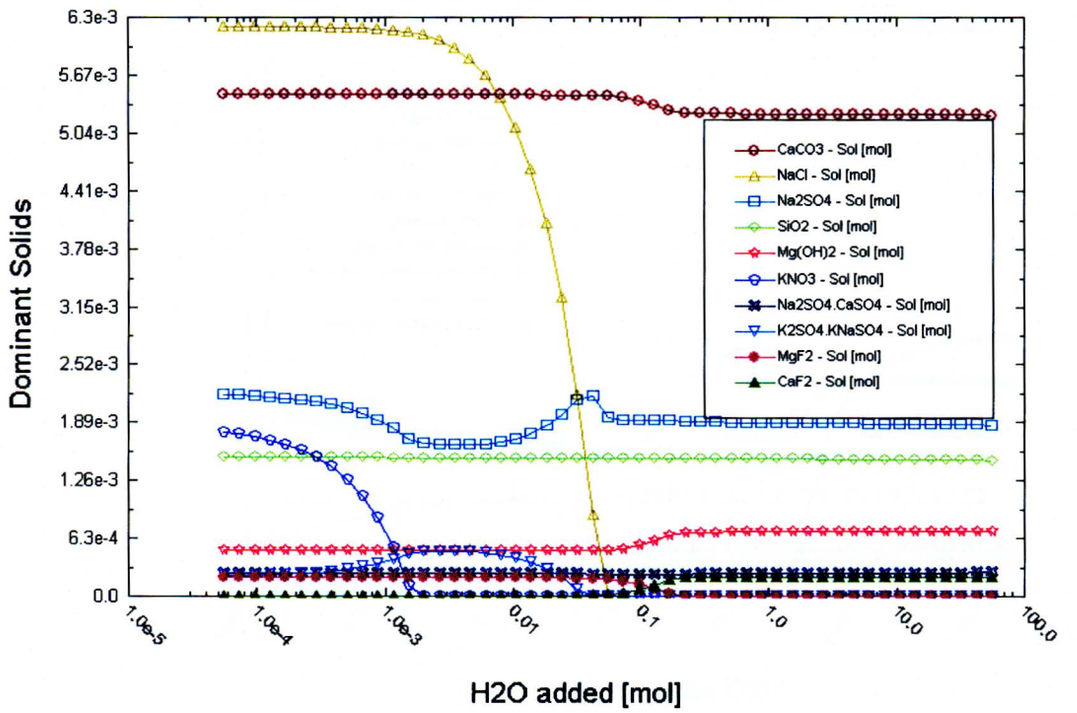
For sample C-186098 at T=110 °C, the results are as follows:



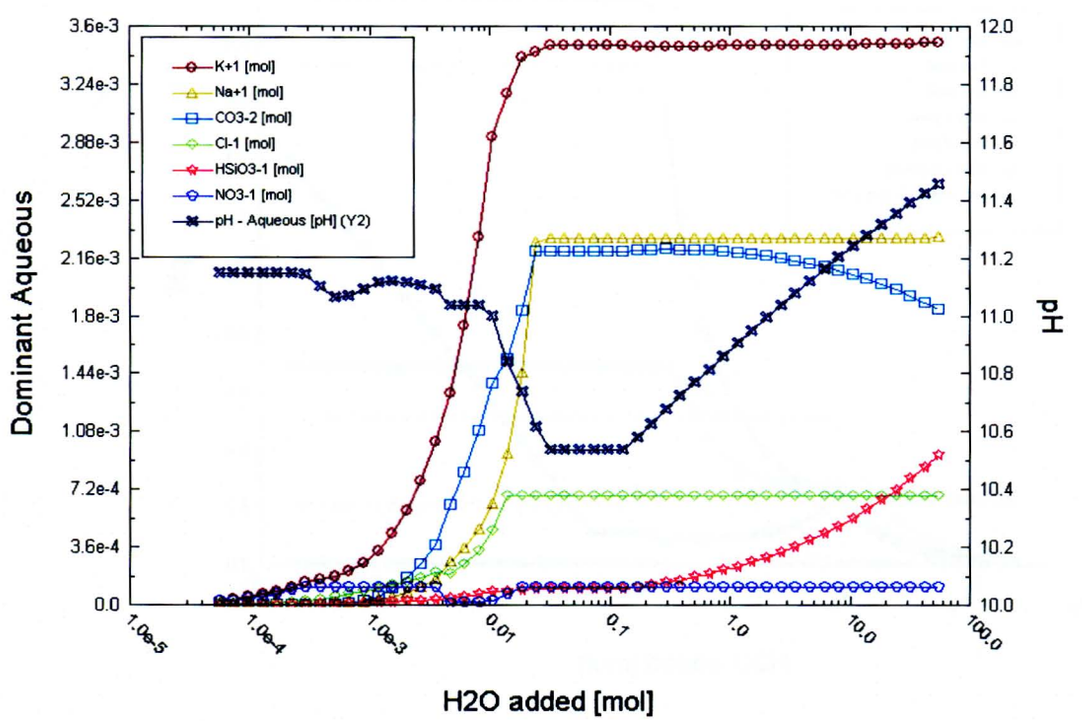


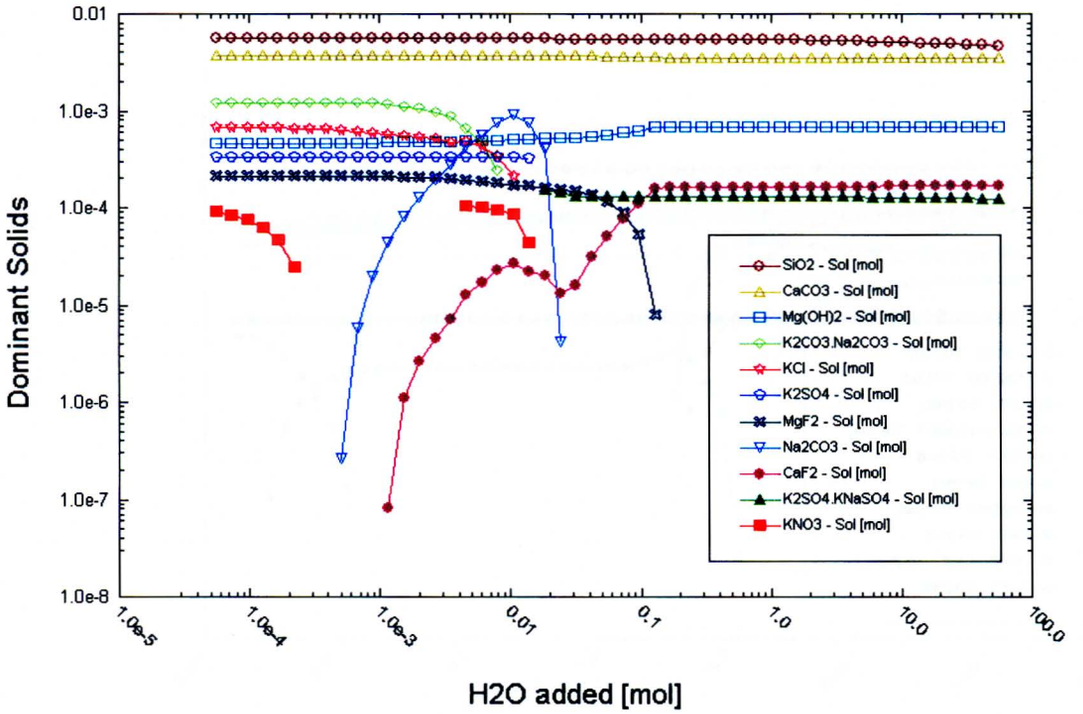
For sample C-186098 at T=110 °C, the results are as follows:



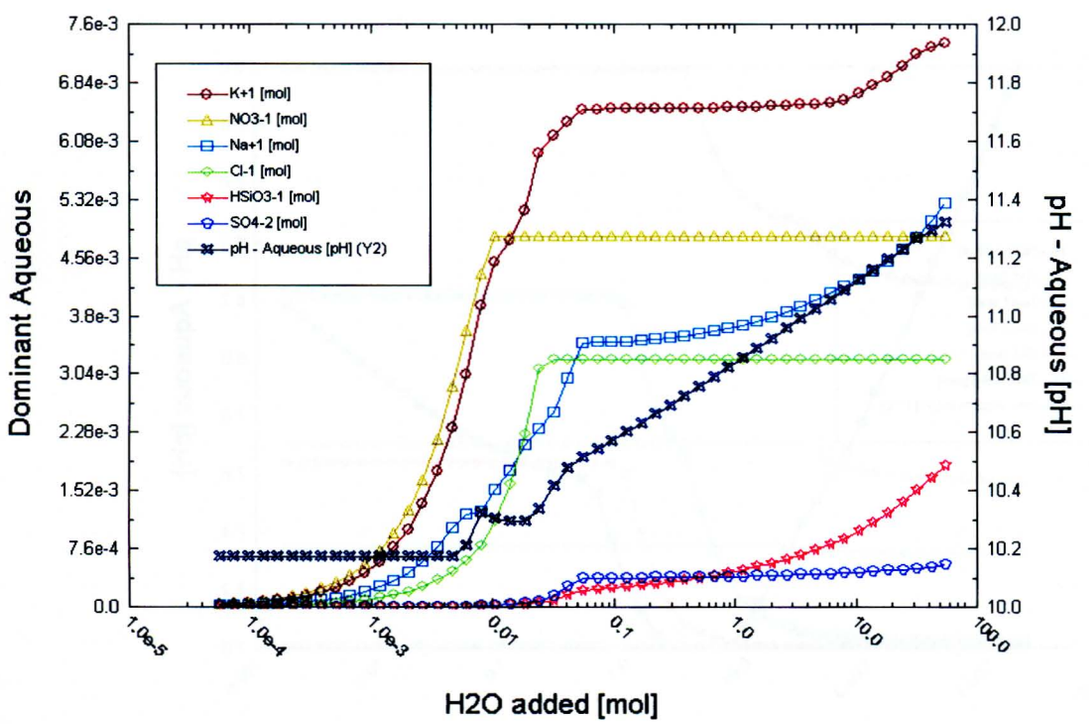


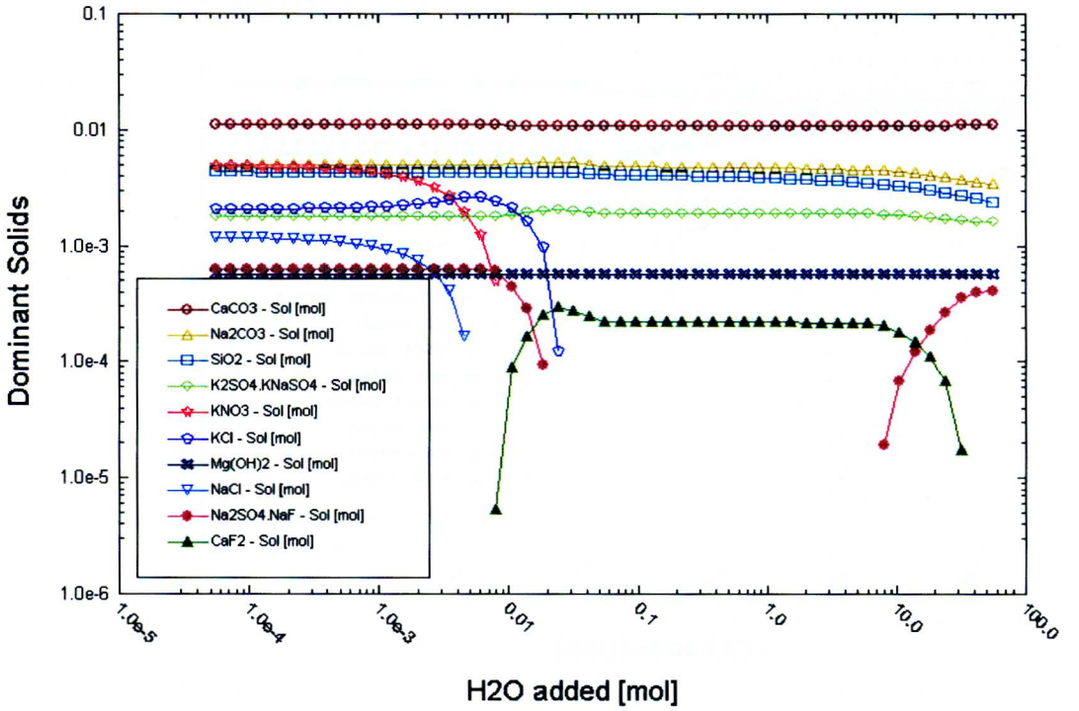
For sample C-203112 at T=110 °C, the results are as follows:



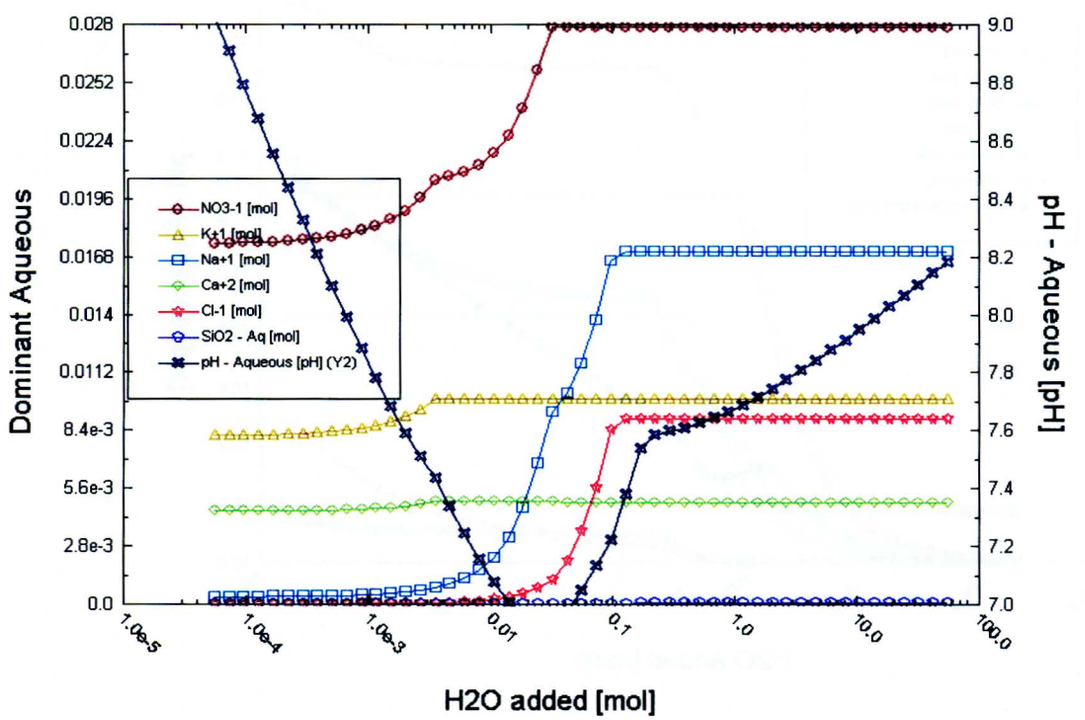


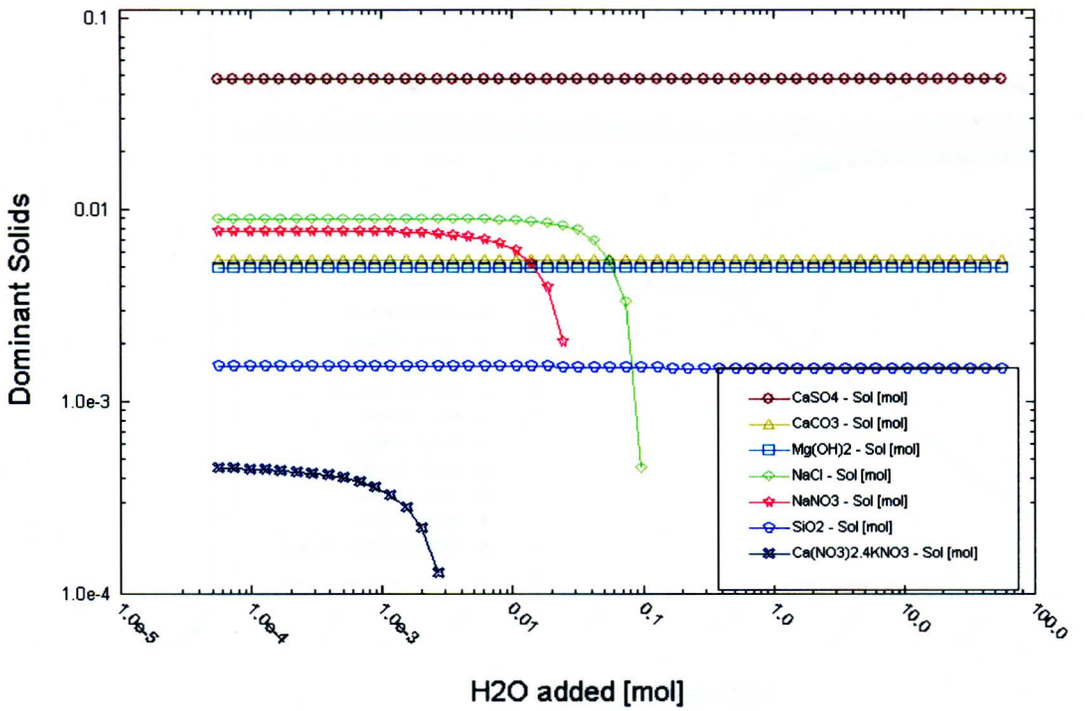
For sample C-186088 at T=110 °C, the results are as follows:



