ELECTRONIC NOTEBOOK #930E

March 1, 2008 through September 30, 2008

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Roberto T. Pabalan

The entries in this electronic scientific notebook #930E document activities conducted during the period March 1, 2008, through September 30, 2008, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.14002.01.071).

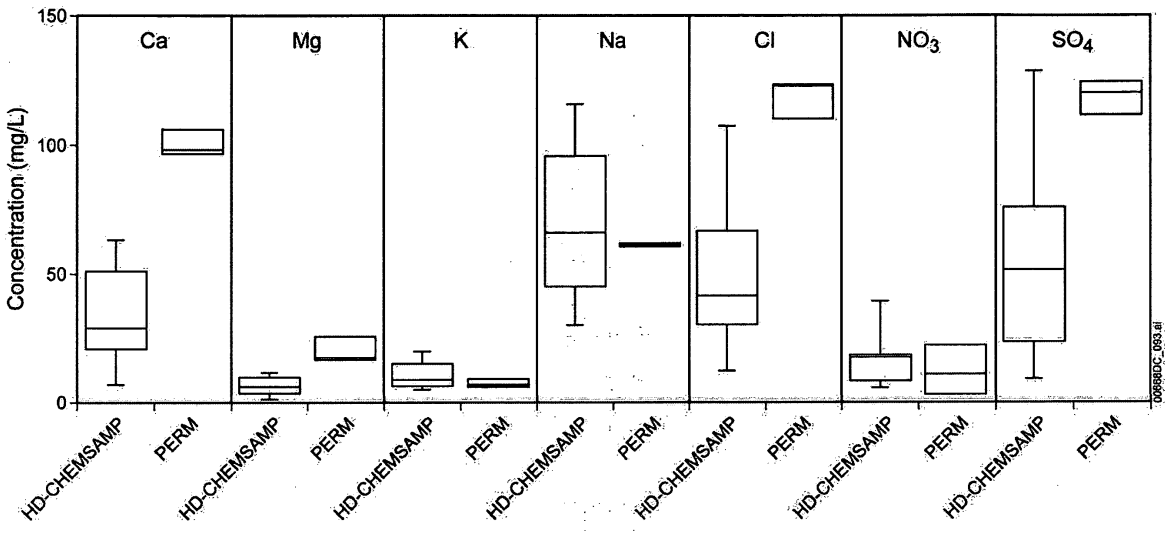
March 12, 2008

A question was raised by Bret Leslie with respect to seepage water chemistry composition assumed in a CNWRA manuscript "Probabilistic Methodology to Estimate Environmental Conditions for Localized Corrosion and Stress Corrosion Cracking of Alloy 22 in a High-Level Radioactive Waste Repository Setting," (AI No. 06002.01.322.710), and the assumption in the paper that the chemical constituents and their ratios in the pore water are indicative of water that flows under thermal condtions and contributes to seepage. According to him, the only known waters that flowed under repository-relevant conditions (e.g. affected by thermal-related FEPS) are those collected and analyzed as part of the Drift Scale Heater test. He suggested that it would be useful to look at the starting compositions and their evolution of Drift-scale water that seeped/flowed down fractures and into open borehole and compare those to pore waters starting and evolved compositions.

To address Bret's concern, an LSN search (www.lsnnet.gov) was done to find DOE data on drift scale test water compositions.

The following pages are tables of chemical compositions of waters DOE sampled from the Drift Scale Test, as reported in Section 6.3.4 of the report "Thermal Testing Measurements Report —Final Check Copy" (TDR-MGR-HS-000002 Rev 01G; February 2007, Table 6.3-25). A copy of this report was downloaded from www.lsnnet.gov, and the table values were cut and pasted onto an Excel file and onto this notebook. Only values listed on pages 6-261 to 6-267 were copied; the concentrations listed on pages 6-268 to 6-271 are mostly very low, indicating the samples are water vapor condensates.

Also copied from the DOE report is the chemical analyses of water extracted from the CHEMSAMP core samples, which were taken from two continuously cored boreholes, one that was drilled into the heated rock mass of the Drift Scale Test (ESF-HD-CHEMSAMP-1) and another drilled into the below-boiling zone above the heated drift (ESF-HD-CHEMSAMP-3). The chemical analyses are listed in Table 6.3-26 of the DOE report and were copied and pasted in this notebook also. A comparison of the CHEMSAMP values with the PERM sample values is given in Figure 6.3-47 of the DOE report (a copy is given below), which indicates both sets of samples have similar overall chemistries, although the calcium and magnesium concentrations are significantly less in the former than in the latter.



Source: DTNs: GS030408312272.002 [DIRS 165226]; GS031008312272.008 [DIRS 166570]; GS041108312272.005 [DIRS 178057]; MO0005PORWATER.000 [DIRS 150930].

NOTE: The boxes represent the 25th through 75th percentiles and the whiskers extend to the complete range of the data.

Figure 6.3-47. Box and Whisker Plots Comparing the Distribution of Chemical Constituents in Water Extracted from HD-CHEMSAMP-1 (N=4) and HD-CHEMSAMP-3 (N=13) with Water Extracted from HD-PERM Core (N=3; Table X)

SMF No.		1002488	1002586	1002525	1527969	0527968	0527977	0527915	0527916	0527917
Collection Date		Preheating	Preheating	Preheating	6/4/1998	6/4/1998	6/4/1998	8/12/1998	08/12198	8/12/1998
Sample ID		PERM-1	PERM-2	PERM-3	BH 60-2	BH 60-2	BH 60-3	BH 60-2	BH 60-3	BH 77-3
Field pH		7.79	8.32	8.31	7.5	N/A	7.7	6.9	6.8	5.5
Na	**(mg/L)**	**60.5**	**61**	**61.5**	**20**	**N/A**	**24**	**20.4**	**17.2**	**2.4**
Si	**(mg/L)**	**37**	**31**	**35**	**56**	**N/A**	**41**	**51.8**	**43.5**	**1.48**
Ca	**(mg/L)**	**98.17**	**106.17**	**96.67**	**20**	**N/A**	**25**	**19.9**	**18.7**	**2.09**
K	**(mg/L)**	**6**	**7**	**9**	**6**	**N/A**	**4.5**	**5.4**	**4.5**	**1.4**
Mg	**(mg/L)**	**26.65**	**16.55**	**17.35**	**2.9**	**N/A**	**5.7**	**1.21**	**4**	**0.21**
Al	(mg/L)	<0.06	<0.06	<0.06	0.12	N/A	0.017	<0.06	0.003	<0.06
B	(mg/L)	3.05	2.75	2.75	1.2	N/A	0.92	1.84	1.14	0.13
S	(mg/L)	42.25	38.6	38.65	5.5	N/A	9.2	4.5	5.2	1.4
Fe	(mg/L)	<0.02	<0.02	<0.02	0.04	N/A	<0.02	0.02	0.12	<0.02
Li	(mg/L)	0.1	0.45	0.05	0.07	N/A	0.07	0.03	0.04	<0.01
Sr	(mg/L)	1.4	1	1.05	0.18	N/A	0.34	0.11	2.21	0.05
HCO3	**(mg/L)**				**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**
F	**(mg/L)**	**0.36**	**0.96**	**0.76**	**N/A**	**1**	**0.82**	**0.71**	**0.43**	**0.41**
Cl	**(mg/L)**	**122.73**	**109.93**	**123.13**	**N/A**	**10**	**16**	**6.14**	**5.52**	**2.15**
Br	**(mg/L)**	**0.6**	**0.76**	**1.2**	**N/A**	**0.84**	**0.73**	**0.05**	**0.21**	**0.03**
SO4	**(mg/L)**	**124.18**	**111.38**	**119.78**	**N/A**	**17**	**30**	**4.88**	**8.81**	**1.86**
PO4	(mg/L)	<0.07	<0.07	<0.07	N/A	<0.07	<0.07	0.25	0.16	1.06
NO2	(mg/L)	<0.04	<0.04	<0.04	N/A	<0.01	<0.01	<0.04	<0.04	<0.04
NO3	**(mg/L)**	**21.72**	**2.52**	**10.4**	**N/A**	**3**	**3.6**	**0.46**	**0.6**	**0.22**

SMF No.		0541803a	0541803a,f	0541804a	0541804a,f	0541805a	0541805a,f	0504397a	0504396a	0527961
Collection Date		11/12/1998	11/12/1998	11/12/1998	11/12/1998	11112/98	11/12/1998	1/26/1999	01126/99	1/26/1999
Sample ID		BH 59-4	BH 59-4	BH 60-3	BH 60-3	BH 186-3	BH 186-3	BH 59-4	BH 60-3	BH 186-3
Field pH		6.63	6.63	6.92	6.92	6.83	6.83	N/A	7.4	7.2
Na	**(mg/L)**	**22.6**	**135**	**10.1**	**20.3**	**105**	**17**	**219**	**19.1**	**25.9**
Si	**(mg/L)**	**33.5**	**44.2**	**60**	**53.8**	**16**	**27.2**	**12**	**65**	**49.3**
Ca	**(mg/L)**	**476**	**450**	**15.3**	**13.9**	**11.5**	**20.2**	**429**	**5.93**	**2.92**
K	**(mg/L)**	**29.5**	**37.8**	**8.7**	**7.8**	**3.5**	**3.9**	**29.7**	**4.1**	**5.9**
Mg	**(mg/L)**	**64.1**	**83.9**	**3.35**	**3**	**5.1**	**5.68**	**164**	**1.17**	**6.32**
Al	(mg/L)	0.01	<0.06	0.033	0.033	0.003	0.003	0.086	<0.06	<0.06
B	(mg/L)	4.47	4.13	1.58	1.41	0.51	0.58	6.68	1.75	0.84
S	(mg/L)	50.7	64.8	11.6	10.5	8.47	9.42	109	6.4	7.9
Fe	(mg/L)	<0.02	<0.02	0.02	<0.02	0.02	<0.02	<0.02	<0.02	0.09
Li	(mg/L)	0.21	0.2	0.04	0.04	0.05	0.05	0.33	0.02	0.05
Sr	(mg/L)	4.02	3.71	0.22	0.2	0.3	0.34	5.84	0.09	0.37
HCO3	**(mg/L)**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**41**	**116**
F	**(mg/L)**	**0.8**	**4.3**	**0.49**	**0.5**	**0.56**	**0.62**	**0.51**	**1.27**	**1.2**
Cl	**(mg/L)**	**1,130**	**1,250**	**19.5**	**19.6**	**18.7**	**18.6**	**1,160**	**10.3**	**23.3**
Br	**(mg/L)**	**1.13**	**<0.07**	**0.6**	**0.51**	**0.67**	**0.6**	**1.51**	**0.15**	**0.32**
SO4	**(mg/L)**	**226**	**213**	**30.6**	**30.8**	**26.3**	**26.2**	**240**	**13.5**	**21**
PO4	(mg/L)	<5	<0.2	<0.2	<0.2	<0.2	<0.2	0.5	<0.05	<0.1
NO2	(mg/L)	<3	<10	<0.10	<0.10	<0.10	<0.10	<0.3	<0.03	<0.05
NO3	**(mg/L)**	**3.12**	**7.81**	**3.38**	**3.17**	**7.47**	**7.27**	**11.6**	**2.56**	**6.73**

SMF No.		0529637-#1	0529637-#2	0529637-#3	0529634	0551100	0551103	0551104	0551105	0551106
Collection Date		3/30/1999	3/30/1999	3/30/1999	3/30/1999	4/20/1999	4/20/1999	5/10/1999	5/10/1999	5/10/1999
Sample ID		BH 60-3	BH 60-3	BH 60-3	BH 77-3	BH 60-3	BH 60-3	BH 60-3	BH 60-3	BH 60-3
Field pH		8	N/A	N/A	4.8	4.19-4.50	4.77	4.78-4.80	4.68	N/A
Na	**(mg/L)**	**11.2**	**11**	**2.2**	**<0.2**	**0.14**	**<0.05**	**1.8**	**2.5**	**0.15**
Si	**(mg/L)**	**62.8**	**59.8**	**12.1**	**1.03**	**0.7**	**<0.5**	**1.1**	**1.2**	**0.6**
Ca	**(mg/L)**	**2.06**	**2.27**	**1.22**	**0.41**	**0.14**	**0.1**	**0.14**	**0.09**	**0.22**
K	**(mg/L)**	**2.4**	**2.4**	**0.5**	**<0.5**	**<0.5**	**<0.5**	**<0.5**	**<0.5**	**<0.5**
Mg	**(mg/L)**	**0.27**	**0.26**	**0.01**	**0.02**	**<0.005**	**<0.005**	**<0.005**	**<0.005**	**<0.005**
Al	(mg/L)	0.36,0.27	0.36,0.27	0.08,0.07	0.005	<0.2	<0.2	<0.2	<0.2	<0.2
B	(mg/L)	2.1	2.11	1.23	0.09	1.7	1	2.3	2.6	0.9
S	(mg/L)	1.83	1.82	0.42	<0.02	<0.5	<0.5	<0.5	<0.5	<0.5
Fe	(mg/L)	<0.02	<0.02	<0.02	0.05	0.02	0.01	<0.01	<0.01	<0.01
Li	(mg/L)	0.02	<0.01	<0.01	<0.01	<4	<4	<4	<4	<4
Sr	(mg/L)	0.02	0.02	0.01	<0.01	<0.05	<0.05	<0.05	<0.05	<0.05
HCO3	**(mg/L)**	**25**	**N/A**	**N/A**	**1.25**	**N/A**	**N/A**	**N/A**	**N/A**	**8.1**
F	**(mg/L)**	**1.02**	**0.97**	**0.11**	**0.01**	**<0.005**	**<0.005**	**<0.005**	**<0.005**	**<0.005**
Cl	**(mg/L)**	**4.15**	**3.92**	**0.72**	**0.3**	**0.05**	**0.08**	**0.06**	**0.05**	**0.11**
Br	**(mg/L)**	**<0.04**	**<0.04**	**<0.04**	**<0.04**	**<0.03**	**<0.03**	**<0.03**	**<0.03**	**<0.03**
SO4	**(mg/L)**	**3.83**	**3.75**	**0.79**	**0.13**	**0.1**	**0.09**	**0.09**	**0.09**	**0.08**
PO4	(mg/L)	<0.05	<0.05	<0.05	<0.05	<0.02	<0.02	0.92	0.84	0.62
NO2	(mg/L)	<0.03	<0.03	<0.03	<0.03	<0.007	<0.007	<0.007	<0.007	<0.007
NO3	**(mg/L)**	**0.92**	**0.84**	**0.17**	**0.065**	**<0.02**	**<0.02**	**<0.02**	**<0.02**	**<0.02**

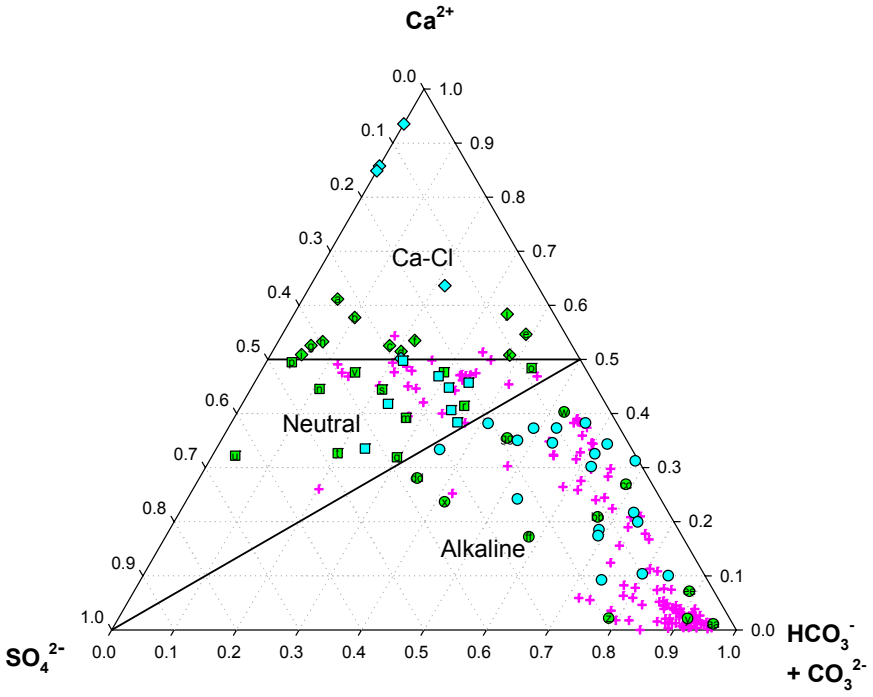
SMF No.		0551107	0551110	0551111	0551154	0551155	0551159	0551160	0551169	0557029
Collection Date		5/10/1999	OS/25/99	OS/25/99	6/24/1999	6/24/1999	8/9/1999	8/9/1999	8/10/1999	10/27/1999
Sample ID		BH 60-3	BH 60-3	BH 60-3	BH 60-3	BH 60-3	BH 59-2(AC)	BH 59-2(BC)	BH 61-3	BH 59-2
Field pH		4.84	4.68	4.75	5.02	N/A	N/A	N/A	N/A	N/A
Na	**(mg/L)**	**2.8**	**1.8**	**1.6**	**1.87**	**2.26**	**30**	**24**	**19**	**N/A**
Si	**(mg/L)**	**1.4**	**2.1**	**0.7**	**6.3**	**3.22**	**78**	**81**	**67**	**N/A**
Ca	**(mg/L)**	**0.15**	**0.13**	**0.09**	**0.69**	**0.23**	**47**	**39**	**14**	**N/A**
K	**(mg/L)**	**<0.5**	**<0.5**	**<0.5**	**0.5**	**<0.5**	**8**	**6**	**5**	**N/A**
Mg	**(mg/L)**	**<0.005**	**<0.005**	**<0.005**	**0.012**	**<0.005**	**13**	**11**	**3.2**	**N/A**
Al	(mg/L)	<0.2	<0.2	<0.2	<0.04	<0.04	<0.2	<0.2	<0.2	N/A
B	(mg/L)	2.8	2	1.9	0.62	1.85	0.8	0.6	1.5	N/A
S	(mg/L)	<0.5	<0.5	<0.5	<0.1	<0.1	22	17	3.1	N/A
Fe	(mg/L)	0.31	<0.01	<0.01	<0.01	<0.01	0.41	0.32	1.2	N/A
Li	(mg/L)	<4	<4	<4	<1	<1	<4	<4	<4	N/A
Sr	(mg/L)	<0.05	<0.05	<0.05	<0.01	<0.01	0.54	0.45	0.14	N/A
HCO3	**(mg/L)**	**N/A**	**8.6**	**8.6**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**23.5**
F	**(mg/L)**	**<0.005**	**<0.005**	**<0.005**	**0.685**	**0.195**	**0.725**	**0.575**	**0.835**	**0.27**
Cl	**(mg/L)**	**0.09**	**0.2**	**0.06**	**0.615**	**0.305**	**88.3**	**71**	**24.1**	**9.5**
Br	**(mg/L)**	**<0.03**	**<0.03**	**<0.03**	**<0.03**	**<0.03**	**0.515**	**0.46**	**0.35**	**0.61**
SO4	**(mg/L)**	**0.12**	**0.09**	**0.07**	**<0.03**	**0.325**	**64.2**	**53.5**	**9.13**	**6.2**
PO4	(mg/L)	<0.02	0.69	0.33	<0.02	<0.02	<0.02	<0.02	<0.02	<0.02
NO2	(mg/L)	<0.007	<0.007	<0.007	<0.007	<0.007	<0.007	<0.007	<0.007	<0.007
NO3	**(mg/L)**	**<0.02**	**<0.02**	**<0.02**	**N/A**	**<0.02**	**3.79**	**2.83**	**0.825**	**1.32**