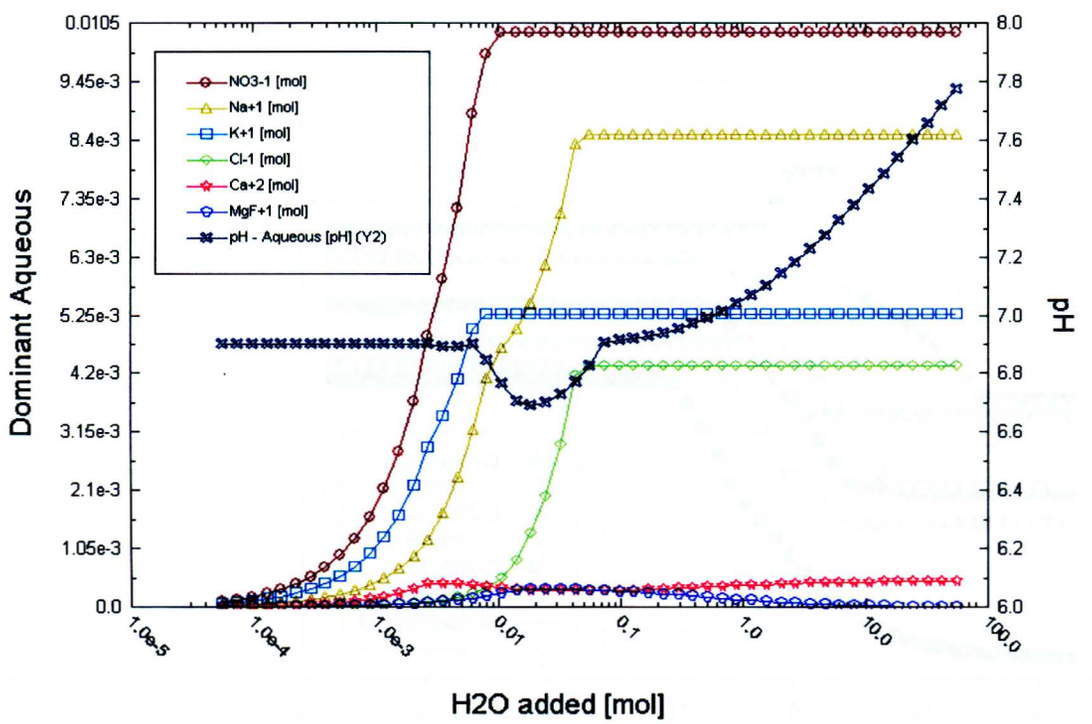


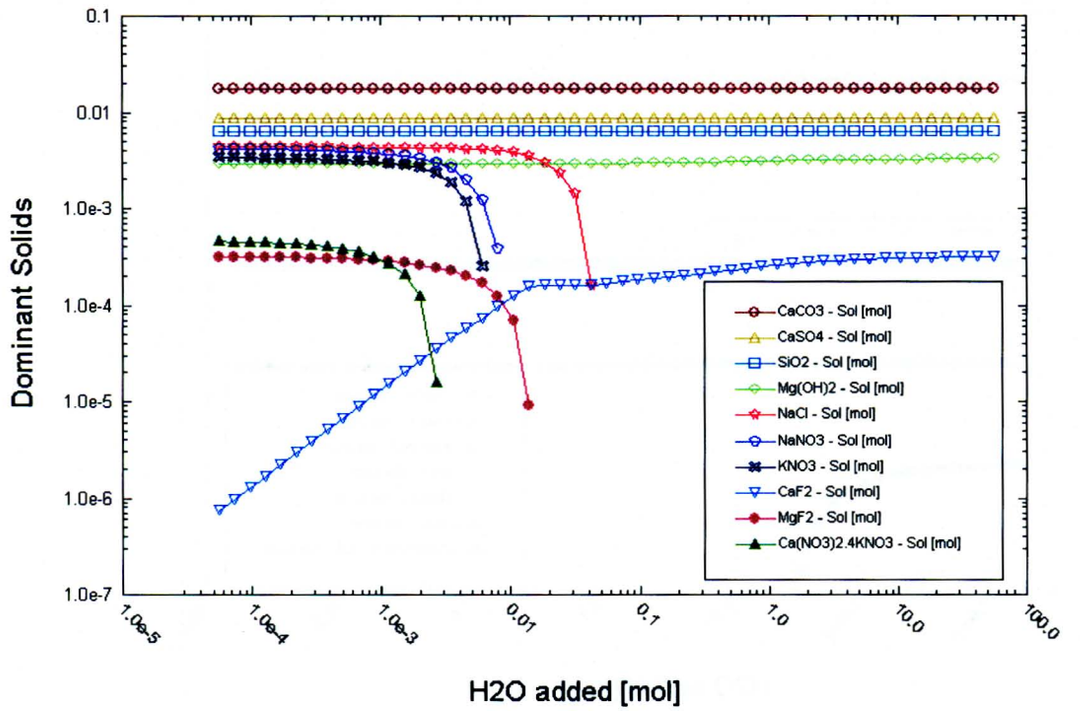
For sample C-203120 at T=110 °C, the results are as follows:



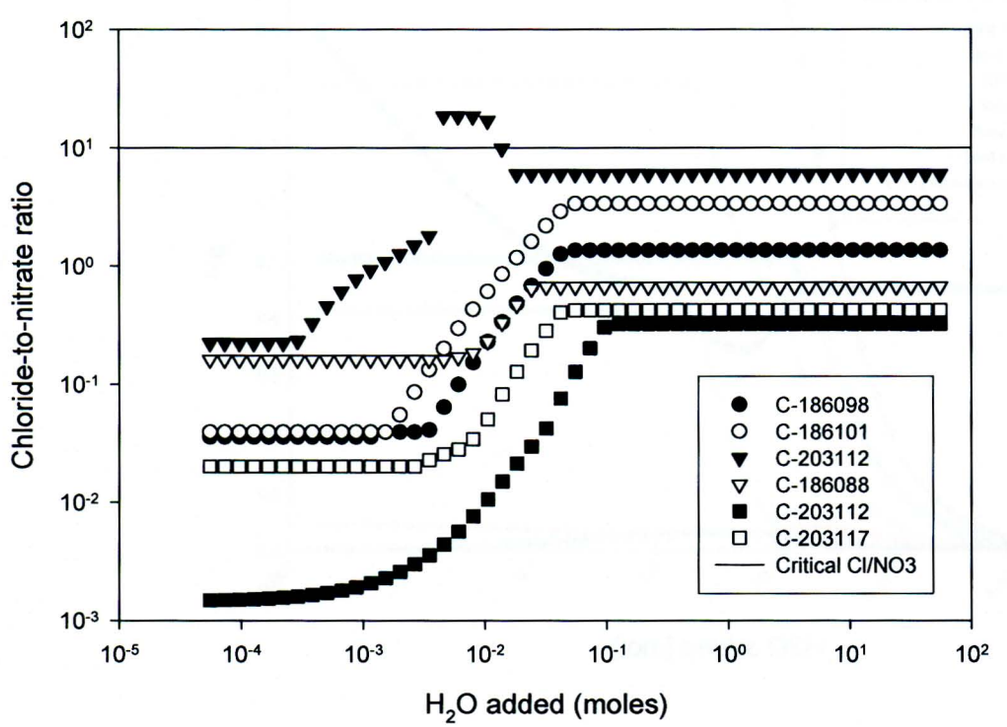


For sample C-203117 at T=110 °C, the results are as follows:





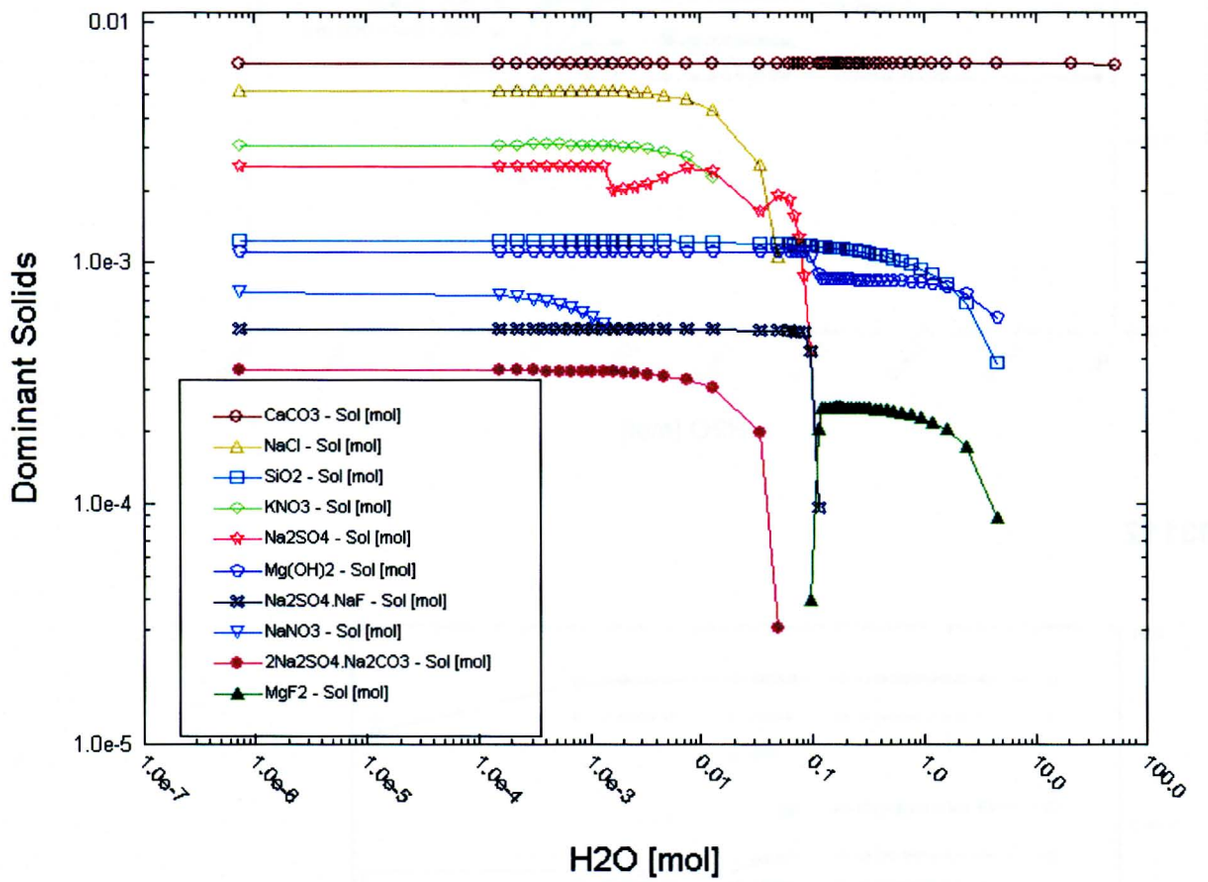
The following figure shows the evolution of chloride-to-nitrate ratio of the six representative samples as H2O is added to the initial dry solids:



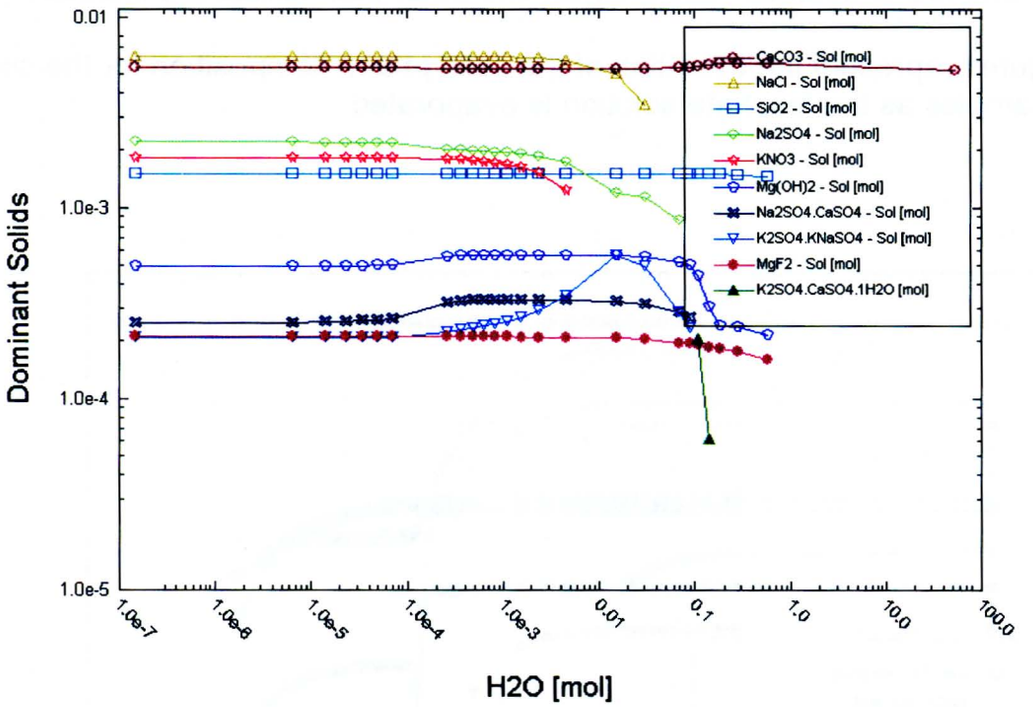
Although the chloride-to-nitrate ratio increases initially, then becomes constant, none except for C-203112, exceed the critical value of 10. As discussed previously, C-203112 has low chloride-to-inhibitor ratio if oxyanions other than nitrate are included.

The following figures represent the evolution of the solid phase composition for the six representative samples as the leachate solution is evaporated.