SMF No.		557032	5570333	557036	557038	557040	557080	557081	557083	552575	557043
Collection Date		10/27/1999	10/27/1999	10/27/1999	10/27/1999	10/27/1999	11/30/1999	11/30/1999	11/30/1999	11/30/1999	11/30/1999
Sample ID		BH 59-2	BH 59-2	BH 59-3	BH 59-3	BH 76-3	BH 59-2	BH 59-2	BH 59-2	BH 59-3	BH 59-3
Field pH		5.93	6.08	N/A	6.64	6.14-6.46	6.86	7.24	N/A	7.47	N/A
Na	**(mg/L)**	**9.2**	**9.2**	**N/A**	**19.3**	**64.5**	**6.6**	**7.7**	**N/A**	**15.6**	**N/A**
Si	**(mg/L)**	**44.5**	**44.9**	**N/A**	**84.2**	**133.4**	**38**	**39.9**	**N/A**	**92.5**	**N/A**
Ca	**(mg/L)**	**7.53**	**7.47**	**N/A**	**13.2**	**59.5**	**4.33**	**5.63**	**N/A**	**2.86**	**N/A**
K	**(mg/L)**	**3.4**	**3.6**	**N/A**	**5.6**	**13.4**	**2.6**	**3**	**N/A**	**3.9**	**N/A**
Mg	**(mg/L)**	**1.81**	**1.72**	**N/A**	**1.49**	**13.8**	**1.02**	**1.38**	**N/A**	**0.29**	**N/A**
Al	(mg/L)	0.033	0.033	N/A	0.04	0.01	0.03	0.03	N/A	0.071	N/A
B	(mg/L)	0.27	0.21	N/A	0.86	2.38	0.14	0.17	N/A	1.06	N/A
S	(mg/L)	2.52	2.5	N/A	14.48	34.55	0.76	1.33	N/A	3.25	N/A
Fe	(mg/L)	0.2	0.19	N/A	<0.02	<0.02	0.09	0.14	N/A	<0.02	N/A
Li	(mg/L)	0.16	0.01	N/A	0.02	0.13	0.01	0.01	N/A	0.02	N/A
Sr	(mg/L)	0.11	0.08	N/A	0.13	0.78	0.06	0.08	N/A	0.03	N/A
HCO3	**(mg/L)**	**N/A**	**23.5**	**12.4**	**12.4**	**N/A**	**N/A**	**N/A**	**22.3**	**N/A**	**20.7**
F	**(mg/L)**	**N/A**	**0.27**	**0.64**	**0.73**	**1.11**	**N/A**	**N/A**	**0.35**	**N/A**	**1.3**
Cl	**(mg/L)**	**N/A**	**9.1**	**12.9**	**12.9**	**81.9**	**N/A**	**N/A**	**5**	**N/A**	**8.8**
Br	**(mg/L)**	**N/A**	**0.58**	**0.89**	**0.51**	**0.97**	**N/A**	**N/A**	**<0.03**	**N/A**	**<0.03**
SO4	**(mg/L)**	**N/A**	**6.3**	**40.7**	**40.3**	**94.6**	**N/A**	**N/A**	**2.8**	**N/A**	**8.2**
PO4	(mg/L)	N/A	<0.02	<0.04	<0.04	<0.02	N/A	N/A	<0.02	N/A	<0.02
NO2	(mg/L)	N/A	<0.007	<0.01	<0.01	<0.007	N/A	N/A	0.007	N/A	<0.007
NO3	**(mg/L)**	**N/A**	**1.4**	**3.06**	**3.05**	**6.42**	**N/A**	**N/A**	**<0.02**	**N/A**	**2.4**

SMF No.		552578	552579	557081	557084	557022	550671	550673	550698	550674	550674
Collection Date		11/30/1999	11/30/1999	11/30/1999	11/30/1999	1/25/2000	01125/00	1/25/2000	01125/00	1/25/2000	1/25/2000
Sample ID		BH 76-3	BH 76-3	BH 77-3	BH 77-3	BH 59-2	BH 59-2	BH 59-2	BH 77-2	BH 77-3	BH 77-3
Field pH		6.94	N/A	N/A	4.68	7.07	6.68	N/A	4.63	3.47	N/A
Na	**(mg/L)**	**28.2**	**N/A**	**N/A**	**0.6**	**8.1**	**6.6**	**N/A**	**<0.3**	**<0.3**	**N/A**
Si	**(mg/L)**	**92.8**	**N/A**	**N/A**	**2.45**	**42.8**	**41.7**	**N/A**	**2**	**2.5**	**N/A**
Ca	**(mg/L)**	**22.3**	**N/A**	**N/A**	**1.27**	**7.54**	**2.89**	**N/A**	**0.17**	**<0.050**	**N/A**
K	**(mg/L)**	**7.4**	**N/A**	**N/A**	**<0.2**	**3.6**	**2.8**	**N/A**	**<0.2**	**<0.2**	**N/A**
Mg	**(mg/L)**	**4.71**	**N/A**	**N/A**	**0.19**	**1.78**	**0.72**	**N/A**	**0.01**	**<0.005**	**N/A**
Al	(mg/L)	0.031	N/A	N/A	0.334	<0.05	0.043	N/A	0.049	0.023	N/A
B	(mg/L)	0.81	N/A	N/A	0.09	0.29	0.21	N/A	0.05	0.04	N/A
S	(mg/L)	9.46	N/A	N/A	0.24	6.44	0.65	N/A	<0.05	<0.05	N/A
Fe	(mg/L)	0.1	N/A	N/A	0.37	0.07	<0.02	N/A	0.25	0.07	N/A
Li	(mg/L)	0.04	N/A	N/A	<0.01	<0.01	<0.01	N/A	<0.01	<0.01	N/A
Sr	(mg/L)	0.26	N/A	N/A	0.02	0.091.	0.036	N/A	<0.005	<0.005	N/A
HCO3	**(mg/L)**	**N/A**	**82.3**	**N/A**	**N/A**	**N/A**	**N/A**	**22.8**	**N/A**	**N/A**	**N/A**
F	**(mg/L)**	**N/A**	**1.3**	**15**	**N/A**	**N/A**	**N/A**	**0.73**	**6.7**	**19.9**	**20.8**
Cl	**(mg/L)**	**N/A**	**19**	**3.5**	**N/A**	**N/A**	**N/A**	**3.8**	**0.6**	**0.8**	**0.29**
Br	**(mg/L)**	**N/A**	**<0.03**	**<0.03**	**N/A**	**N/A**	**N/A**	**<0.1**	**<0.1**	**<0.1**	**<0.1**
SO4	**(mg/L)**	**N/A**	**26**	**1.6**	**N/A**	**N/A**	**N/A**	**1.8**	**0.39**	**<0.1**	**<0.1**
PO4	(mg/L)	N/A	<0.02	<0.02	N/A	N/A	N/A	0.62	0.64	4	2.9
NO2	(mg/L)	N/A	<0.007	<0.007	N/A	N/A	N/A	<0.05	<0.05	<0.05	<0.06
NO3	**(mg/L)**	**N/A**	**2.5**	**<0.02**	**N/A**	**N/A**	**N/A**	**0.77**	**<0.1**	**0.2**	**0.18**

SMF No.		550681	550682	550684	550687	550697	550679	550693	550694	550691
Collection Date		OS/23/00	OS/23/00	OS/23/00	OS/23/00	OS/23/00	OS/23/00	6/29/2000	6/29/2000	6/29/2000
Sample ID		BH 59-2	BH 59-2	BH 59-2	BH 59-3	BH 76-3	BH 76-4	BH 59-2	BH 59-2	BH 59-2
Field pH		6.96	6.96	6.95	5.19	6.92-6.96	N/A	6.99-7.08	6.99-7.08	7
Na	**(mg/L)**	**17**	**18**	**17**	**<2.4**	**29**	**<2.4**	**16**	**15**	**<4.8**
Si	**(mg/L)**	**59.4**	**59.2**	**59.3**	**<0.46**	**96**	**3.4**	**62.7**	**57.5**	**36.3**
Ca	**(mg/L)**	**4.7**	**4.4**	**4.5**	**<0.17**	**7.1**	**1.5**	**4.3**	**3.8**	**2**
K	**(mg/L)**	**4.3**	**4.4**	**4.4**	**<0.095**	**6.5**	**0.7**	**4.7**	**4.2**	**2.5**
Mg	**(mg/L)**	**1.1**	**1.1**	**1.1**	**<0.042**	**1.4**	**0.14**	**1.1**	**1**	**0.54**
Al	(mg/L)	<0.053	<0.053	<0.053	<0.053	<0.053	<0.053	<0.053	<0.053	<0.11
B	(mg/L)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
S	(mg/L)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Fe	(mg/L)	<0.038	<0.038	<0.038	<0.038	<0.038	<0.038	<0.038	<0.038	<0.076
Li	(mg/L)	0.022	0.021	<	0.0007	0.045	0.0037	0.019	0.018	0.01
Sr	(mg/L)	<0.013	<0.013	<0.013	<0.013	<0.013	<0.013	<0.013	<0.013	<0.026
HCO3	**(mg/L)**	**31.4**	**31.4**	**31.4**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**	**N/A**
F	**(mg/L)**	**0.58**	**0.55**	**0.49**	**0.15**	**0.76**	**0.13**	**N/A**	**N/A**	**N/A**
Cl	**(mg/L)**	**10.15**	**10.6**	**10.15**	**0.07**	**14.5**	**2.75**	**N/A**	**N/A**	**N/A**
Br	**(mg/L)**	**<0.1**	**0.38**	**<0.1**	**<0.1**	**<0.1**	**<0.1**	**N/A**	**N/A**	**N/A**
SO4	**(mg/L)**	**2.9**	**3.18**	**3.1**	**<0.1**	**4.98**	**2.24**	**N/A**	**N/A**	**N/A**
PO4	(mg/L)	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	N/A	N/A	N/A
NO2	(mg/L)	<0.06	<0.06	<0.06	<0.06	<0.06	<0.06	N/A	N/A	N/A
NO3	**(mg/L)**	**0.56**	**0.54**	**0.71**	**0.38**	**1.47**	**0.85**	**N/A**	**N/A**	**N/A**

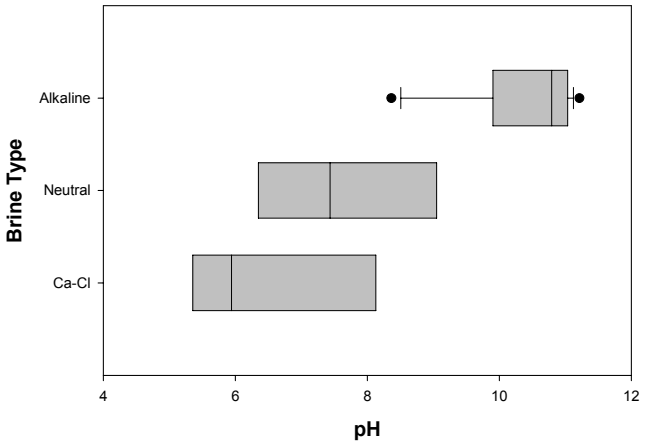
The following figure plots the DST water compositions (light blue symbols), together with the YM unsaturated porewater compositions (red crosses; also green symbols that were used in earlier evaporation simulations). There are five DST waters that are Ca–Cl-type, eight that are neutral-type, and nineteen that are alkaline-type.



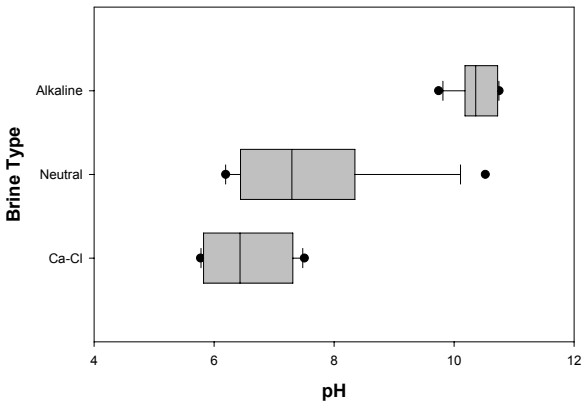
Thermodynamic calculations were conducted to simulate the evaporation of selected Drift Scale Test waters (highlighted in yellow in the previous tables; light blue in the figure above). The calculations were done using StreamAnalyzer Version 2.0 (Aqueous H+ model) for a temperature of 110 °C and a temperature of 0.85 atm (or higher if the calculation does not converge at 0.85 atm).

The StreamAnalyzer results were cut and pasted onto an Excel file, and summary information extracted and pasted onto a Sigmaplot file for plotting purposes. The following figures show the results of the calculations. The results of evaporation simulations for YM unsaturated pore waters (from notebook ESN#697, starting from page 158) are shown for comparison.

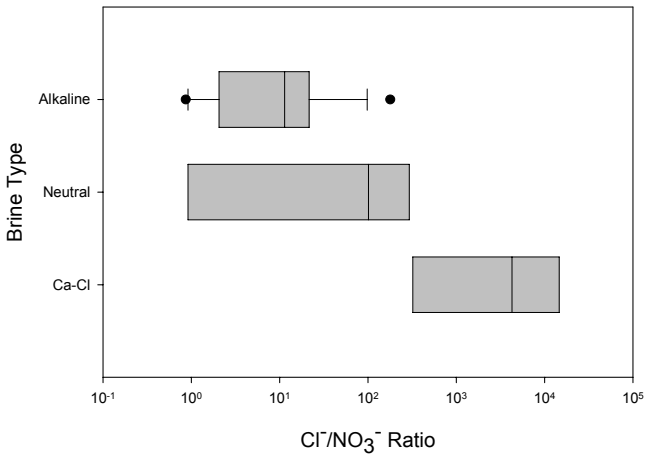
pH (at 110 °C) of Evaporated DST Waters



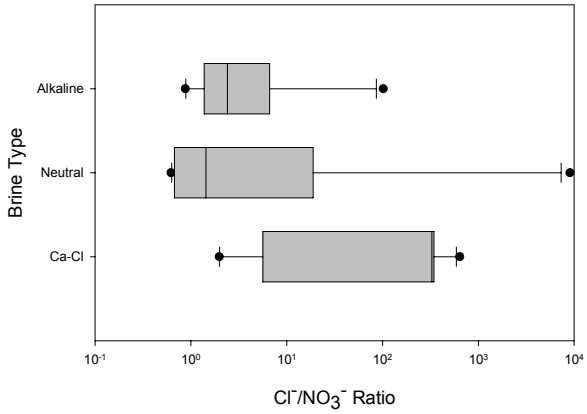
pH (at 110 °C) of Evaporated YM Waters



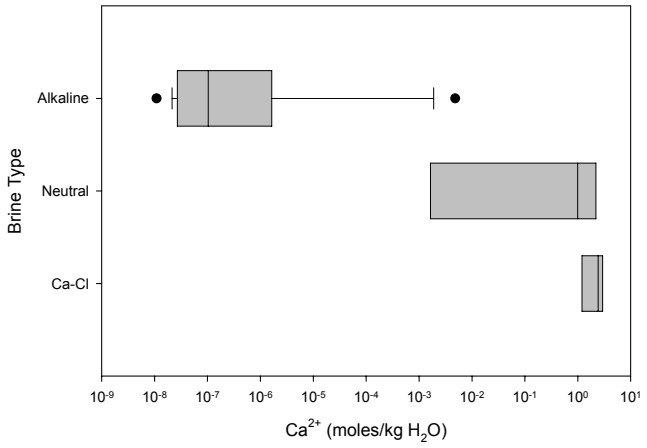
Cl^-/NO_3^- Ratio (at T=110 °C) of Evaporated DST Waters



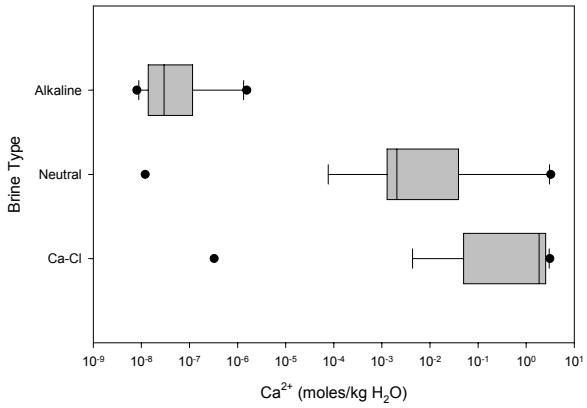
Cl^-/NO_3^- Ratio (at T=110 °C) of Evaporated YM Waters



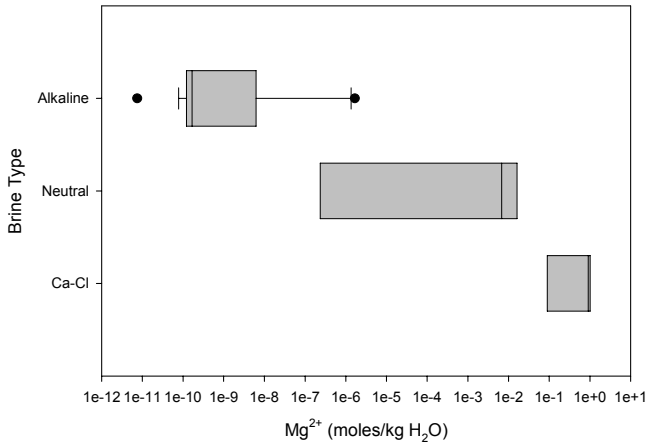
Calcium Conc. (at T=110 °C) of Evaporated DST Waters



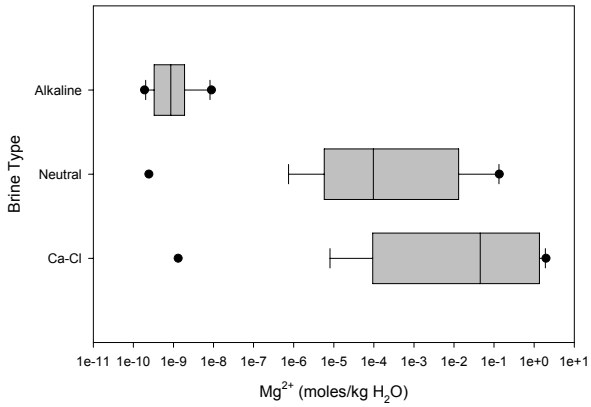
Calcium Conc. (at T=110 °C) of Evaporated YM Waters



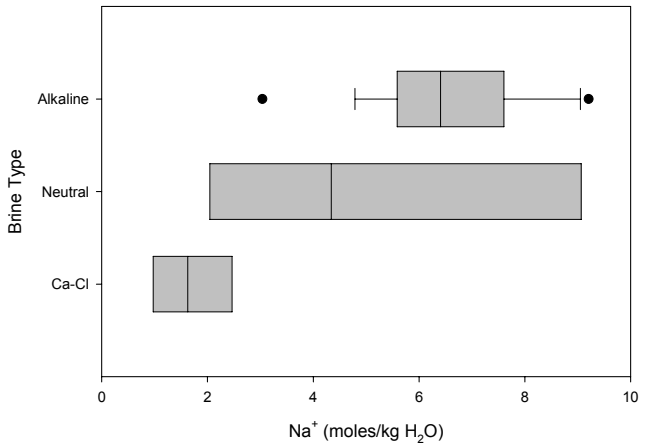
Magnesium Conc. (at T=110 °C) of Evaporated DST Waters



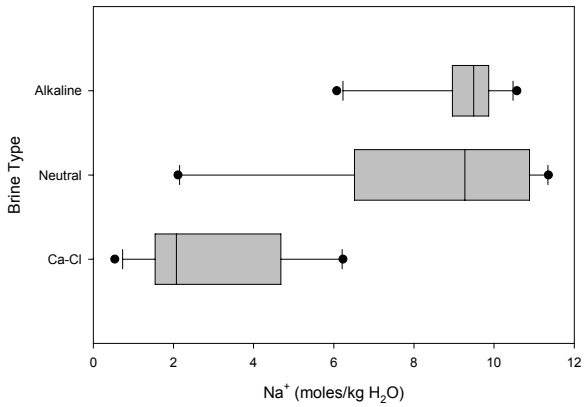
Magnesium Conc. (at T=110 °C) of Evaporated YM Waters



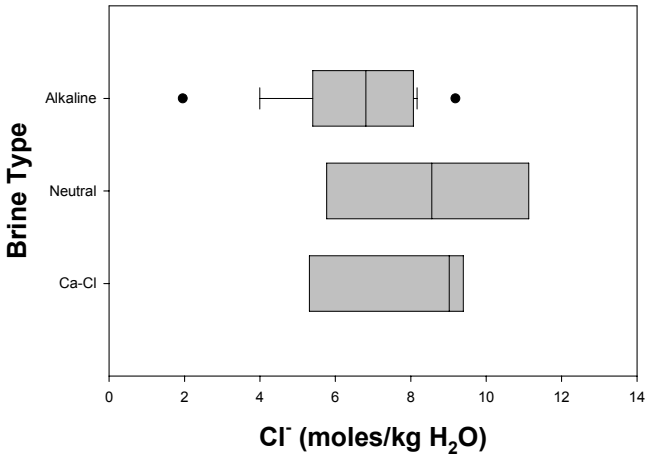
Sodium Conc. (at T=110 °C) of Evaporated DST Waters



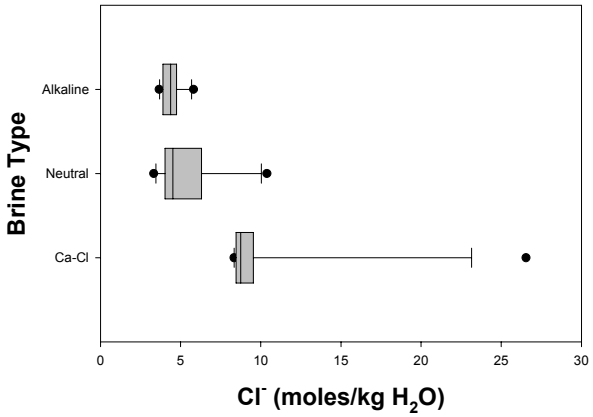
Sodium Conc. (at T=110 °C) of Evaporated YM Waters



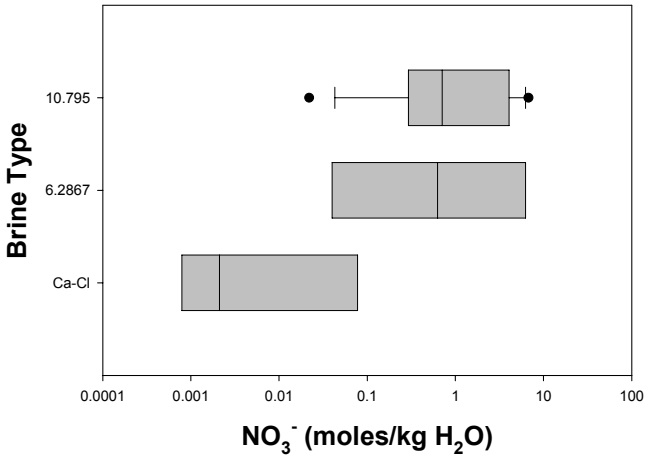
Chloride Conc. (at T=110 °C) of Evaporated DST Waters



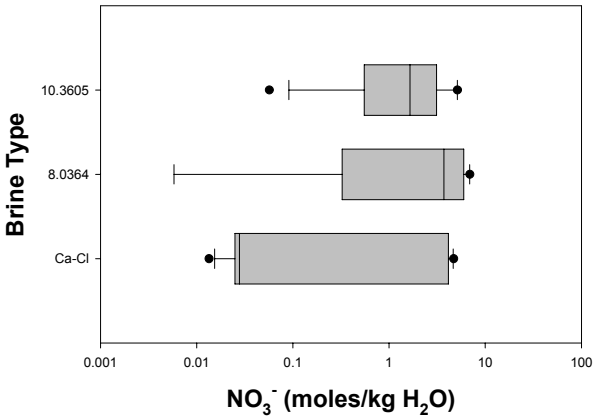
Chloride Conc. (at T=110 °C) of Evaporated YM Waters



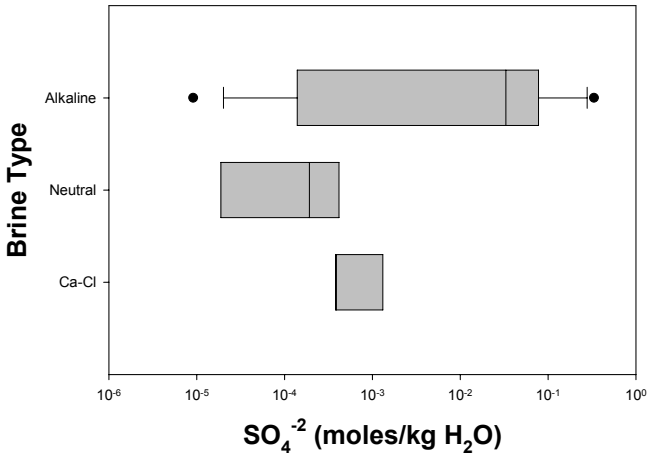
Nitrate Conc. (at T=110 °C) of Evaporated DST Waters



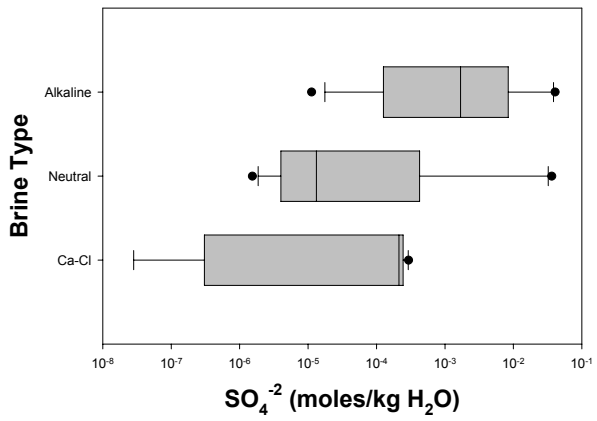
Nitrate Conc. (at T=110 °C) of Evaporated YM Waters



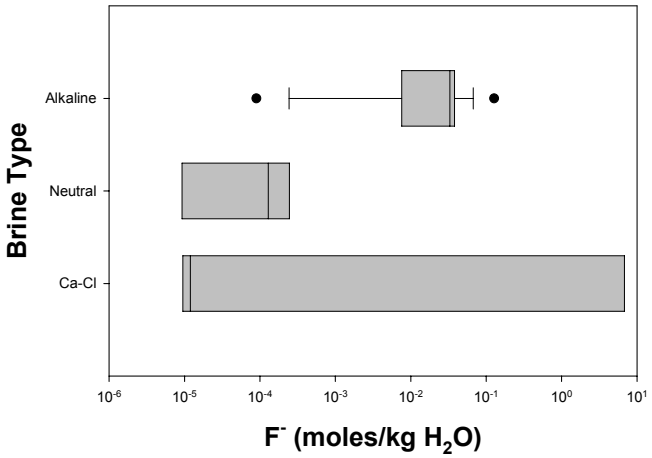
SO_4^{-2} Conc. (at T=110 °C) of Evap. DST Waters



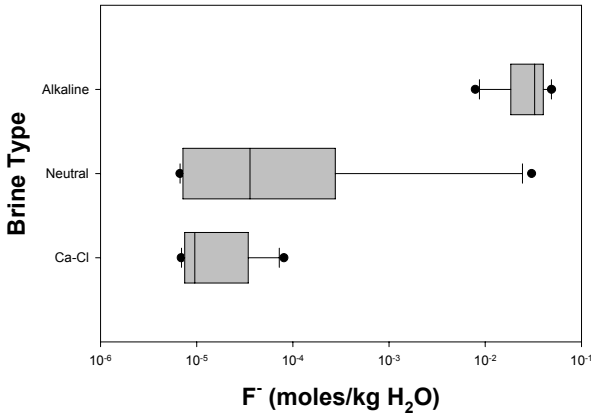
SO_4^{-2} Conc. (at T=110 °C) of Evap. YM Waters



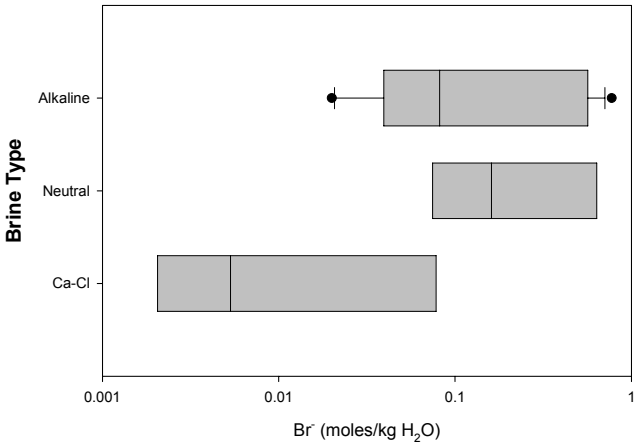
Fluoride Conc. (at T=110 °C) of Evaporated DST Waters



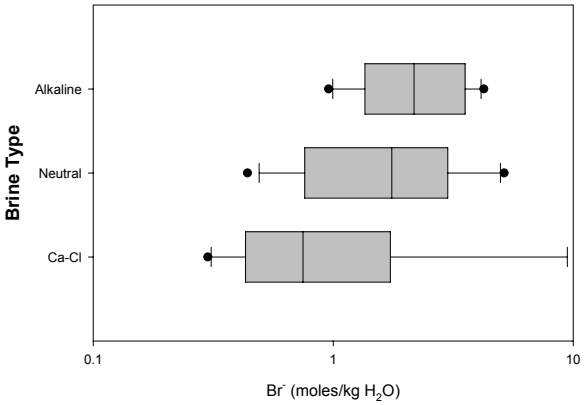
Fluoride Conc. (at T=110 °C) of Evaporated YM Waters



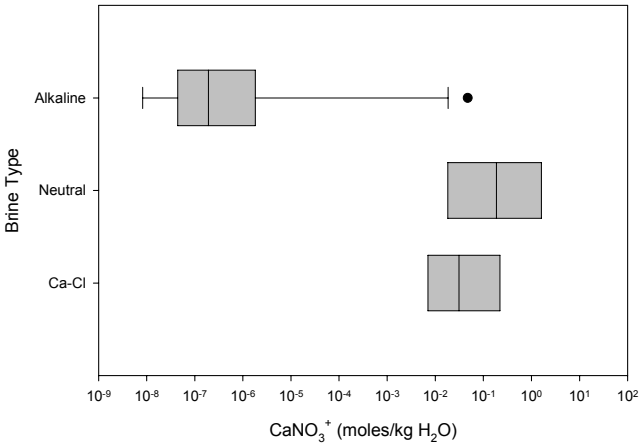
Bromide Conc. (at T=110 °C) of Evaporated DST Waters



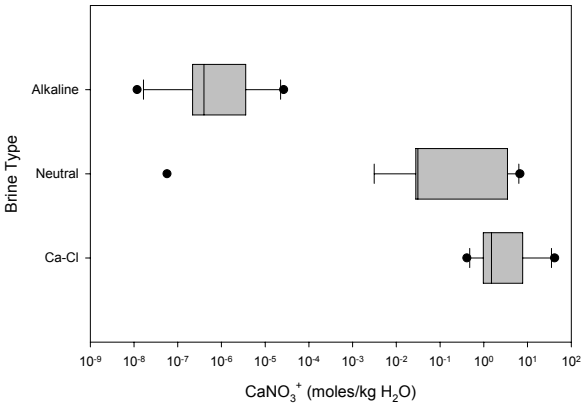
Bromide Conc. (at T=110 °C) of Evaporated YM Waters

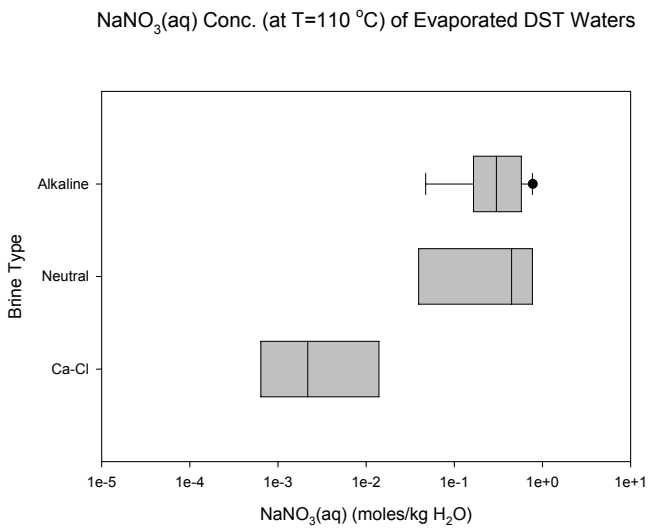


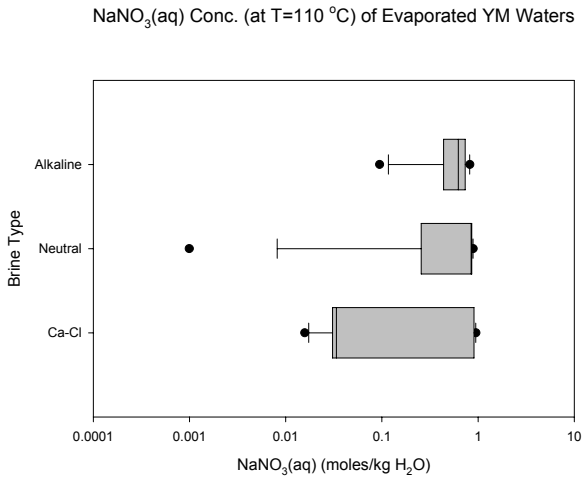
$CaNO_3^+$ Conc. (at T=110 °C) of Evap. DST Waters

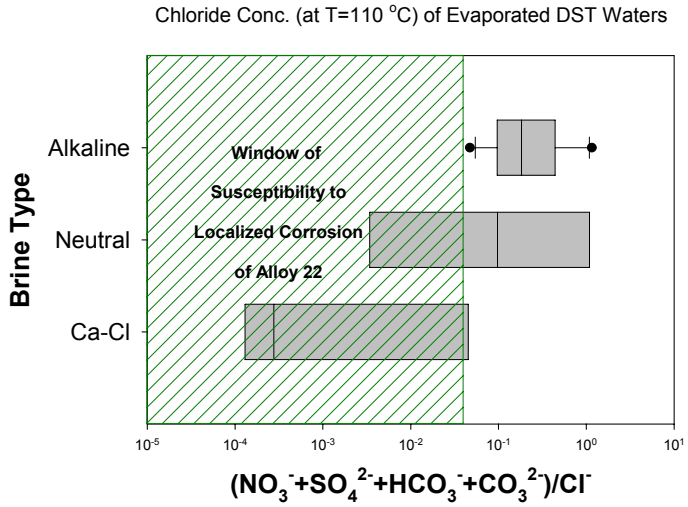


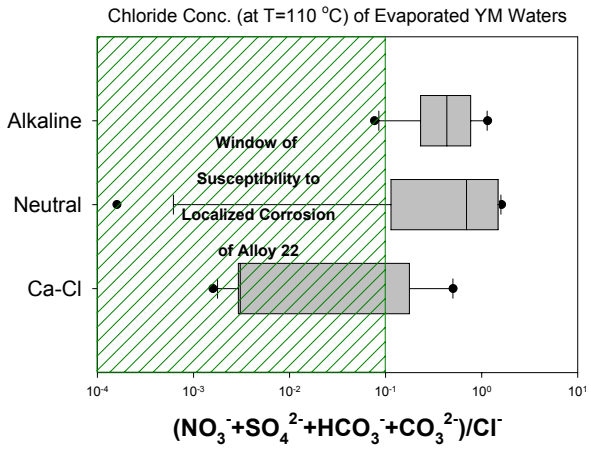
$CaNO_3^+$ Conc. (at T=110 °C) of Evap. YM Waters




NaNO3(aq) Conc. (at T=110 °C) of Evaporated DST Waters
Brine Type
Alkaline
Neutral
Ca-Cl
1e-5
1e-4
1e-3
1e-2
1e-1
1e+0
1e+1
NaNO3(aq) (moles/kg H2O)


NaNO3(aq) Conc. (at T=110 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0.0001
0.001
0.01
0.1
1
10
NaNO3(aq) (moles/kg H2O)


Chloride Conc. (at T=110 °C) of Evaporated DST Waters
Brine Type
Alkaline
Neutral
Ca-Cl
Window of
Susceptibility to
Localized Corrosion
of Alloy 22
10-5
10-4
10-3
10-2
10-1
100
101
(NO3-+SO42-+HCO3-+CO32-)/Cl-


Chloride Conc. (at T=110 °C) of Evaporated YM Waters
Alkaline
Neutral
Ca-Cl
Window of
Susceptibility to
Localized Corrosion
of Alloy 22
10-4
10-3
10-2
10-1
100
101
(NO3-+SO42-+HCO3-+CO32-)/Cl-

May 5, 2008

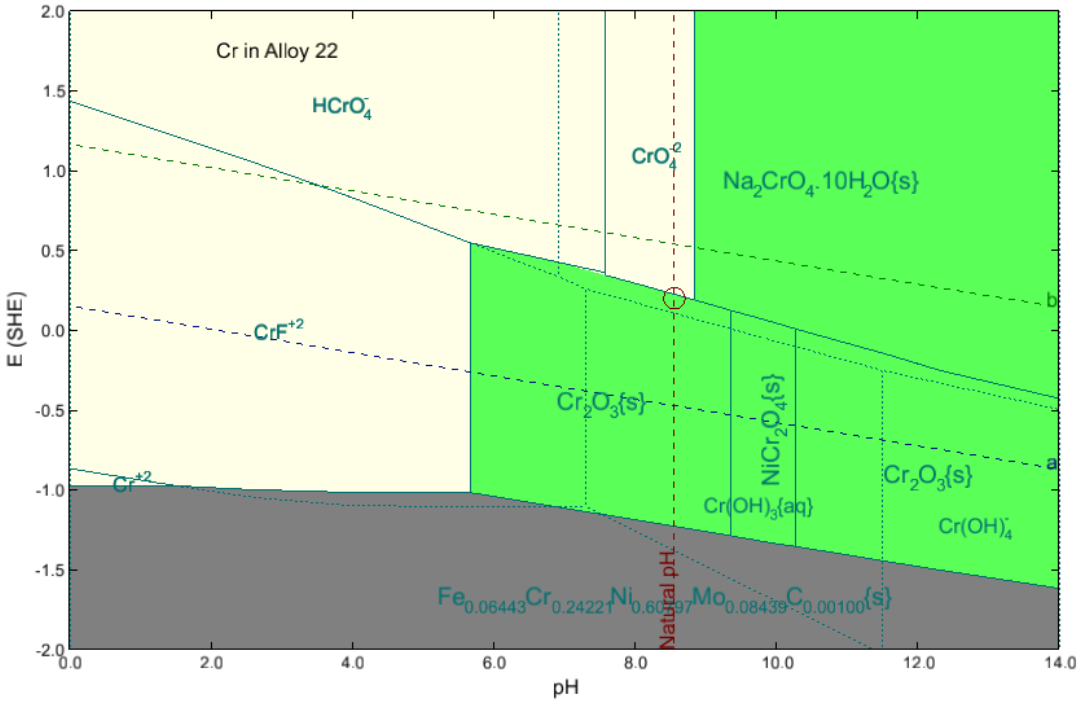
From Mintz et al. (2007):

"The passivity of Alloy 22 is attributed to the presence of a chromium-rich oxide film. A thermodynamic analysis was conducted to analyze the formation of the chromium-rich passive film. Solution compositions examined by other investigators where chromium oxides were not detected have been evaluated with commercial software to develop potential-pH diagrams. The thermodynamic data indicate that a chromium-nickel oxide ($NiCr_2O_4$) is thermodynamically stable and may be a likely contributor to the observed low corrosion rates."