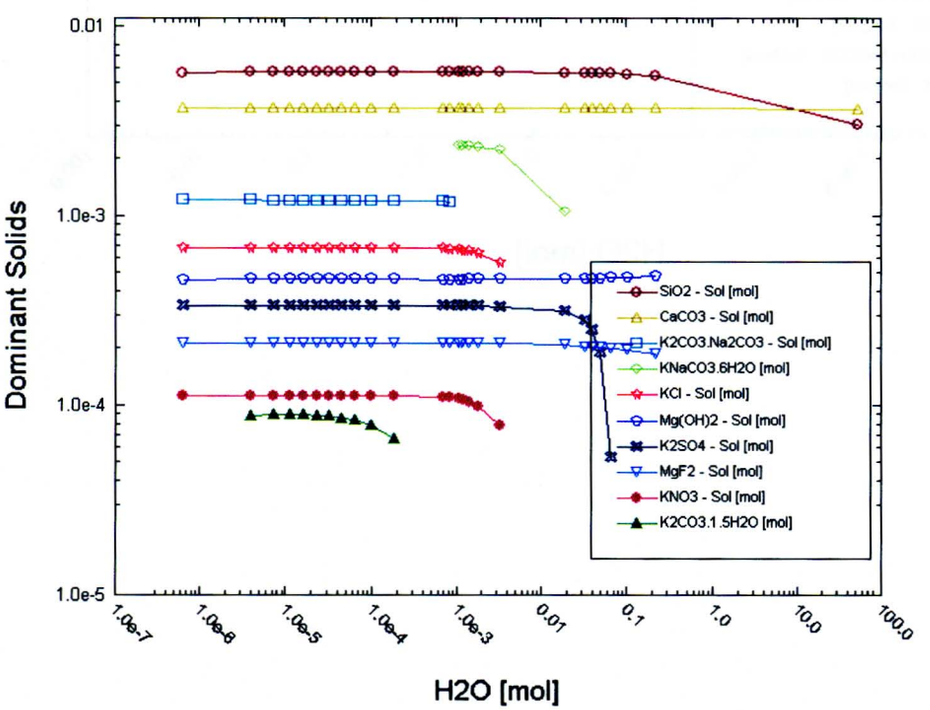
C-186098



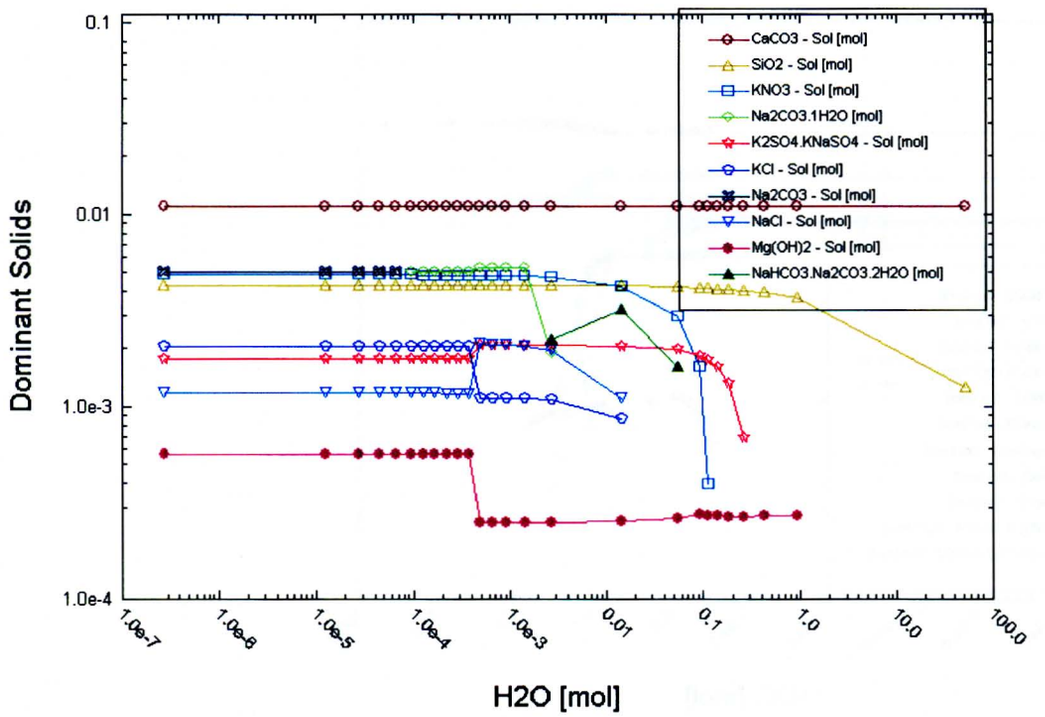
C-186101



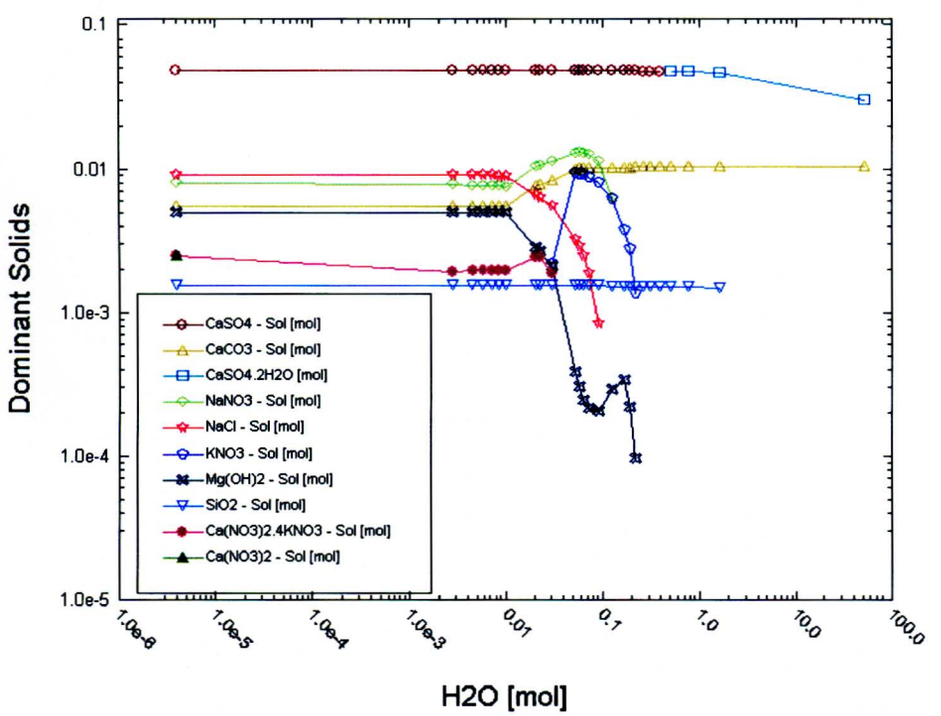
C-203112



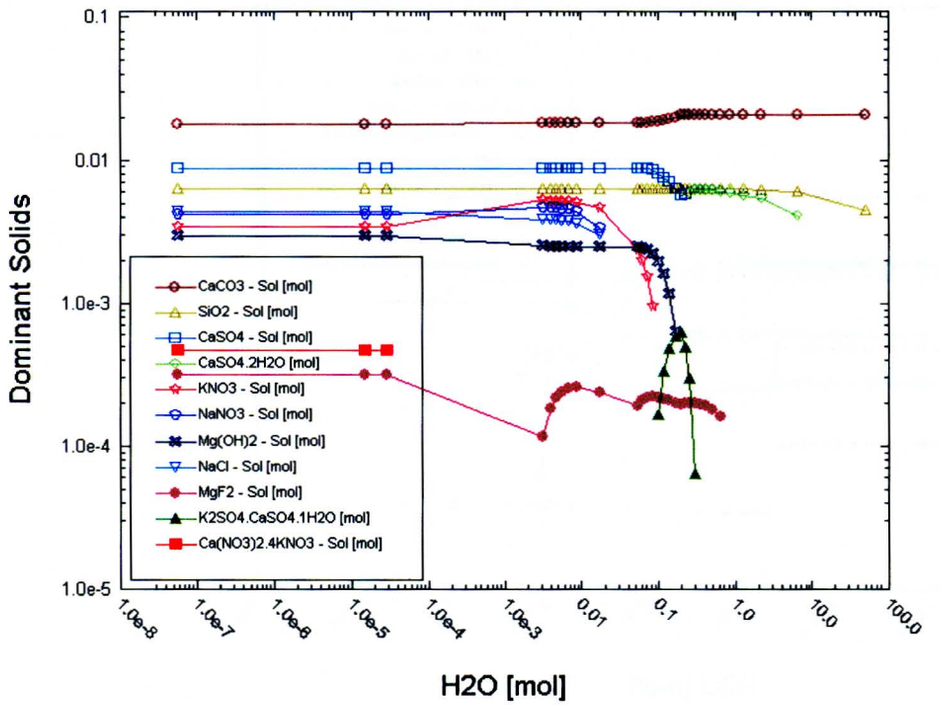
C-186088



C-203120



C-203117


Dominant Solids
0.1
0.01
1.0e-3
1.0e-4
1.0e-5
1.0e-8
1.0e-7
1.0e-6
1.0e-5
1.0e-4
1.0e-3
0.01
0.1
1.0
10.0
100.0
H2O [mol]
CaCO3 - Sol [mol]
SiO2 - Sol [mol]
CaSO4 - Sol [mol]
CaSO4.2H2O [mol]
KNO3 - Sol [mol]
NaNO3 - Sol [mol]
Mg(OH)2 - Sol [mol]
NaCl - Sol [mol]
MgF2 - Sol [mol]
K2SO4.CaSO4.1H2O [mol]
Ca(NO3)2.4KNO3 - Sol [mol]

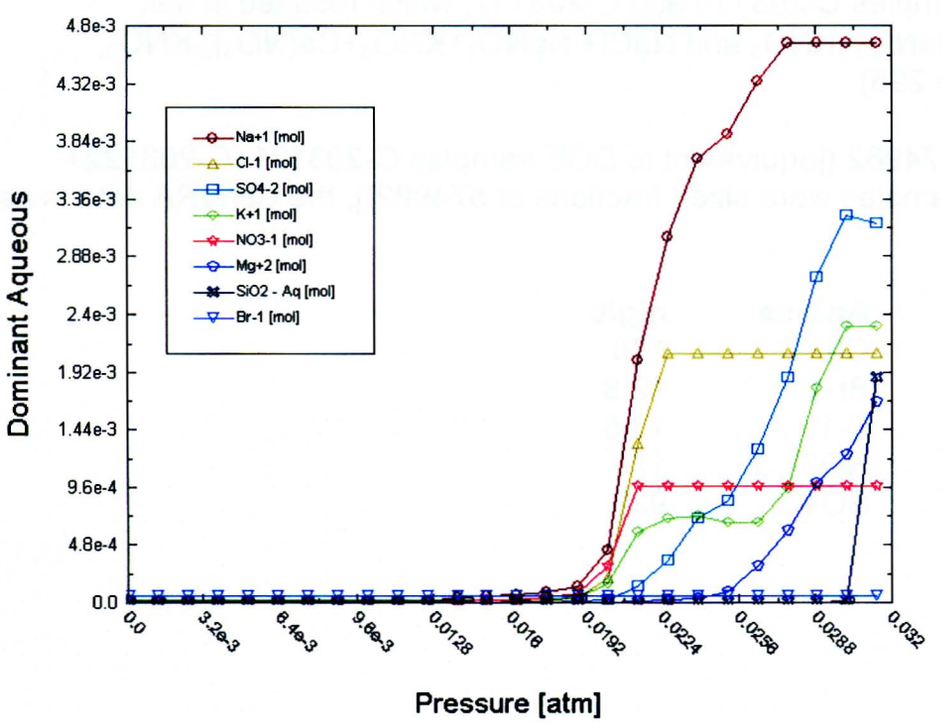
February 11, 2008

Additional StreamAnalyzer Version 2.0 calculations were conducted using CNWRA leachate chemistry data as input. The CNWRA data are lower in nitrate to chloride ratio compared to DOE results. The new calculations were done to see if the salt assemblage that forms will be different compared to the calculations that used DOE leachate chemistry data.

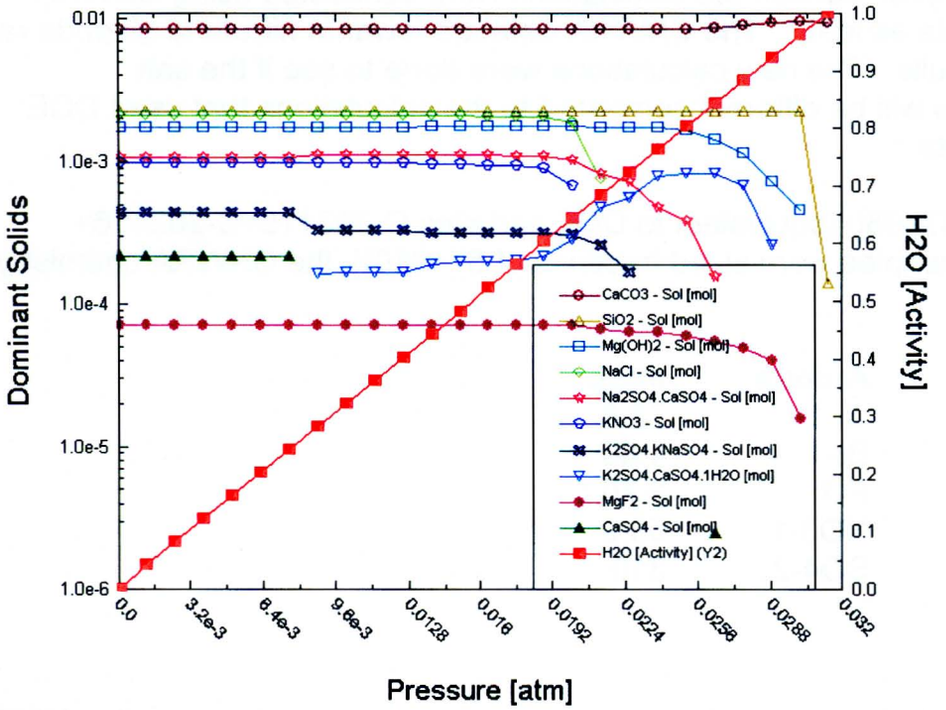
For CNWRA sample 574980 [equivalent to DOE samples C-203115+C-203116+ C-203117 (the DOE samples were sized fractions of 574980)], the CNWRA chemistry data is as follows:

Cations	**mg/L**	**Anions**	**mg/L**
Ca+2	389	Cl-1	73.6
Mg+2	44.1	Br-1	4.66
K+1	89.8	F-1	2.70
Na+1	107	NO3-1	59.9
		SO4-2	310
Neutrals	**mg/L**		
SiO2	134		

Evaporation at 25 °C of a leachate solution with the above composition was simulated using StreamAnalyzer by decreasing the total pressure from 3.13849e-002 to 3.13849e-005 atm. A plot of the dominant aqueous species as a function of total pressure is shown below:



The dominant solids and water activity are as follows:

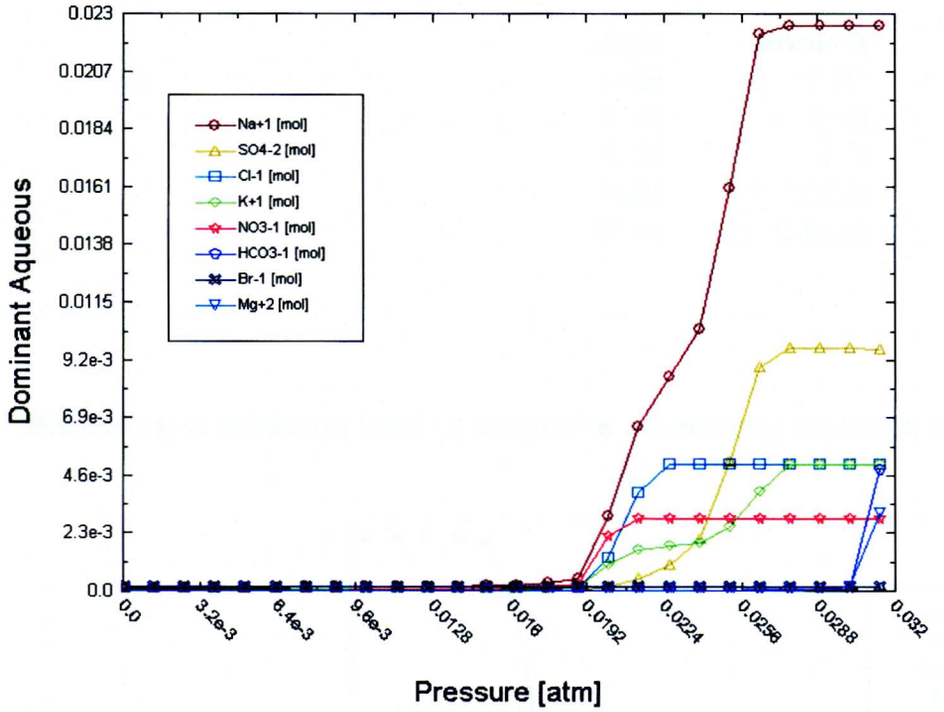


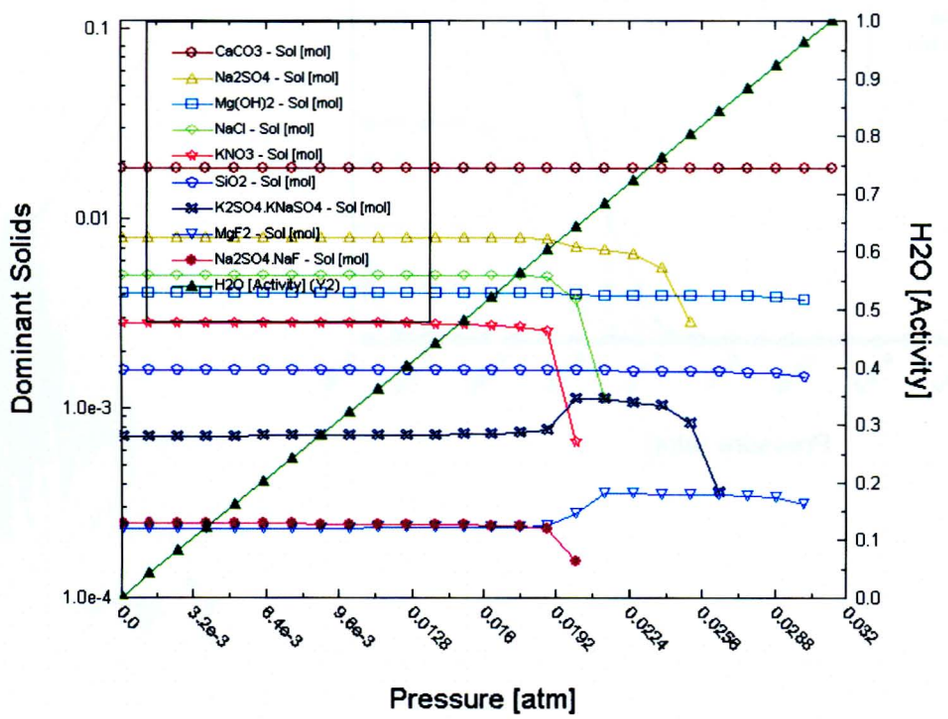
As shown in the above figure, the deliquescent salt assemblage that results by evaporation of the initially dilute leachate solution (CNWRA sample 574980) is $NaCl+KNO_3$. This result is the same as for DOE sample C-203115 but different from the results for DOE samples C-203116 and C-203117, which resulted in salt assemblages $NaCl+ NaNO_3+KNO_3$ and $NaCl+ NaNO_3+KNO_3+Ca(NO_3)_2{\cdot}KNO_3$, respectively (see page 295).

For CNWRA sample 574982 ([equivalent to DOE samples C-203121+C-203122+ C-203123 (the DOE samples were sized fractions of 574982)], the CNWRA data is as follows:

Cations	**mg/L**	**Anions**	**mg/L**
Ca+2	737	Cl-1	178
Mg+2	104	Br-1	12.8
K+1	196	F-1	13.5
Na+1	518	NO3- 1	176
		SO4-2	926
Neutral	**mg/L**		
SiO2	95.2		

The dominant aqueous, solids, and water activities of the evaporated CNWRA sample 574982 (equivalent to DOE samples C-203121+C-203122+ C-203123) are as follows:



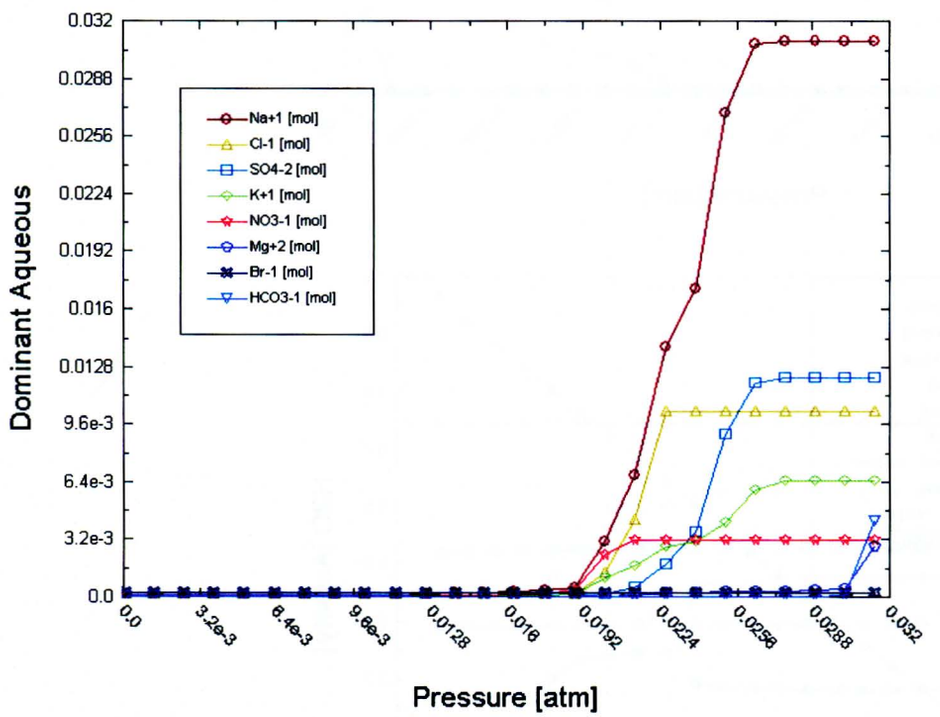


As indicated in the above figure, the resulting salt assemblage is $NaCl+KNO_3$. This result is the same as that for DOE sample C-203121 but not for C-203122 and C-203123. The latter samples yielded the salt assemblage $NaCl+NaNO_3+KNO_3$ (see page 295).

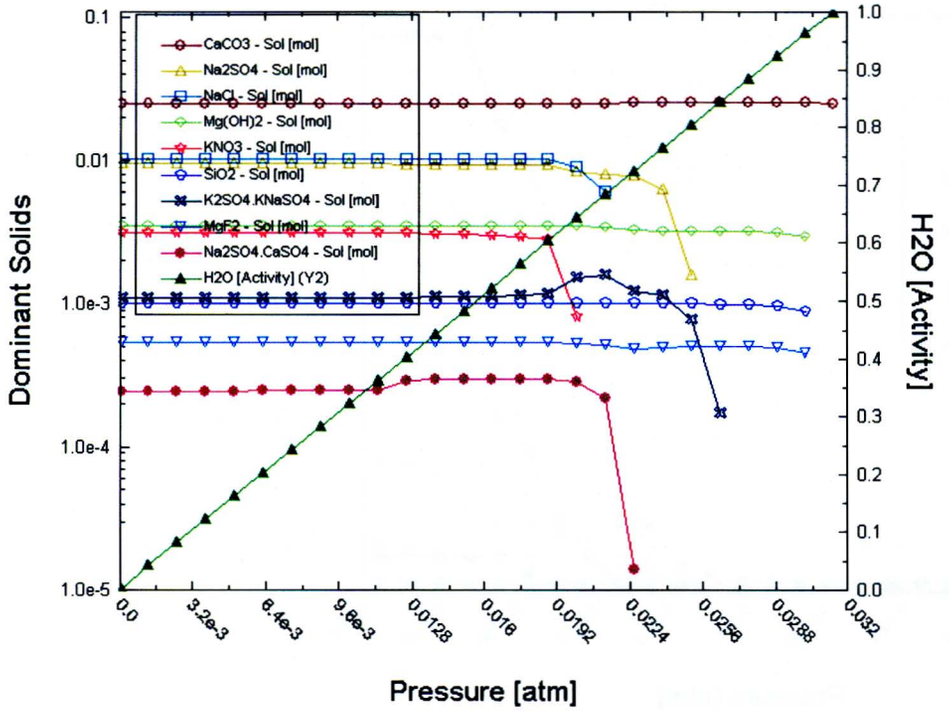
For CNWRA sample 574983 [equivalent to DOE samples C-203124+C-203125+ C-203126 (the DOE samples were sized fractions of 574983)], the CNWRA chemistry data is as follows:

Cations	**mg/L**	**Anions**	**mg/L**
Ca+2	1010	Cl-1	364
Mg+2	98.5	Br-1	15.7
K+1	253	F-1	20.2
Na+1	710	NO3- 1	194
		SO4-2	1170
Neutral	**mg/L**		
SiO2	60.6		

The resulting dominant aqueous species as a function of total pressure is as follows:



The dominant solids and water activity upon evaporation of CNWRA sample 574983 (equivalent to DOE samples C-203124+C-203125+ C-203126) is as follows:

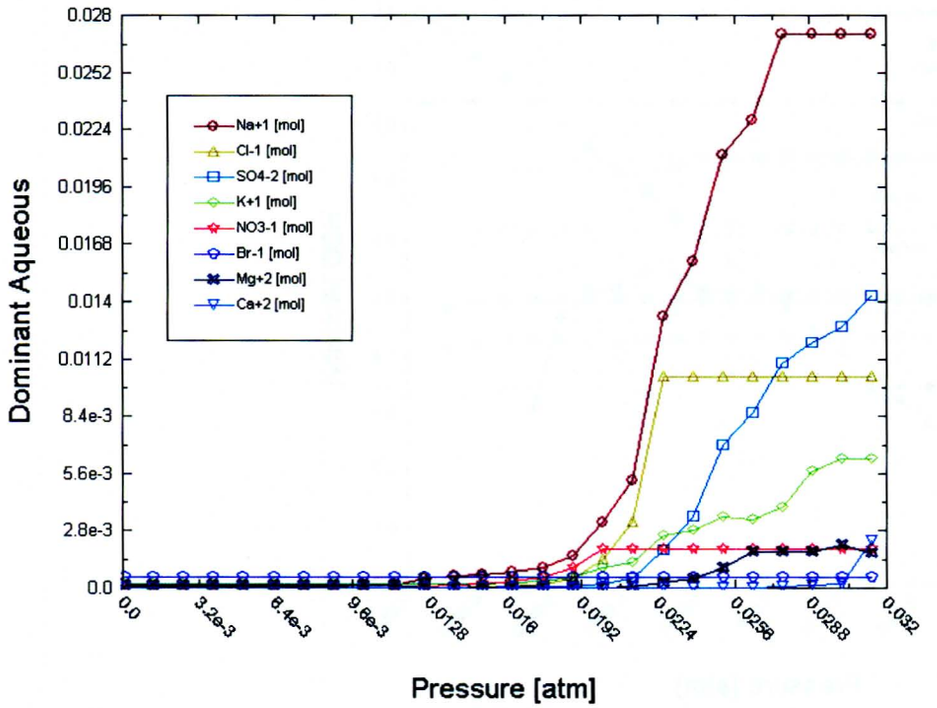


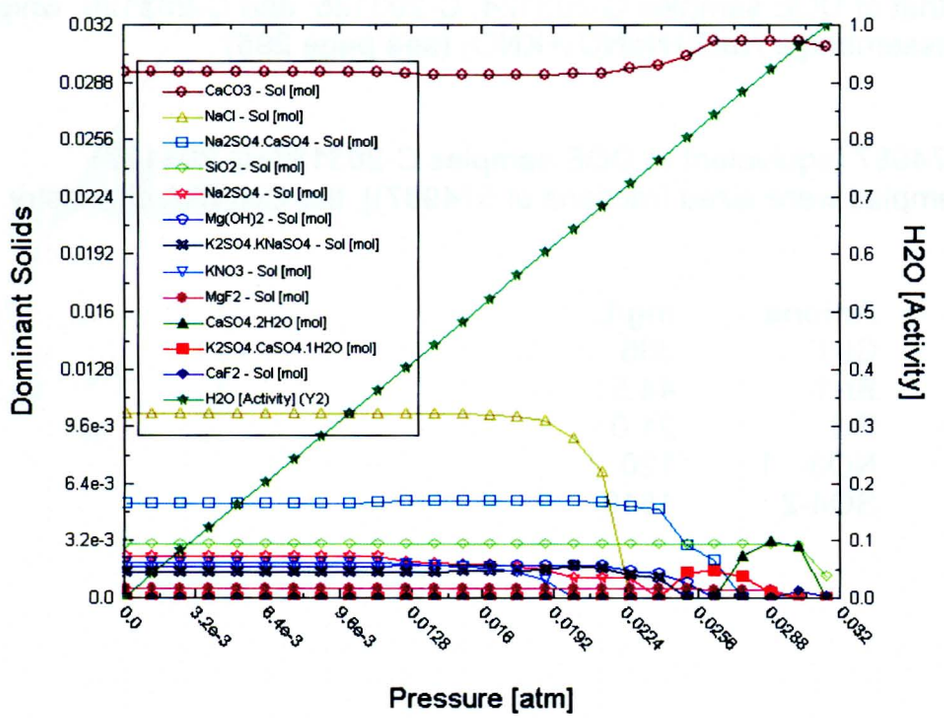
As indicated in the above figure, the resulting salt assemblage is NaCl+KNO_3. This result is different from that of DOE samples C-203124, C-203125, and C-203126, which all resulted in the salt assemblage NaCl+$NaNO_3$+KNO_3 (see page 295).

For CNWRA sample 574987 [equivalent to DOE samples C-203136+C-203137+ C-203138 (the DOE samples were sized fractions of 574987)], the CNWRA chemistry data is as follows:

Cations	**mg/L**	**Anions**	**mg/L**
Ca+2	1390	Cl-1	366
Mg+2	58.3	Br-1	44.5
K+1	247	F-1	21.0
Na+1	622	NO3- 1	120
		SO4-2	1510
Neutral	**mg/L**		
SiO2	180		

The dominant aqueous, solids, and water activities of the evaporated CNWRA sample 574987 (equivalent to DOE samples C-203136+C-203137+ C-203138) are as follows:





As indicated in the above figure, the resulting salt assemblage is $NaCl+KNO_3$. This result is the same as that for DOE sample C-203136 but not for C-203137 and C-203138. The latter samples yielded the salt assemblage $NaCl+NaNO_3+KNO_3$ (see page 295).

Although the CNWRA analysis of dust leachates had lower nitrate to chloride ratio compared to DOE leachates of equivalent splits of dust samples, the calculated salt assemblages using the CNWRA chemistry data all yielded the salt assemblage $NaCl+KNO_3$. Deliquescence of this salt assemblage would have low chloride to nitrate ratio (see table on page 332).

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February 15, 2008
-----Original Message----

From: Lietai Yang [mailto:ltyang@cnwra.swri.edu]
Sent: Friday, February 15, 2008 4:16 PM
To: rpabalan@cnwra.swri.edu
Subject: RE: Chapter 2 revisions

As discussed, enclosed is the file for the composition. We know the pH (T=room)=4.4 for the diluted sample. What would be the pH of the original solution at the system temperature. The solution was diluted by approximately 10 times by weight (from 35.6 gram to 300 mL).

Thanks - Lietai

The original data see notebook #737, page 31							
							in 17 mL volume, 35 g
	Sample ID, after diluted to 300 mL			L=300 mL			17
	Sol-A-150°C-Nov. 3, 05				Ratio	300	Moles/L
	Sample Result	Reporting Limit		mM		mMol in 300 mL	M in the 17 mL at system temp
Analysis	(mg/L)	(mg/L)					
Chloride	1880	100	35.5	53.0		15.9	0.935
Nitrate-N	15400	100	14	1100.0	20.8	330.0	19.41
Phosphate-P	1970	100	30.97	63.6		19.1	1.12
Potassium	22900	150	39.1	585.7		175.7	10.34
Sodium	14800	150	23	643.5		193.0	11.36
Sulfate	<100	100					
pH of the diluted dilution 4.4						Cl–	0.935
			33.18			NO–3	19.41
						PO4–3	1.12
						Sum(Anion moles)	23.71
						K	10.34
						Na	11.36
						Sum(Cation moles)	21.69

February 18, 2008

The dilute aqueous concentrations and pH were input into StreamAnalyzer Version 2.0. Charge balance was reconciled, using prorate and pH-reconciled options.

Part of the StreamAnalyzer report is a follows:

Reconciliation Summary

	Specification
Charge Balance Method	Prorate
pH Reconciliation Type	Not specified

	Measured	Calculated	Difference %
Temperature, °C	25.0000		
Pressure, atm	1.00000		
pH	0.0	13.1324	100.00
Density, g/ml	0.0	1.44925	
Water, mol H2O	55.5087	55.5087	

Stream Inflows

	Input	Calculated		% Diff
H2O	55.5087	55.5087	mol	
Na+1	11.3600	12.4096	mol	9.23963
K+1	10.3400	11.2954	mol	9.23963
Cl-1	0.935000	0.935000	mol	
NO3-1	19.4100	19.4100	mol	
PO4-3	1.12000	1.12000	mol	

Charge Balance

Cation Charge:	21.700000 eq
Anion Charge:	-23.705000 eq
Imbalance:	-2.005000 eq
Adjusted Species:	Na+1 K+1

Charged Species	Input mol	Balanced mol	Difference %
Na+1	11.3600	12.4096	9.24
K+1	10.3400	11.2954	9.24
Cl-1	0.935000	0.935000	
NO3-1	19.4100	19.4100	
PO4-3	1.12000	1.12000	

The reconciled composition was added as a stream in StreamAnalyzer for further calculations.