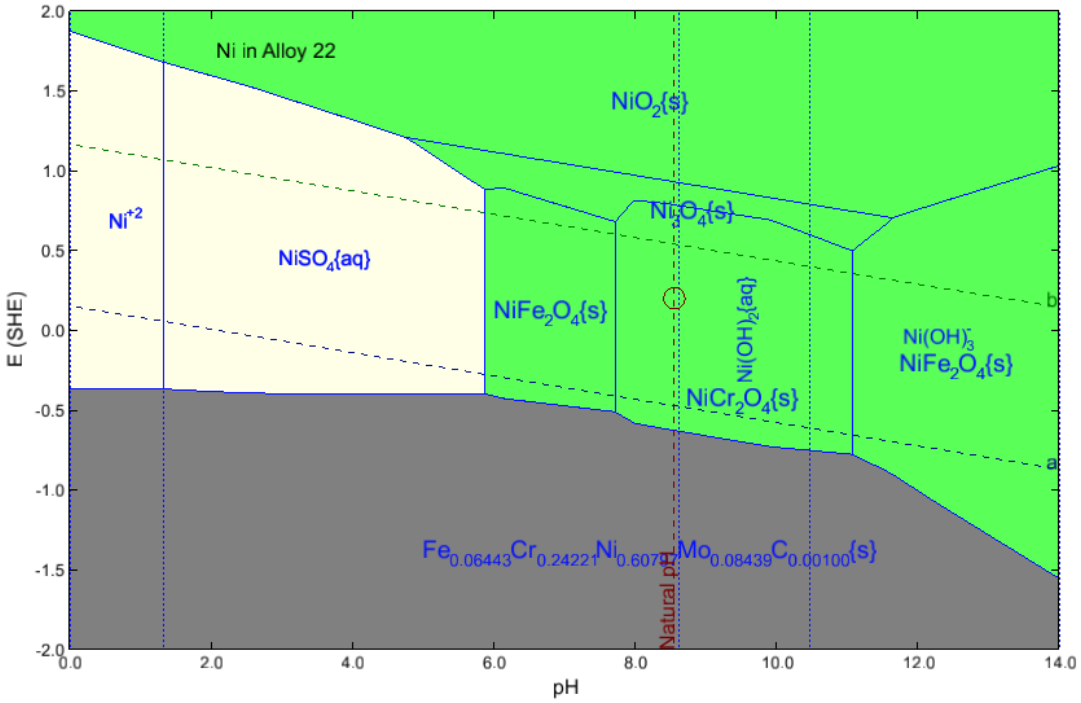
CorrosionAnalyzer 2.0 was used to calculate a Pourbaix diagram representing the Eh–pH of a system of a Saturated Concentrated Water in contact with Alloy 22. The SCW composition was taken from Table 3 of Mintz et al. (2007) and listed below:

Na+1	1.63000	molarity
K+1	0.0800000	molarity
Cl-1	0.180000	molarity
NO3-1	0.1000000	molarity
SO4-2	0.0800000	molarity
F-1	0.0600000	molarity
HCO3-1	0.610000 (0.769998)*	molarity
CO3-2	0.220000	Molarity
*Value in parentheses is after charge balancing. Values in Mintz et al. (2007) are in moles/kgH2O and were assumed equal to moles/L solution.		

The Pourbaix diagram calculated at 95 °C is shown below, indicating only the chromium species:

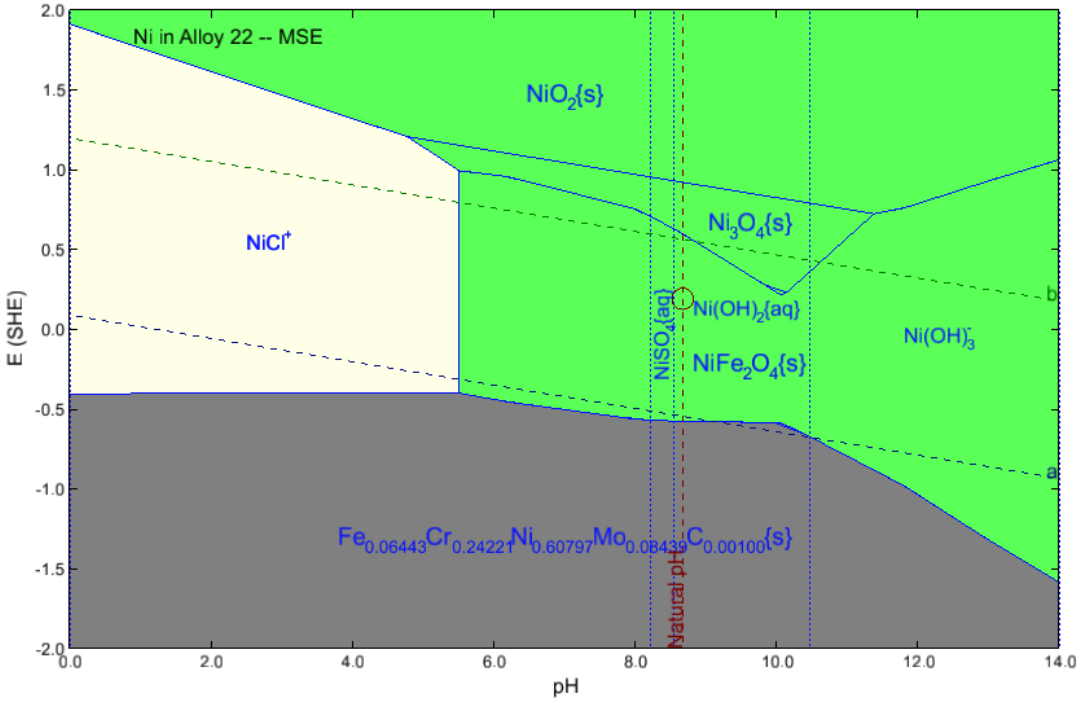


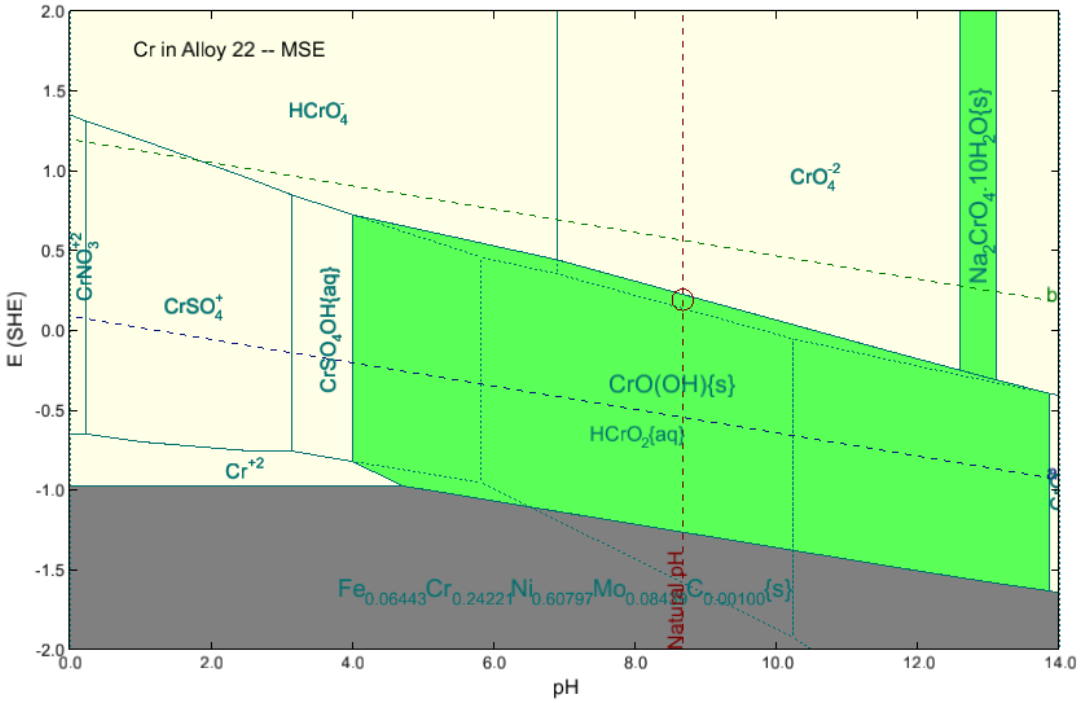
The nickel species are shown below:



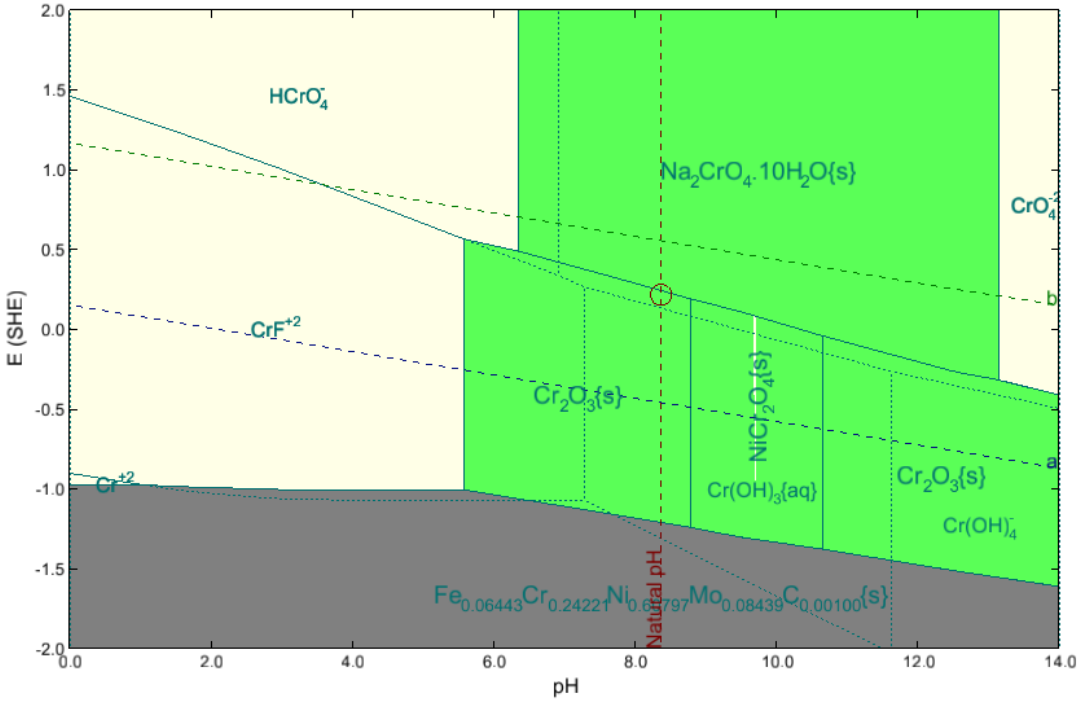
The above figures are somewhat different from those of Mintz et al. (2007) because the current calculations use an updated thermodynamic database.

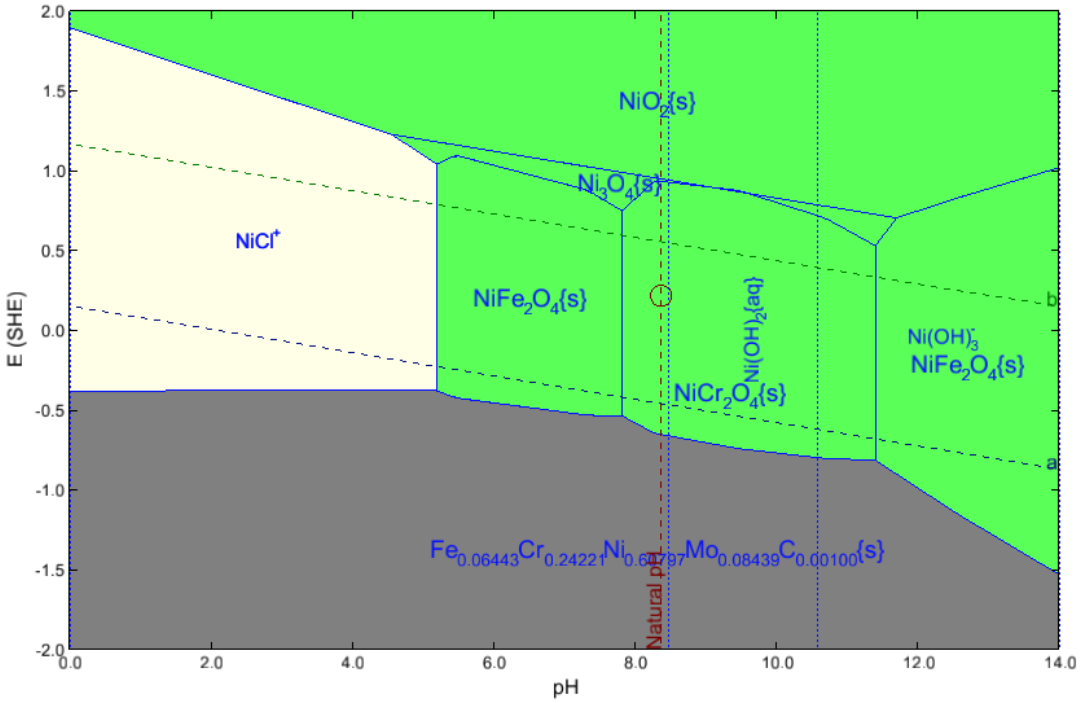
The Pourbaix diagram was recalculated using Mixed Solvent Electrolyte model (MSE Corrosion database). The results are shown below:



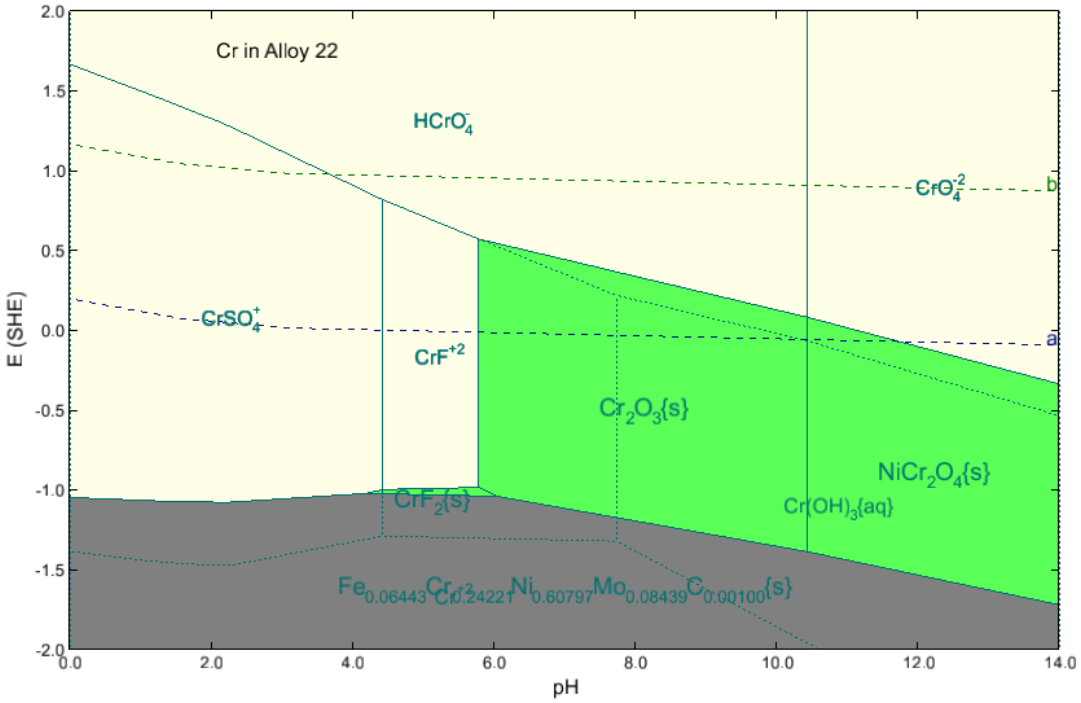


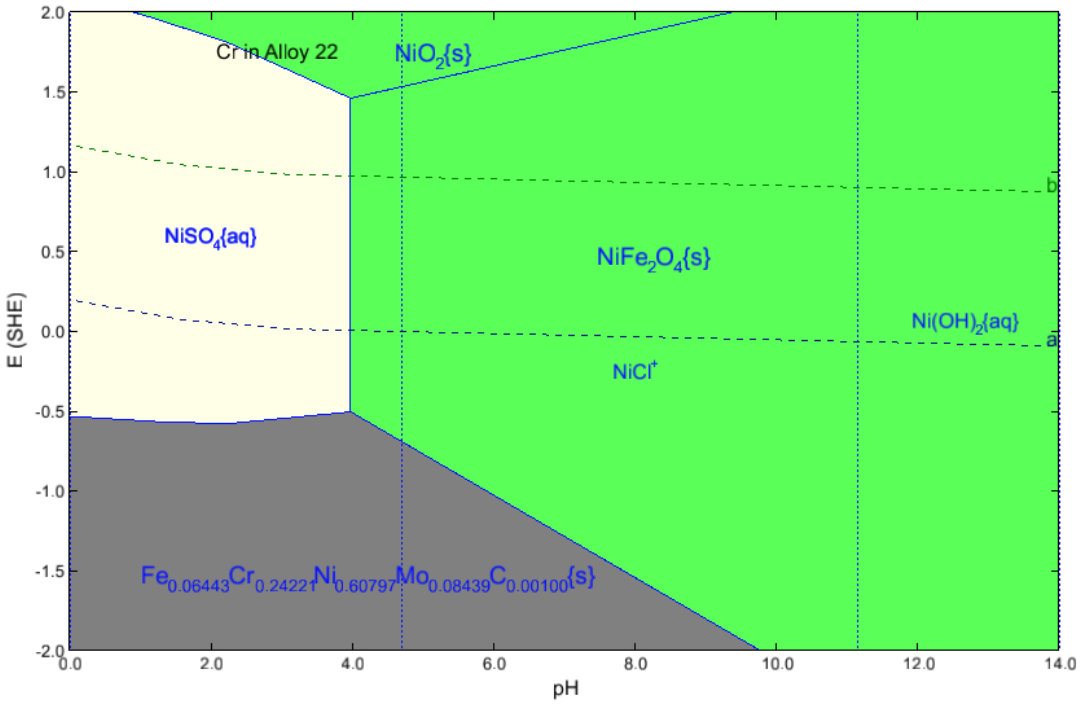
Pourbaix diagram — SCW + 6 M NaCl; Aq. H+ model





Pourbaix diagram — SCW; 125 °C





From:

Anderko, A. and M. Jakab (2007) Prediction of Corrosion of Advanced Materials and Fabricated Components, DE-FC36-04GO14043 Final Report 09/29/2007 OLI Systems Inc. (http://www.osti.gov/bridge/purl.cover.jsp?purl=/916966-5j09Ye/)

Chloride ions cause the breakdown of the passive film on the Cu-Ni alloys leading to localized corrosion (Milosev and Metikos-Hukovic, 1991; Metikos-Hukovic and Milosev, 1992). The structure, composition and thickness of the passive film influence the extent of localized corrosion (Milosev and Metikos-Hukovic, 1992). Several stages of the localized corrosion were identified (Milosev and Metikos-Hukovic, 1992). First, the chloride ions adsorb inside the pores of the outer oxide layer. This time period is known as the pit incubation period. During pit nucleation, the Cl- ions are incorporated into the outer oxide layer and penetrate to the inner oxide layer. This chloride ion incorporation is thought to modify the oxide lattice. The Cl- ions replace the O2- ions in the lattice and enhance cation diffusion through the oxide layer (Milosev and Metikos-Hukovic, 1991). The charge imbalance caused by the ion substitution is neutralized by ejection of a Cu+ ion into the solution creating a cation vacancy (Milosev and Metikos-Hukovic, 1991):

$$Cu^{+}_{metal} + O^{2-}_{oxide} + Cl^{-}_{electrolyte} + 2H^{+}_{electrolyte} = Cu^{+}_{electrolyte} + Cl^{-}_{oxide} + H_2O \qquad (4)$$

The copper ion dissolution causes the formation of a porous film over the dissolution site (Hettiarachchi and Hoar, 1979). At the pit induction time, the Cl- ions completely perforate the inner oxide layer. This stage is followed by steady pit growth. The critical potentials characteristic of localized corrosion, i.e., pitting potential and repassivation potential, were found to be linearly dependent on the logarithm of the chloride ion concentration (Metikos-Hukovic and Milosev, 1992).