The sample taken by L. Yang at 150 °C is approximately 17 mL, which was diluted to 300 mL prior to chemical analysis. Thus, there was a 300/17 (=17.647) dilution. To determine the composition of the original 17 mL sample, the reconciled (stream) composition derived in the previous page was subjected to a vapor-amount type of calculation using StreamAnalyzer Version 2.0. The water in the system was allowed to evaporate such that only 17/300 (=0.0567) of 1-L of water remained in the aqueous phase. Thus, the vapor amount of water was specified to be 55.5087×(1.0–0.0567) (=52.363 mol), leaving only 3.145 moles water in the aqueous phase. The temperature was specified equal to 150 °C.

Part of the StreamAnalyzer report is as follows:

Calculation Summary

SinglePoint Evaporate so 17/300 mL vol is left Calculation for Work2

Unit Set: Default

Automatic Chemistry Model
MSE (H30+ ion) Databanks:
MSE (H3O+ ion)
Using Helgeson Direct

Vapor Amount Calculation

Temperature	150.000	°C
Pressure	2.57098	atm

Stream Inflows

H2O	55.1620	mol
HCl	0.179796	mol
KOH	0.640306	mol
N2O5	0.550000	mol
Na2O	0.351747	mol
P2O5	0.0318000	mol

Stream Parameters

Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	56.9157	mol
Temperature	150.000	°C
Pressure	2.57098	atm

Aqueous Properties

pH	4.18152	pH
Ionic Strength	0.230445	mol/mol
Osmotic Pressure	1049.24	atm
Electrical Cond, specific	0.140976	1/(ohm-cm)
Viscosity, absolute	4.56394	cP

	Total	Aqueous	Vapor	Solid	2nd Liquid
		g/ml	g/ml	g/ml	g/ml
Density		1.39829	1.36094e-3	0.0	0.0

Scaling Tendencies

Row Filter Applied: Only Non Zero Values

solids within temperature range		**Temperature Range**	
NaCl	0.331085	data valid through range	inside range
KNO3	0.281536	data valid through range	inside range
NaNO3	0.244346	data valid through range	inside range
KCl	0.150074	data valid through range	inside range

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total mol	Aqueous mol	Vapor mol
H2O	**55.5087**	**3.14873**	**52.3599**
HCl	3.02E-05	2.38E-08	3.02E-05
KOH	1.19E-16	1.19E-16	0
N2O5	3.43E-16	9.09E-18	3.34E-16
P2O5	1.88E-22	1.88E-22	0
H3PO4	5.88E-04	5.88E-04	0
H4P2O7	8.67E-24	8.67E-24	0
H5P3O10	2.72E-33	2.72E-33	0
HNO3	2.52E-05	6.40E-07	2.46E-05
Cl-1	**0.179766**	**0.179766**	**0**
H2P2O7-2	1.56E-20	1.56E-20	0
H2P3O10-3	6.34E-30	6.34E-30	0
H2PO4-1	0.061965	0.061965	0
H3O+1	7.10E-07	7.10E-07	0
H3P2O7-1	6.02E-22	6.02E-22	0
H3P3O10-2	3.19E-30	3.19E-30	0
H4P3O10-1	3.18E-31	3.18E-31	0
HP2O7-3	2.47E-23	2.47E-23	0
HP3O10-4	1.50E-32	1.50E-32	0
HPO4-2	1.05E-03	1.05E-03	0
K+1	**0.640306**	**0.640306**	**0**
Na+1	**0.703494**	**0.703494**	**0**
NO3-1	**1.09997**	**1.09997**	**0**
OH-1	3.43E-10	3.43E-10	0
P2O7-4	2.67E-29	2.67E-29	0
P3O10-5	5.10E-37	5.10E-37	0
PO4-3	**2.13E-11**	**2.13E-11**	**0**
Total (by phase)	58.1959	5.83588	52.36

Species Activity/Fugacity Coefficients

Species	**γ x-based**	**γ m-based**
H2O	1.03215	0.556895*

*water activity

The calculated molal concentrations of the major species at 150 °C are as follows:

Species	moles/kgH2O
Cl-1	3.17
H2PO4-1	1.09
HPO4-2	0.02
NO3-1	19.4
K+1	11.3
Na+1	12.4
pH	**4.18**

To determine the pH of the undiluted sample at 25 °C, the preceding calculation was rerun at a temperature of 25 °C. The calculated pH is 3.95, lower than the value of 4.4, the measured pH of the diluted sample.

May 5, 2008

The following email from Andre Anderko, OLI Systems, Inc. (Morris Plains, New Jersey) is copied into this notebook to show permission was granted by OLI Systems, Inc. to use the figures on pages 3 through 103 of this notebook.

-----Original Message-----
From: Andre Anderko [mailto:aanderko@olisystems.com]
Sent: Monday, May 05, 2008 3:30 PM
To: rpabalan@cnwra.swri.edu
Subject: RE: request permission to use OLI figures

Bobby:

Yes, feel free to include the figures in the public-domain version of your notebook.

In general, we treat the spreadsheets as a part of the deliverables (on a non-exclusive basis) that we send to our clients in conjunction with a project. Since you funded a large part of this work several years ago, there is absolutely no problem with placing the figures in your report.

Best regards,
Andre

From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Monday, May 05, 2008 3:30 PM
To: 'Andre Anderko'
Subject: request permission to use OLI figures

Andre,

In 2004, I received several Excel files from OLI Systems comparing experimental solubility data with MSE results. I included many of the figures in the Excel files into my scientific notebook, as part of my effort to validate the OLI software. Because my scientific notebook will be in the public domain (www. lsnnet.gov), I need to either get permission to use the figures or else redact them from the notebook. Please let me know if I have your company's permission to include the figures in my notebook. A list of the figures is given below.

Thanks.

Bobby Pabalan
SwRI

Binary Systems	Page #	Ternary Systems	Page #	Ternary Systems (Cont'd)	Page #	Ternary Systems (Cont'd)	Page #
NaCl	3	NaH2PO4	32	MgCl2-KNO3	65	NaH2PO4-KH2PO4	91
KCl	4	Na2HPO4	33	CaCl2-KNO3	66	H2SO4-(NH4)2SO4	92
MgCl2	5	KH2PO4	34	MgCl2-Mg(NO3)2	67	H2SO4(saltfree)-(NH4)2SO4	93
CaCl2	6	K2HPO4	35	CaCl2-Ca(NO3)2	68		

AlCl3	7						
		NaF	36	Na2SO4-NaCl	69	NaF-NaCl	94
NaNO3	8	KF	37	CaSO4-NaCl	70	KF-NaCl	95
KNO3	9	MgF2	38	Al2(SO4)3-NaCl	71	MgF2-NaCl	96
Mg(NO3)2	10	CaF2	39	CaSO4-CaCl2	72	CaF2-NaCl	97
Ca(NO3)2	11	AlF3	40			AlF3-NaCl	98
Al(NO3)3	12			Na2SO4-NaNO3	73	KF-KCl	99
		KOHvp	41			NaF-KCl	100
Na2SO4	13	KOHphi	42	Na2SO4-K2SO4	74		
K2SO4	14	KOHhdil	43	Na2SO4-CaSO4	75	Al(OH)3-NaOH	101
(NH4)2SO4	15	KOHcp	44	Na2SO4-Al2(SO4)3	76	Al(OH)3-NaCl	102
MgSO4	16			K2SO4-CaSO4	77	AlOOH-NaCl-constNaCl	103
CaSO4	17	NaCl-KCl	45			AlOOH-NaCl-ConstT	104
Al2(SO4)3	18	NaCl-MgCl2	46	NaCl-CaCO3	78		
		NaCl-CaCl2	47	CaCl2-CaCO3	79	Al(OH)3,AlOOH vs pH	105
Na2CO3	19	NaCl-AlCl3	48				
K2CO3	20	KCl-MgCl2	49	Na2CO3-K2CO3	80	**Acids**	
MgCO3	21	KCl-CaCl2	50	Na2CO3-MgCO3	81		
CaCO3	22	MgCl2-CaCl2	51	Na2CO3-CaCO3	82	TPA	106
		AlCl3-HCl	52			Na2TPT	107
NaHCO3	23			Na2CO3-NaHCO3	83	IPA	108
KHCO3	24	NaNO3-KNO3	53	K2CO3-KHCO3	84	TMA	109
		NaNO3-Mg(NO3)2	54			NA	110
NaOH	25	NaNO3-Ca(NO3)2	55	Na2CO3-Na2SO4	85,86	Na2NT	111
KOH	26	KNO3-Mg(NO3)2	56				
CaOH2	27	KNO3-Ca(NO3)2	57	MgCO3 vs pCO2	87	H2SO4-SO3vp300h	112
Al(OH)3	28	Mg(NO3)2-Ca(NO3)2	58	CaCO3 vs pCO2	88	H3PO4vp	113
H3PO4	29	NaCl-NaNO3	59	NaOH-NaCl	89		
Na3PO4	30	NaCl-KNO3	60	NaOH-Na2SO4	90		
K3PO4	31	NaCl-Ca(NO3)2	61				
		NaCl-Al(NO3)2	62				
		KCl-KNO3	63				
		KCl-Ca(NO3)2	64				

Entries into Scientific Notebook No. 679E for the period October 1, 2007, through February 29, 2008, have been made by

Roberto T. Pabalan / Date 5/14/2008

No original entry into this Scientific Notebook has been removed.

Roberto T. Pabalan / Date 5/14/2008

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 679

Document Date:	9/27/2004
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" ☐ Sensitive ☐"Non-Sensitive - Copyright" ☐ Sensitive - Copyright
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Media Type: (CDs, 3 ½, 5 1/4 disks, etc.)	2 CD
File Types: (.exe, .bat, .zip, etc.)	xls, STA
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