MessageFrom: Andre Anderko [aanderko@olisystems.com]
Sent: Tuesday, May 06, 2008 1:01 PM
To: rpabalan@cnwra.swri.edu
Cc: Berthold
Subject: RE: Corrosion Analyzer MSE vs H+

Dear Bobby:

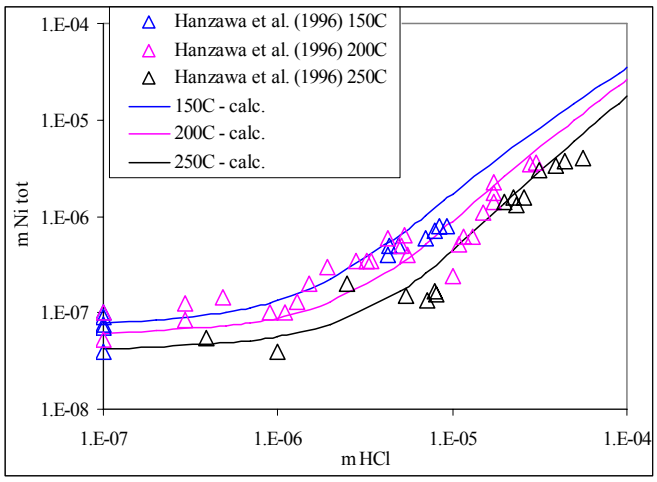
The reason for the difference lies in the somewhat different thermochemical parameters for NiFe2O4. About a year ago, we made an analysis of solubility data for NiFe2O4 in the MSE model, which resulted in somewhat different thermochemical parameters. I am attaching a spreadsheet that compares the calculated and experimental solubilities. In the aqueous model, we kept the thermochemical properties that were simply taken from the literature.

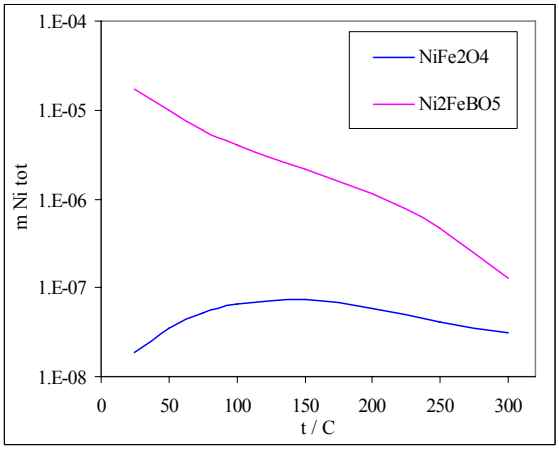
To be absolutely sure which solid should appear, we should make a similar analysis for NiCr2O4. We are planning to do it in approximately a month or so (it is a project sponsored by one of our clients) but I am not sure whether we will be able to find any solubility data. If we do not, we will have no choice but to keep our current literature data for NCr2O4. So, I believe that the current MSE predictions are already better but they may still change.

I think that the real passive film can be probably approximated by a somewhat continuous mixture (or a solid solution) of the various multicomponent oxides. So, I agree that the solubility calculations are a good thing to do but we are still on a somewhat shaky ground for oxides other than Cr2O3 and NiFe2O4.

Best regards,

Andre





From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Tuesday, May 06, 2008 11:44 AM
To: 'Andre Anderko'
Cc: 'James Berthold'
Subject: RE: Corrosion Analyzer MSE vs H+

Dear Andre,

I'm specifically interested in C-22. When I generate the Pourbaix diagram for C-22 in contact with what DOE calls Saturated Concentrated

Water (at 95 C), NiCr2O4(s) is present in the pH range ~8 to 10 if Aq. H+ model is used, whereas NiFe2O4(s) shows up instead using MSE. So I'm just trying to understand what would cause the difference -- maybe you can point me to some published papers describing the basis for the CorrosionAnalyzer models.

Also, do you think that NiCr2O4(s) [or perhaps NiFe2O4(s)] are useful analogs for the passive oxide film protecting Alloy 22. Some of my colleagues think so. If it is, would it be useful to calculate the solubilities of these oxides as a function of temperature and chemistry, as a qualitative measure of the corrosion resistance of Alloy 22?

Thanks.

Bobby

-----Original Message-----
From: Andre Anderko [mailto:aanderko@olisystems.com]
Sent: Tuesday, May 06, 2008 9:50 AM
To: 'James Berthold'; rpabalan@cnwra.swri.edu
Subject: RE: Corrosion Analyzer MSE vs H+

Dear Bobby:

As Jim has indicated, the MSE predictions are usually more accurate if the relevant parameters have been already regressed. Among the metals of metallurgical importance for which Pourbaix diagrams are typically generated, we have completed comprehensive parameter evaluation projects for Cr, Mo, W, Al, and Pb. Partial project have been completed for Fe, Sn, and Ni. Therefore, predictions for these for metals are better in MSE. Currently, a comprehensive project is under way for Ni and Cu, for which parameters will be available starting with build 59. For other transition metals, there should be no significant difference between the quality of predictions for MSE and the aqueous model. I can provide you with more detailed information if you let me know which particular system you are interested in.

Best regards,

Andre

From: James Berthold [mailto:jberthold@olisystems.com]
Sent: Tuesday, May 06, 2008 7:45 AM
To: rpabalan@cnwra.swri.edu
Cc: 'Andre Anderko'
Subject: RE: Corrosion Analyzer MSE vs H+

Dear Bobby,

There is a limitation in MSE with the Corrosion Analyzer in that that rates of corrosion are not yet supported in MSE. Stability diagrams, on the other hand, are supported. The differences between the AQ model (H+) and MSE (H3O+) is that we have changed the solubility parameters for the MSE model. The data fitting is more exact in MSE.

To comment further I would need to know the specific system you are studying. I have cc'd Andre Anderko (OLI) in case he wants to add any additional comments.

Jim

Jim Berthold
Director of Customer Relations
OLI Systems, Inc.
jberthold@olisystems.com
www.olisystems.com
http://support.olisystems.com

Check out our new Video Tutorials
http://support.olisystems.com/Media.shtml

+973-539-4996 x 24 8 AM (0800) to 5 PM (1700) M-F
All E-mails are virus scanned prior to sending.

From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Monday, May 05, 2008 3:33 PM
To: 'Jim Berthold'
Subject: Corrosion Analyzer MSE vs H+

Jim,

Do you have any advice with respect to using MSE versus Aq. H+ model in CorrosionAnalyzer? I get different results in the Pourbaix diagram stability fields (both aqueous and solid phases) if I switch from one to the other using the same aqueous composition.

Thanks.

Bobby Pabalan

May 7, 2008

This following is the approximate composition of Simulated Concentrated Water taken from Gdowski (1997; UCRL-ID- 132286). According to Gdowski, the "Simulated Concentrated Water (SCW) has a ionic composition that is nominally a factor of a thousand higher than that of "representative" water of Yucca Mountain. J-13 well water is obtained from ground water that is in contact with the Topopah Spring tuff, which is the repository horizon rock. The thousand times higher ionic content was chosen to simulate the water that may result from wetting of salts and minerals that have been deposited on the container surfaces."

Table 1. Compositions of "representative" Yucca Mountain waters J-13 well water and "perched" water, and the estimated composition of the simulated concentrated water.

Constituent	J-13 (mg/l) (mg/l)	"Perched" (mg/l)	Simulated Concentrated Water (estimated)
Na	45.80	36	40,900
Si	28.5	37	27 (60C); 49 (90C)
Ca	13.0	25	< 1
K	5.04	1.7	3,400
Mg	2.01	2.2	< 1
F^-	2.18	0.7	1,400
Cl^-	7.14	6.3	6,700
NO_3^-	8.78	4	6,400
SO_4^{2-}	18.4	15	16,700
HCO_3^-	128.9	147	70,000
$CaCO_3$	—	—	47,500 (precipitate)
$MgCO_3$			7,300 (precipitate)
pH	7.41	8.1	

Four porewater compositions selected by DOE for its Near-field Chemistry Model will be used to simulate the composition of seepage water that evaporates and interacts with Alloy 22 waste package material. The compositions are given in the DOE EBS PC&E AMR.

Composition of sample ESF-Thermalk-017/26.5-26.9/UC:

Cations

Na+1	45.0000	mg/L
K+1	14.4000	mg/L
Mg+2	7.90000	mg/L
Ca+2	62.0000	mg/L

Anions

Cl-1	67.0000	mg/L

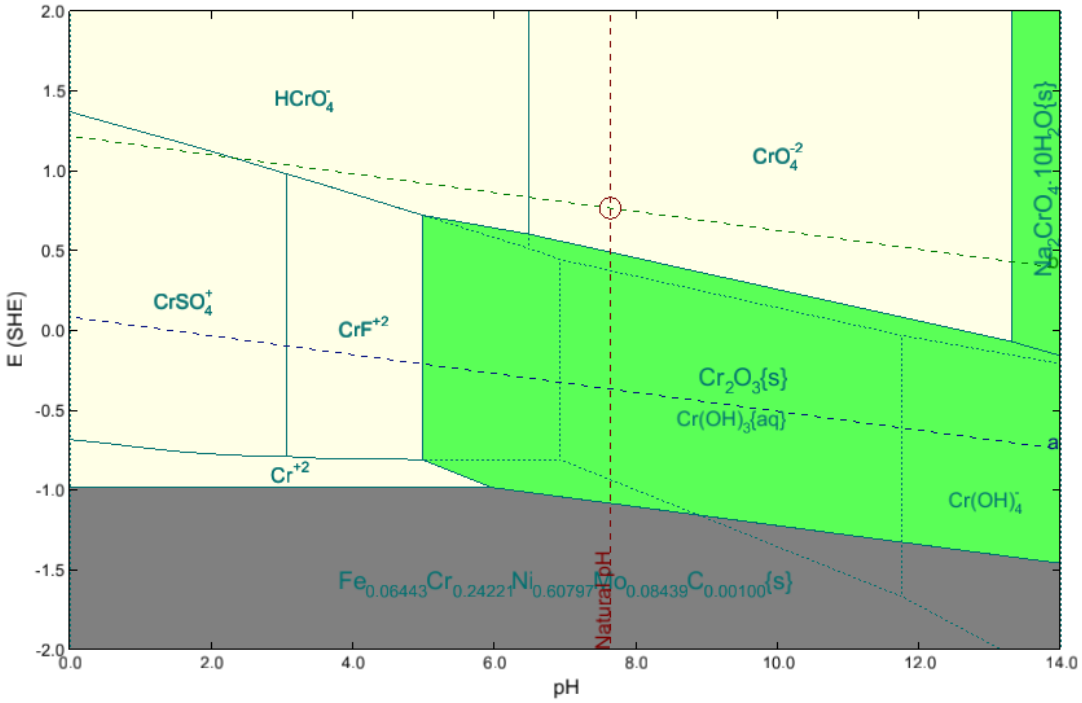
SO4-2 82.0000 mg/L
HCO3-1 126.000 mg/L
NO3-1 44.0000 mg/L
F-1 1.40000 mg/L

Neutral Species
SiO2 52.0000 mg/L

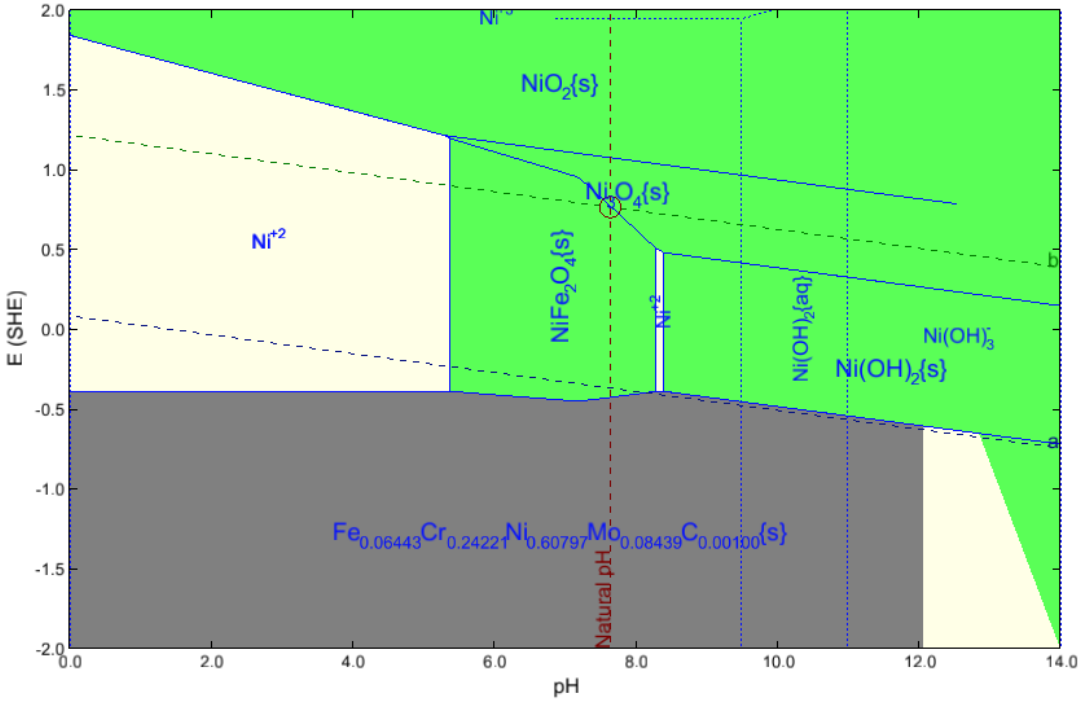
The above composition was inputted into CorrosionAnalyzer as a SCOREAnalysis. In addition, the following gas compositions were specified: N2 = 0.7897 atm; O2 = 0.21 atm; and CO2 = .0003 atm. A water/gas ratio of 0.1 was specified. Charge balance was done using prorated proportions of the cations. H+ aqueous model was used.

A stability diagram calculation (25 C; 1 atm) was specified, with C-22 as the contact surface.

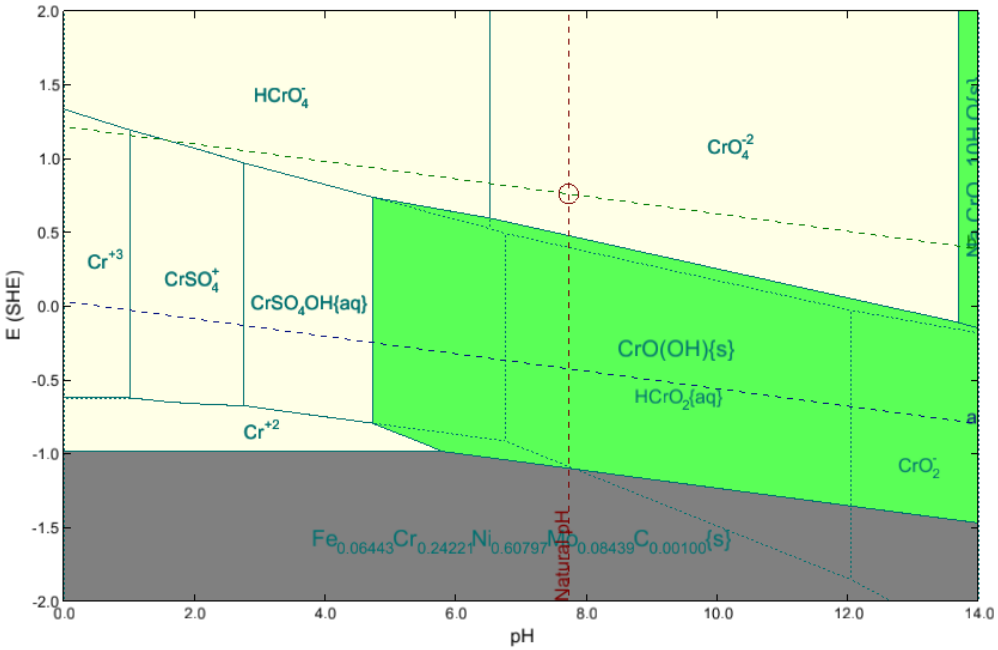
The chromium speciation is as follows:

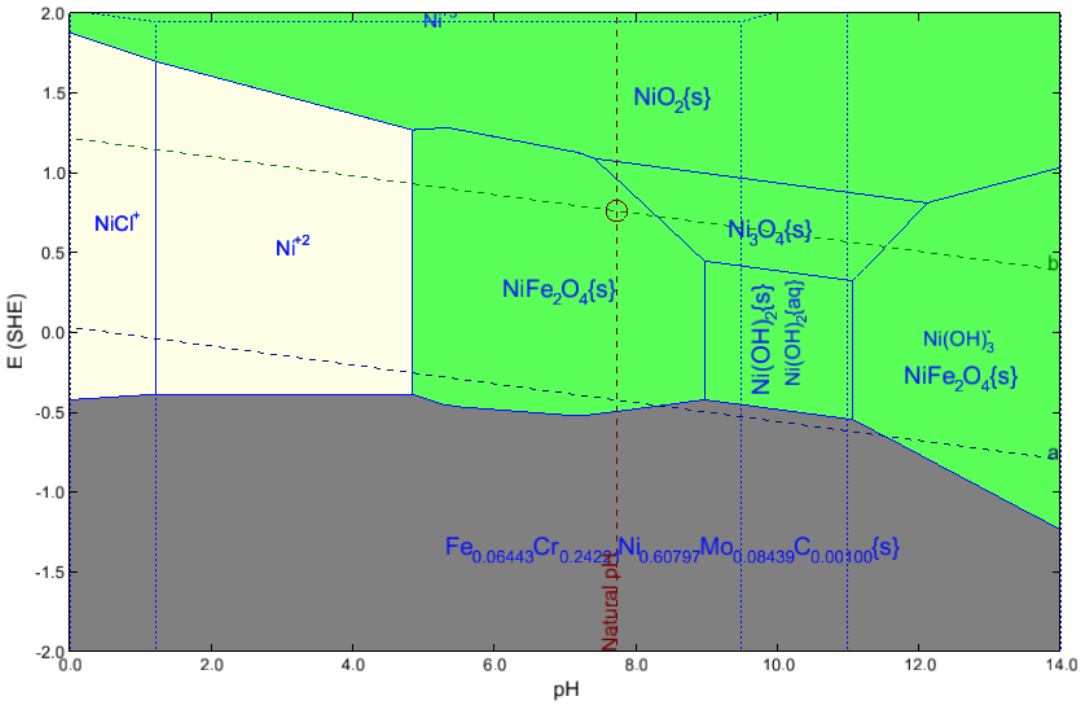


The nickel speciation is as follows:

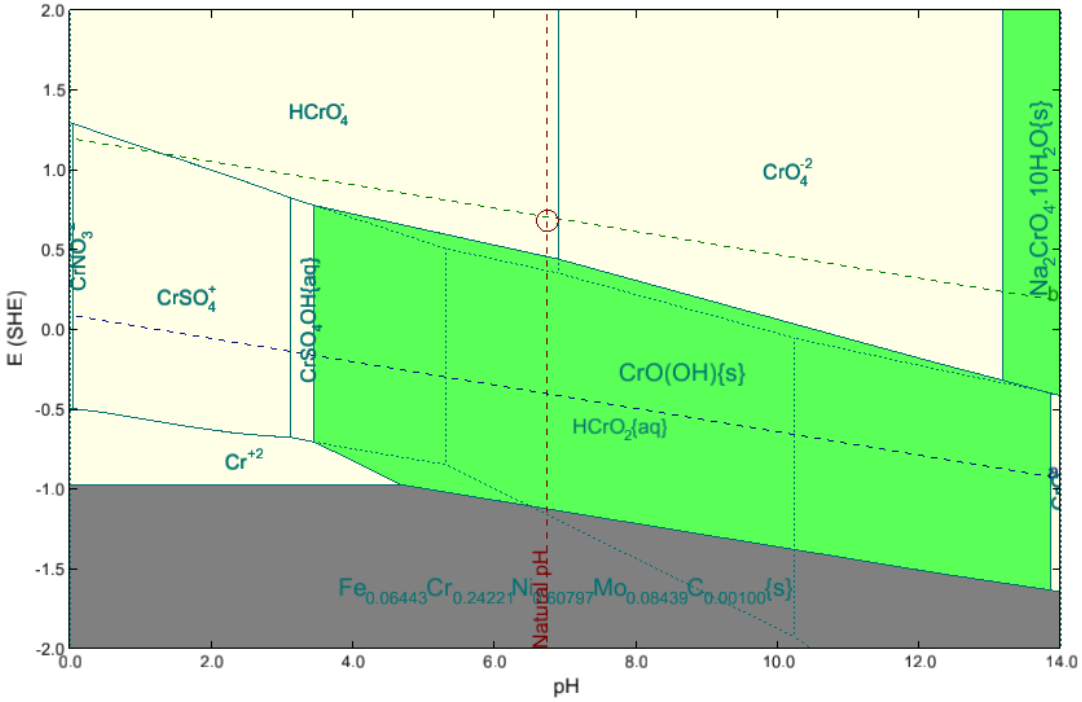


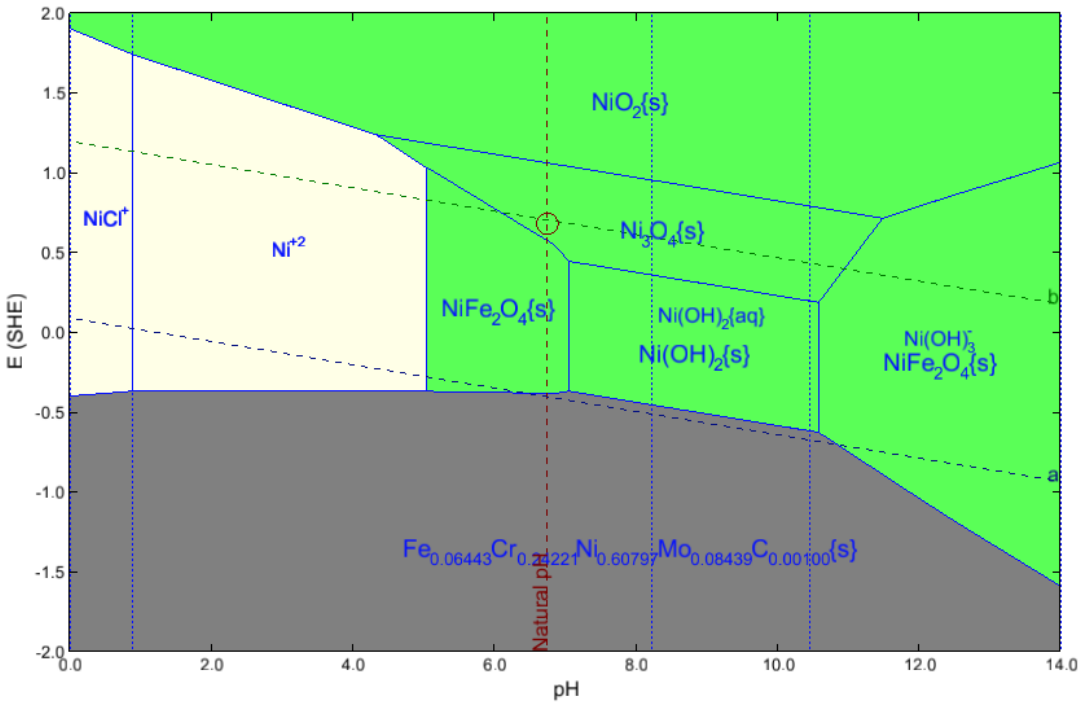
The SCOREAnalysis data were copied into another icon, and MSE model was specified for charge balancing and stability diagram calculations (25 C, 1 atm). The chromium and nickel speciation are as follows:



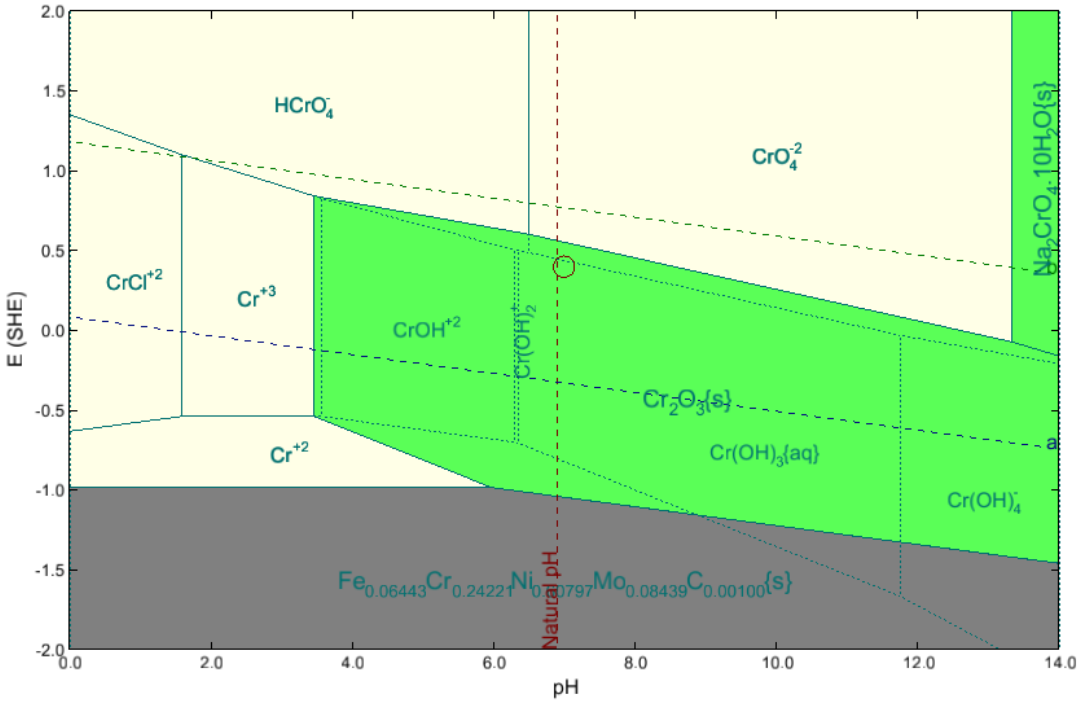


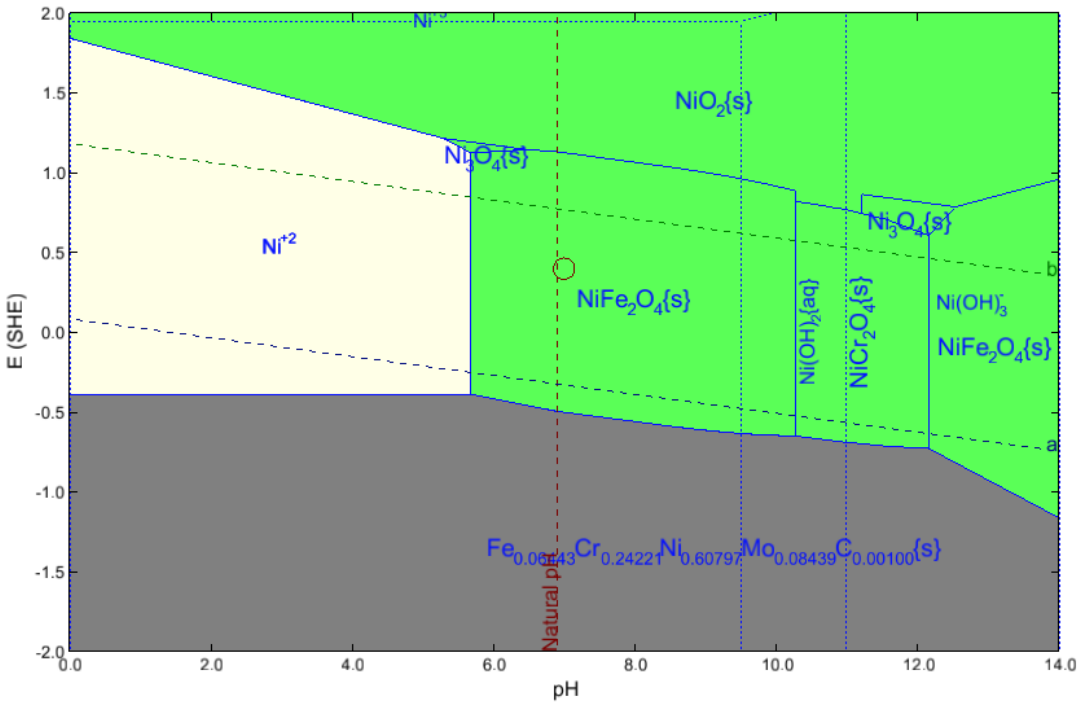
New calculations at 95 C and 0.85 atm; MSE; charge balancing is prorated. Chromium and nickel speciation are as follows:



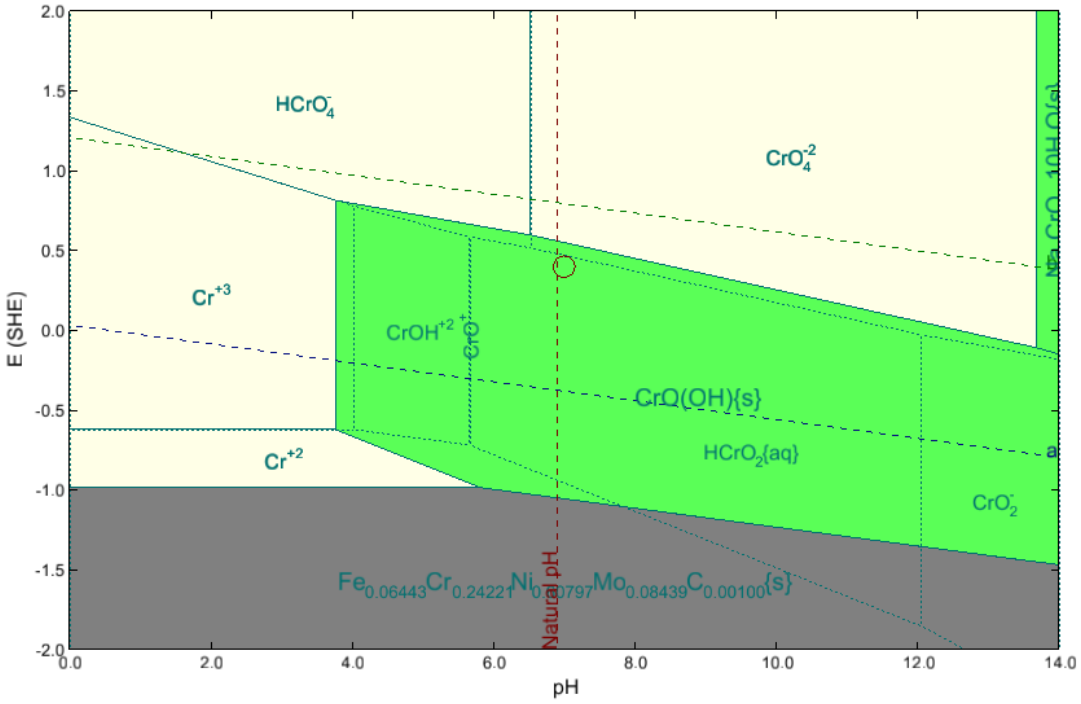


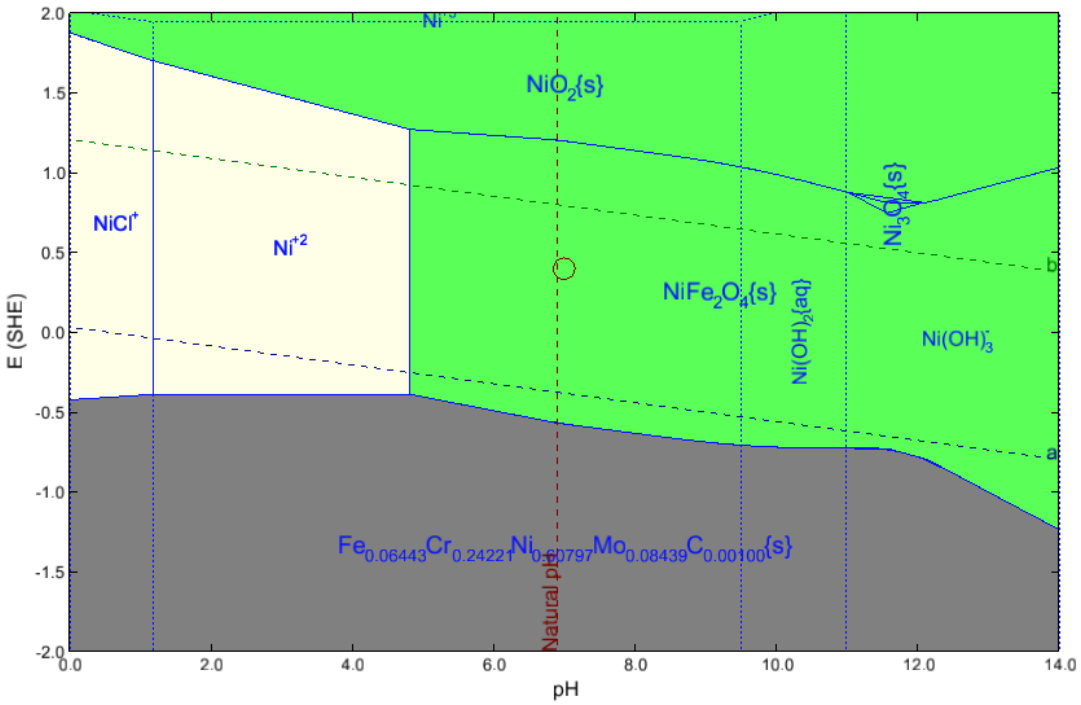
The following is for pure water at 25 C, 1 atm; H+ aqueous model:

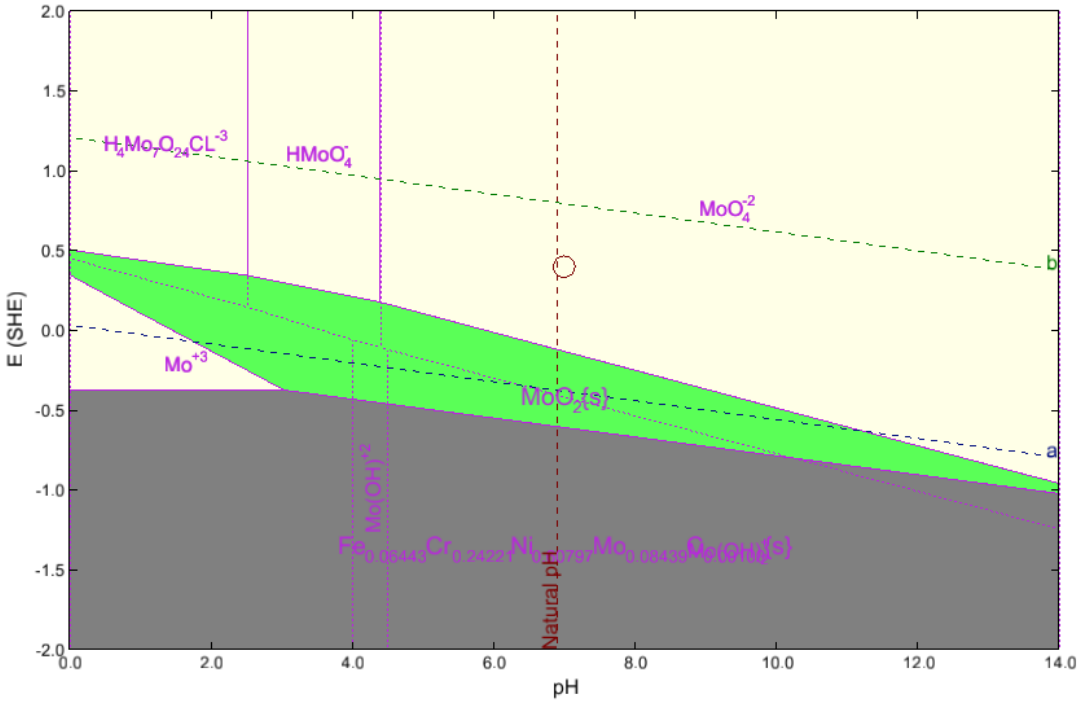


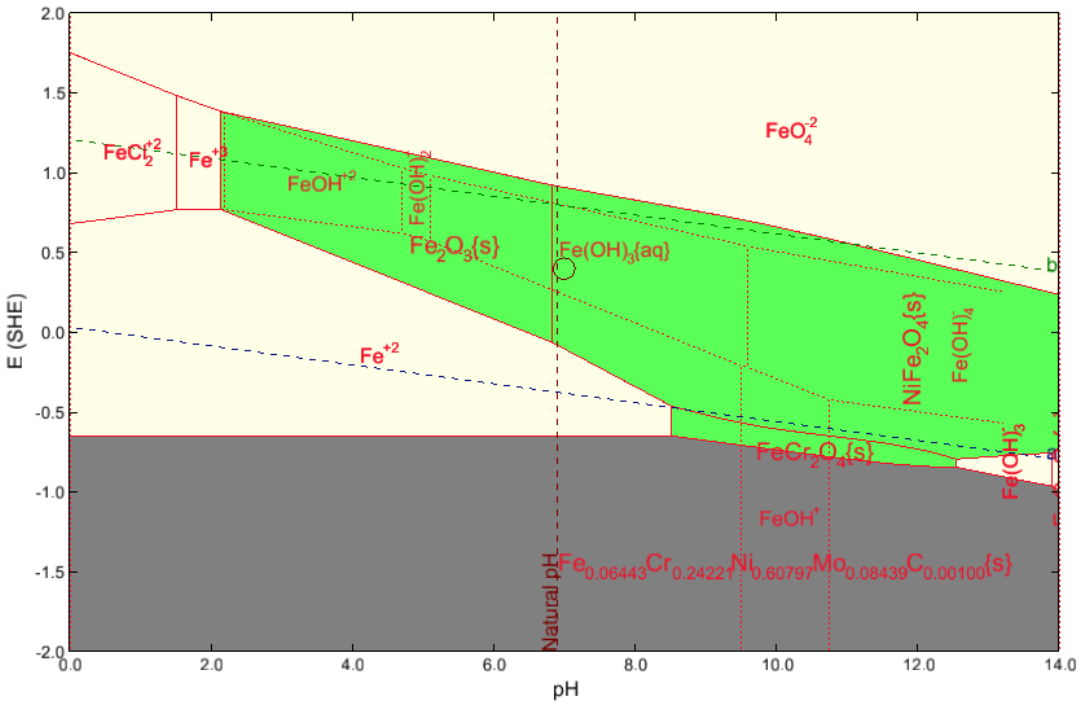


The following are for pure water at 25 C, 1 atm; MSE model:

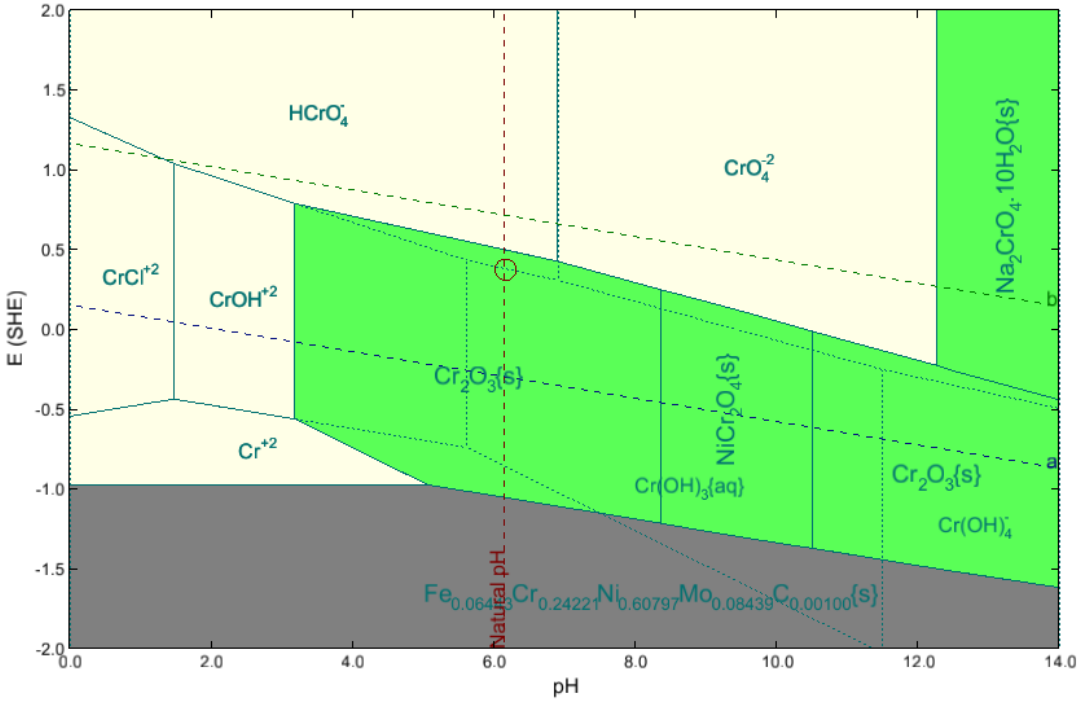


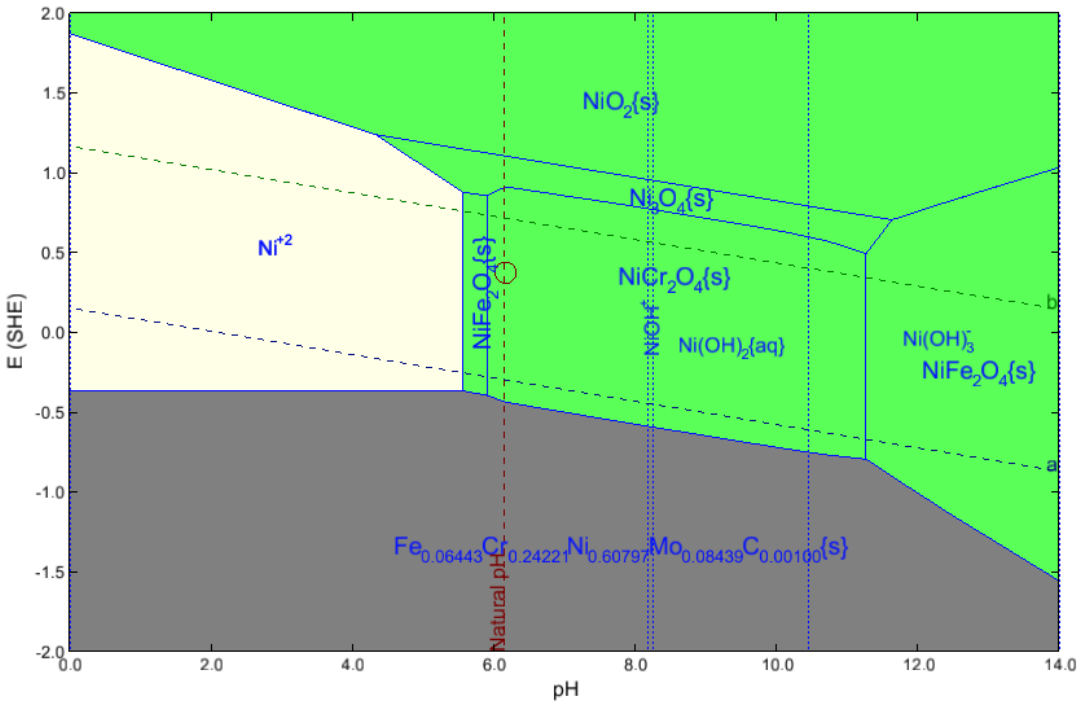

Ni
NiO2{s}
NiCl+
Ni+2
NiFe2O4{s}
Ni3O4{s}
Ni(OH)2{aq}
Ni(OH)3-
Fe0.06443Cr0.24221Ni0.10797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH


H4Mo7O24CL-3
HMoO4-
MoO4-2
Mo+3
MoO2{s}
Mo(OH)+2
Natural pH
E (SHE)
pH

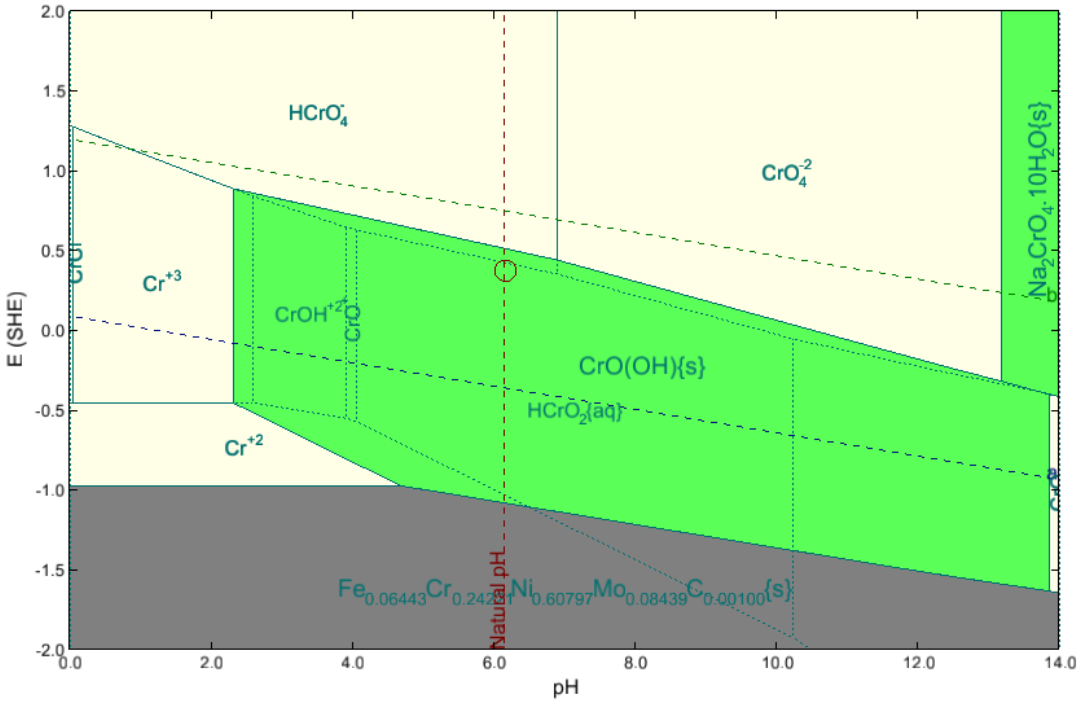


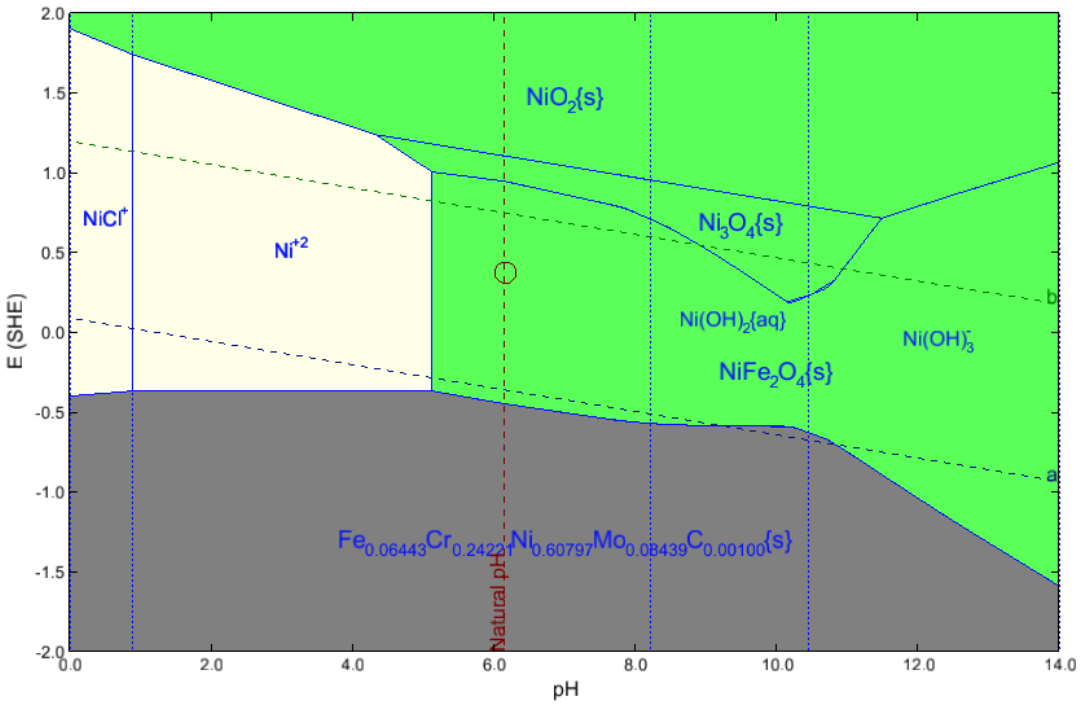
The following are for pure water, 95 C, 1 atm, H+ aqueous model:

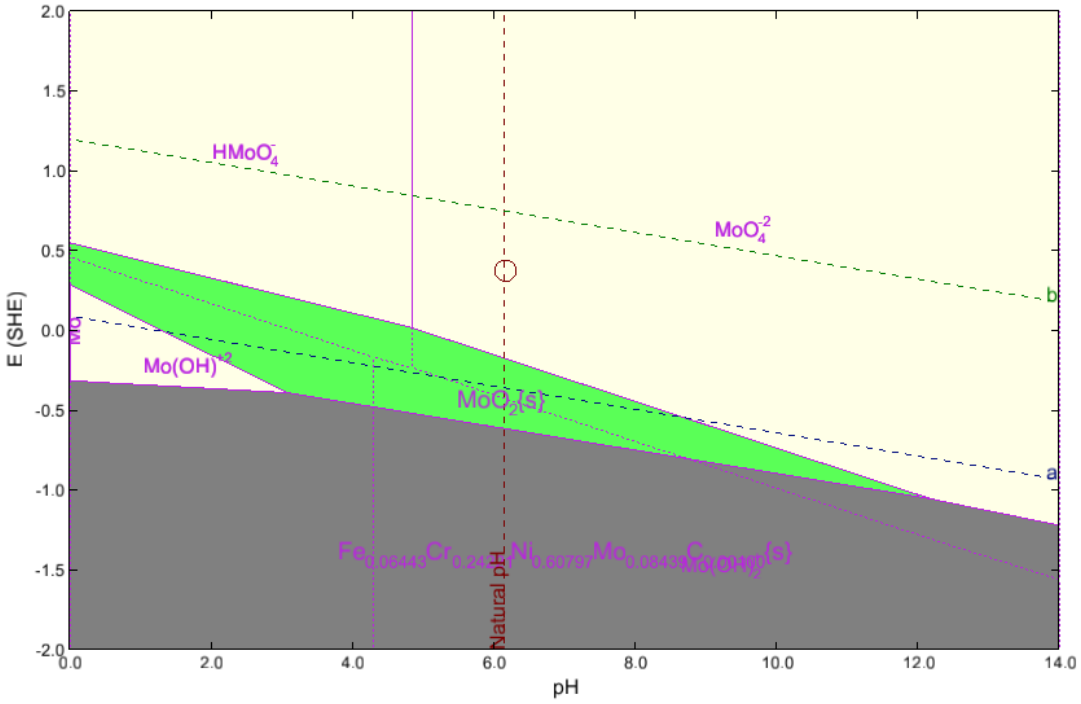


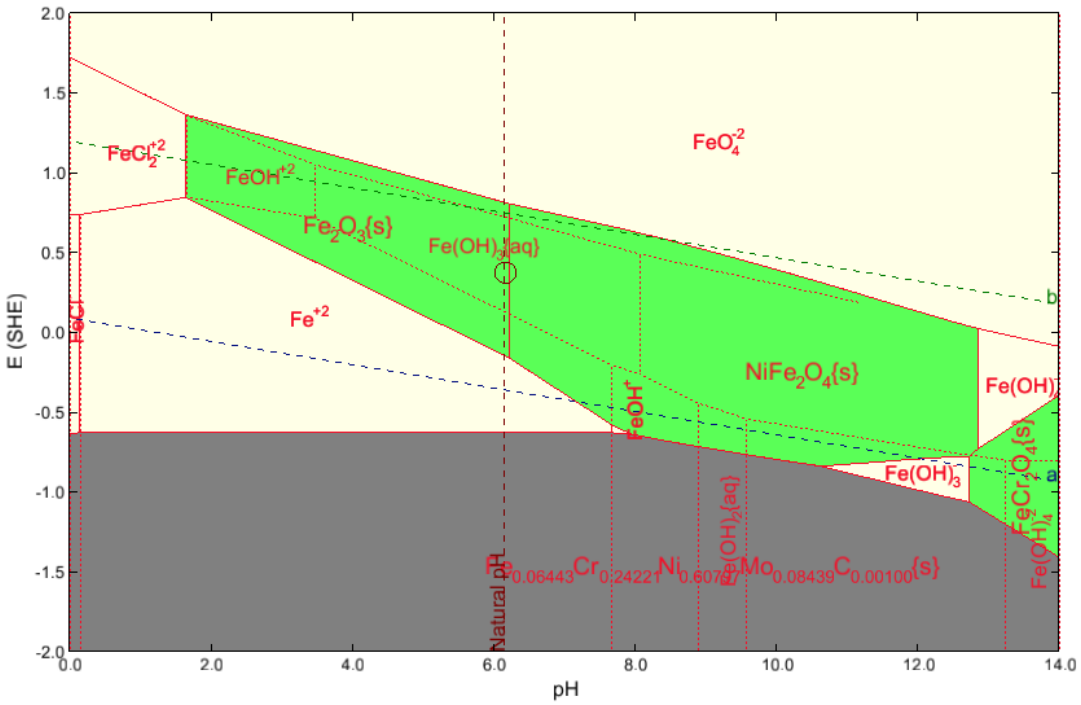


The following are for pure water, 95 C, 1 atm; MSE model:

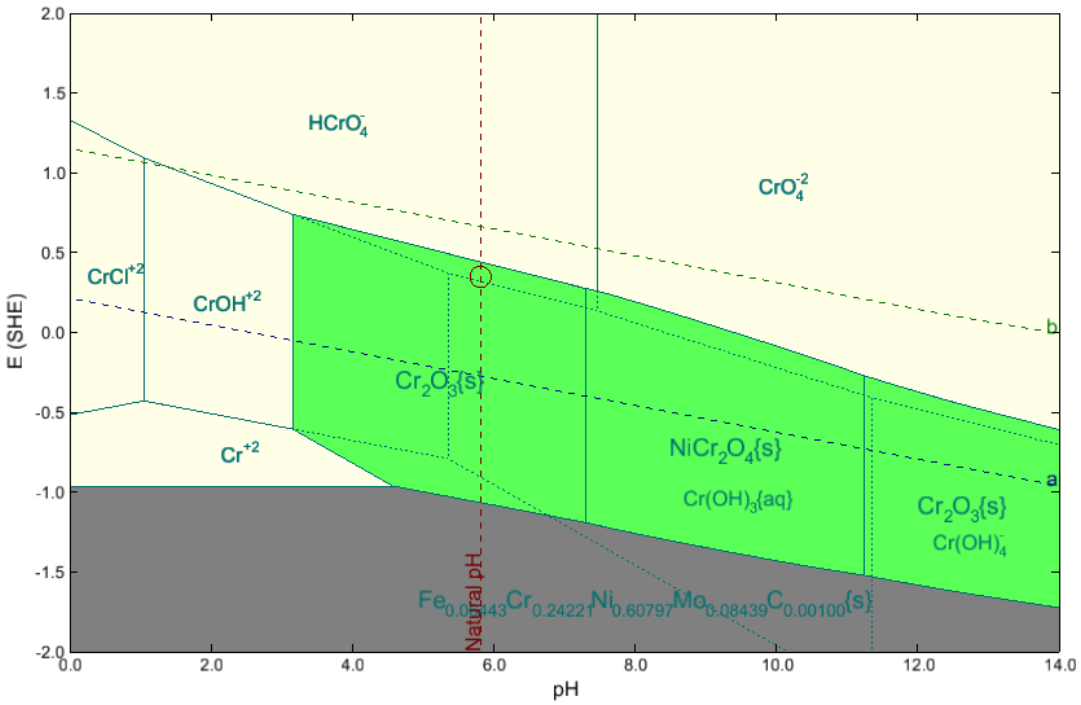


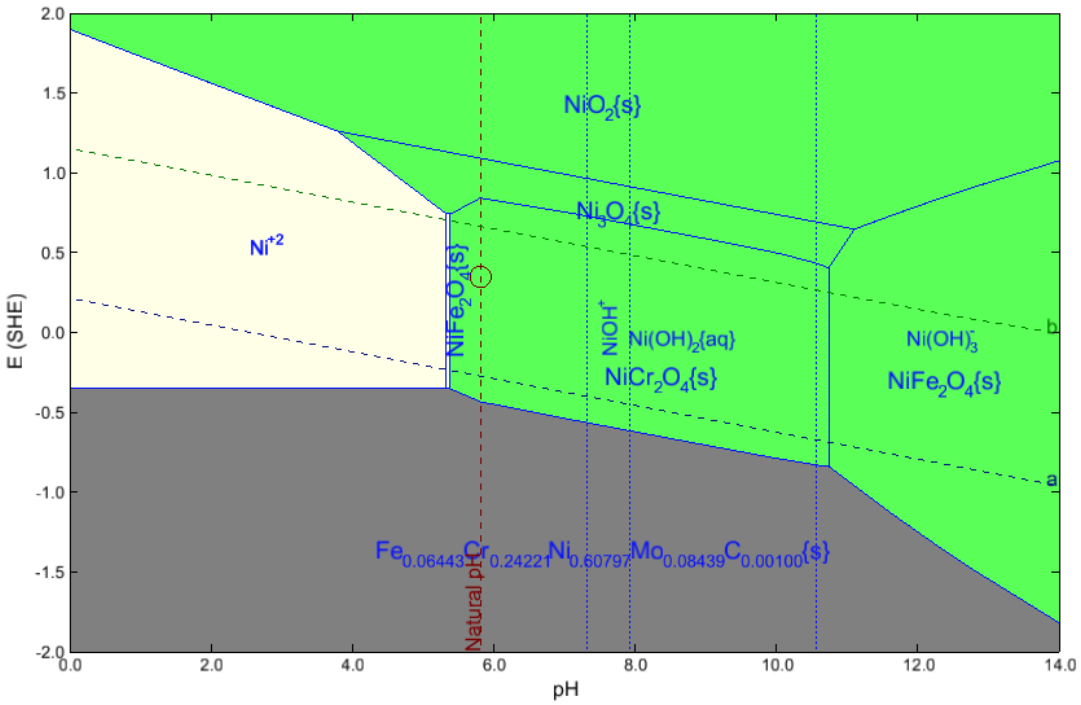

NiO2{s}
NiCl+
Ni+2
Ni3O4{s}
Ni(OH)2{aq}
Ni(OH)3-
NiFe2O4{s}
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH


HMoO4-
MoO4-2
MoO3
Mo(OH)+2
MoO2{s}
Natural pH
E (SHE)
pH

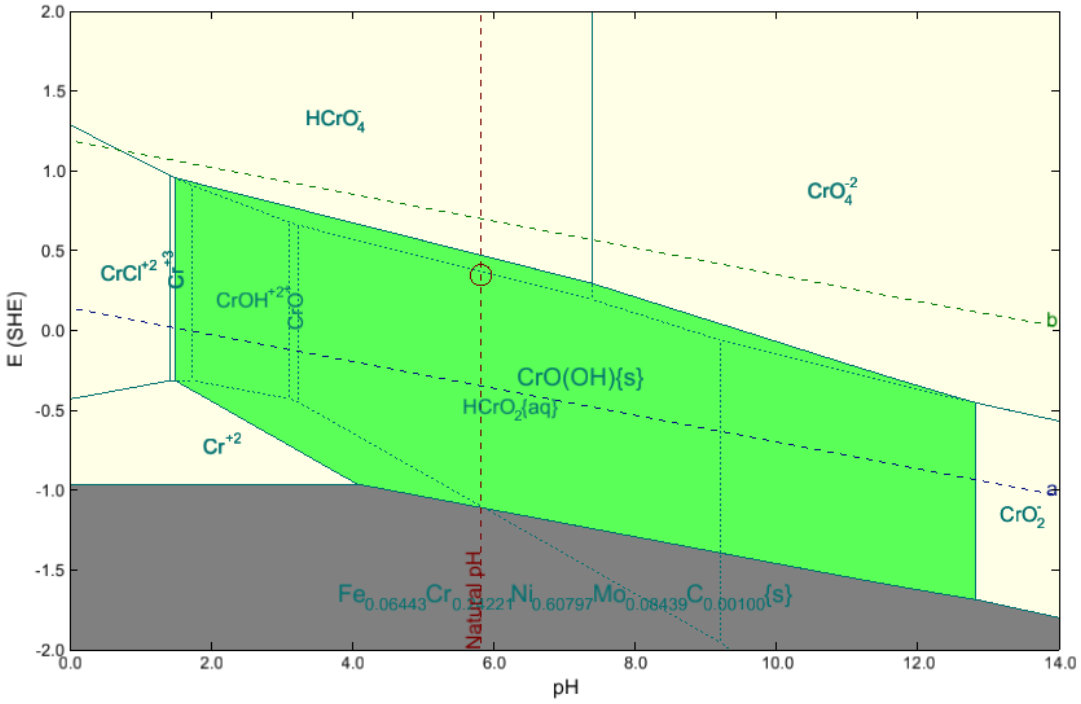


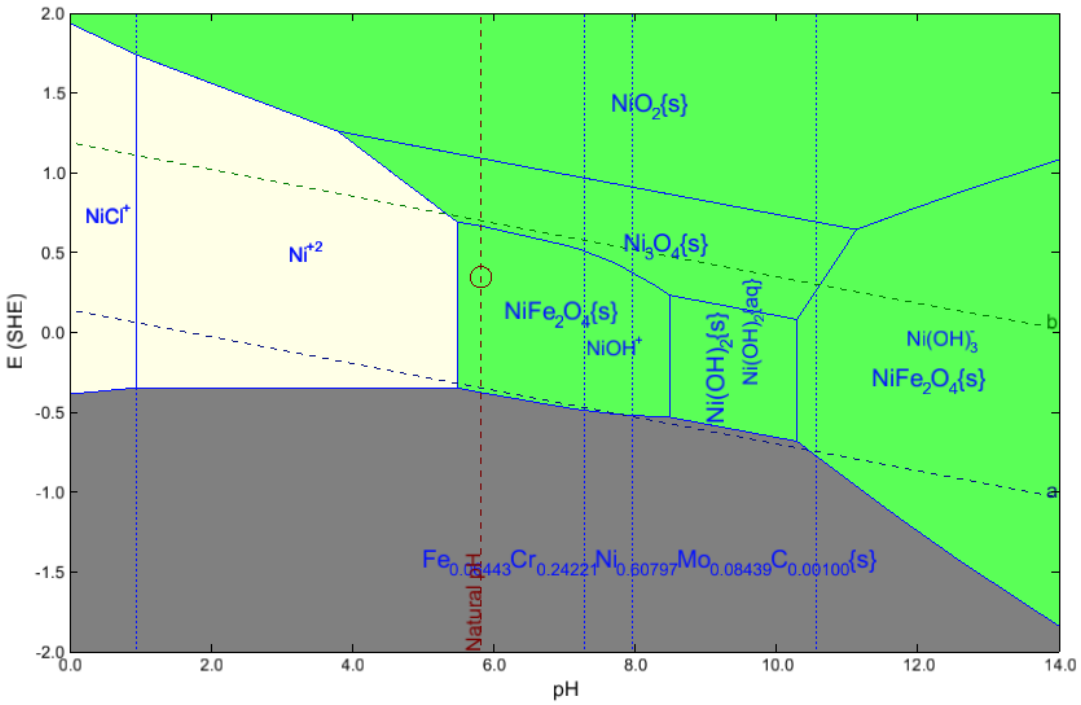
The following are for pure water, 150 C, 5 atm, H+ aqueous model:

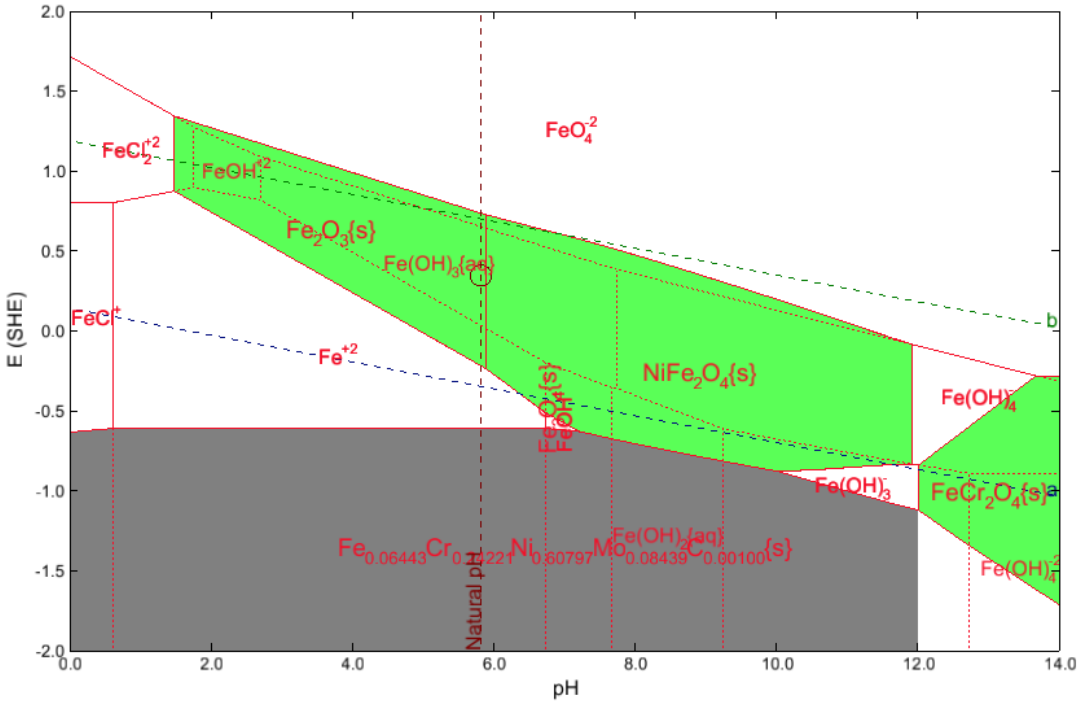




The following are for pure water, 150 C, 5 atm, MSE model:




E (SHE)
pH
NiO2{s}
NiCl+
Ni+2
Ni3O4{s}
NiFe2O4{s}
NiOH+
Ni(OH)2{s}
Ni(OH)2{aq}
Ni(OH)3-
NiFe2O4{s}
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
a
b


E (SHE)
pH
FeO4-2
FeCl2+2
FeOH+2
Fe2O3{s}
Fe(OH)3{aq}
FeCl+
Fe+2
NiFe2O4{s}
Fe(OH)4-
Fe(OH)3
FeCr2O4{s}
Fe(OH)2{aq}
Fe(OH)4-2
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
a
b

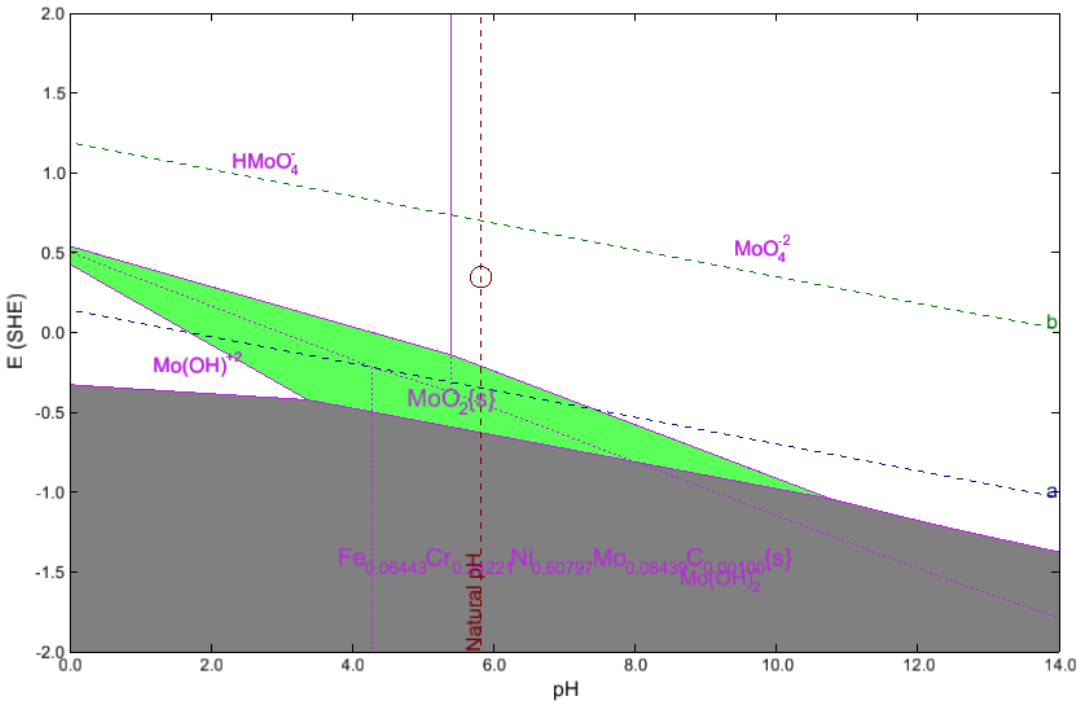
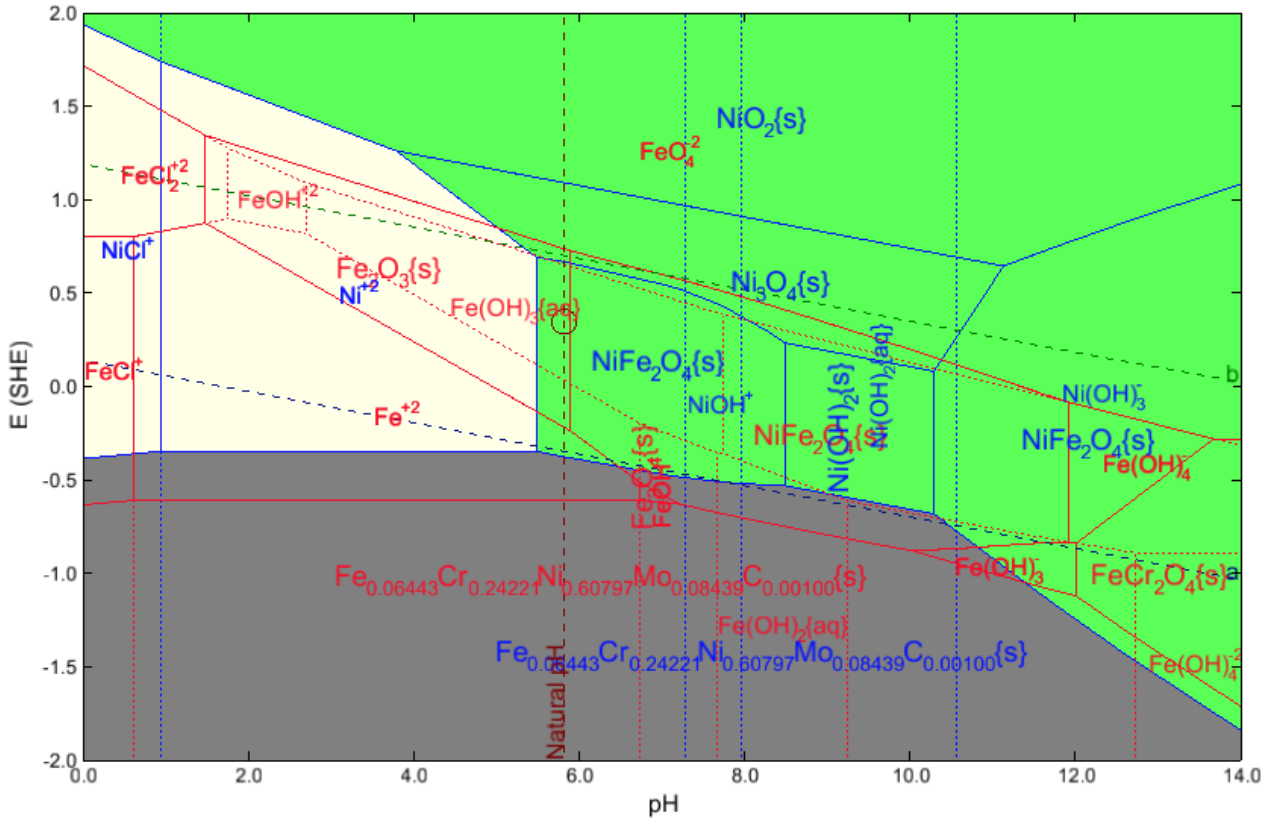


Figure showing both iron and nickel:



May 8, 2008

After charge balance reconciliation in CorrosionAnalyzer at 25 C, 1 atm using MSE aqueous model, the aqueous stream was exported as input to evaporation and metal oxide dissolution simulations at 95 C, a temperature 1 degree Celsius below the seepage threshold temperature of DOE. The simulation was done by specifying an Isothermal Calculation and a total pressure in the input file that would result in an output relative humidity (or water activity) equal to a specified relative humidity. That is,

$P_{Total} = RH_{specified} \times pH_2O°(T)$

Temperature, T, is 95 °C. $pH_2O°$ at 95 °C is 0.832599 atm. $RH_{specified}$ was varied such that a range of degrees of evaporation is achieved.

The table below gives the input total pressure corresponding to the relative humidity values of interest:

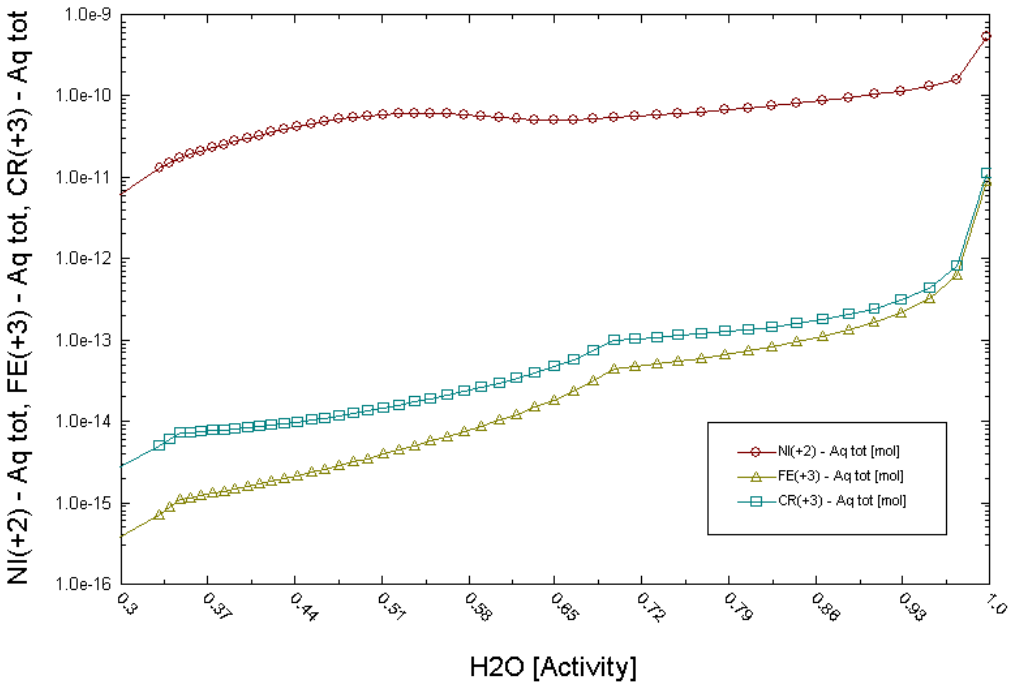
RH	pH2O	Ptot
1	0.8326	0.832599
0.95	0.8326	0.790969
0.9	0.8326	0.749339
0.8	0.8326	0.666079
0.7	0.8326	0.582819
0.6	0.8326	0.499559
0.5	0.8326	0.4163
0.4	0.8326	0.33304
0.3	0.8326	0.24978

A survey calculation was done at 95 C in CorrosionAnalyzer. The total pressure was varied from 0.832599 atm to 0.24978 atm (logarithmic spacing was used) corresponding to a relative humidity range of 30 to 100 percent RH.

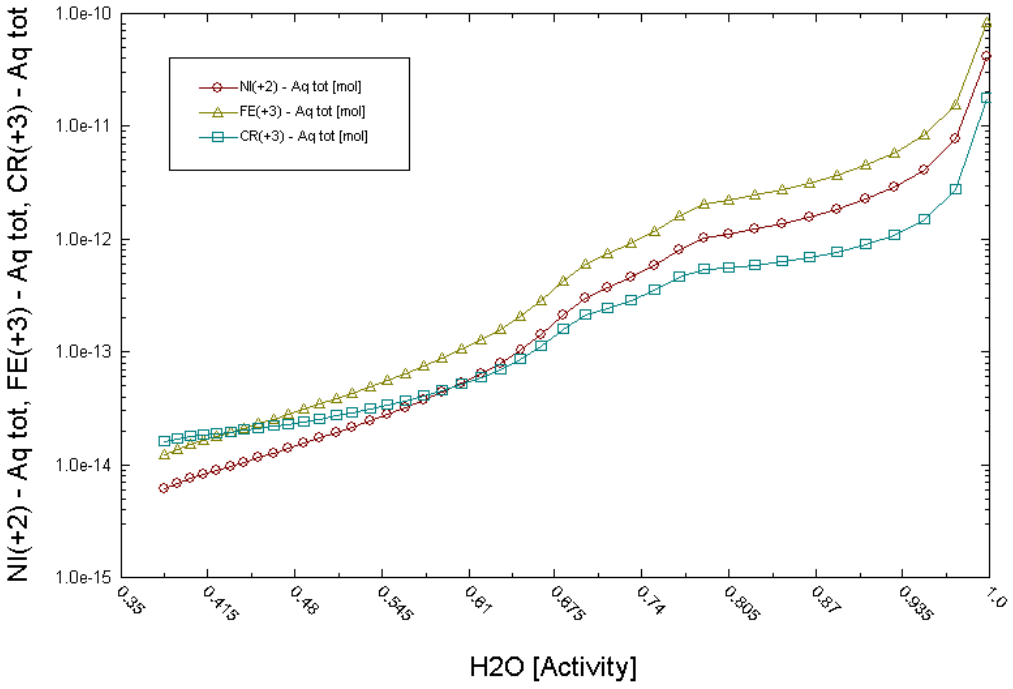
MSE Corrosion database was added to the model. MSE aqueous model was specified. The two solids, CrO(OH) and NiFe2O4, were added to the list of reactants (given 1 mole each).

The following figures show the calculated solubilities of CrO(OH) and NiFe2O4 as plots of total aqueous concentrations of nickel, iron, and chromium as a function of water activity (or relative humidity):

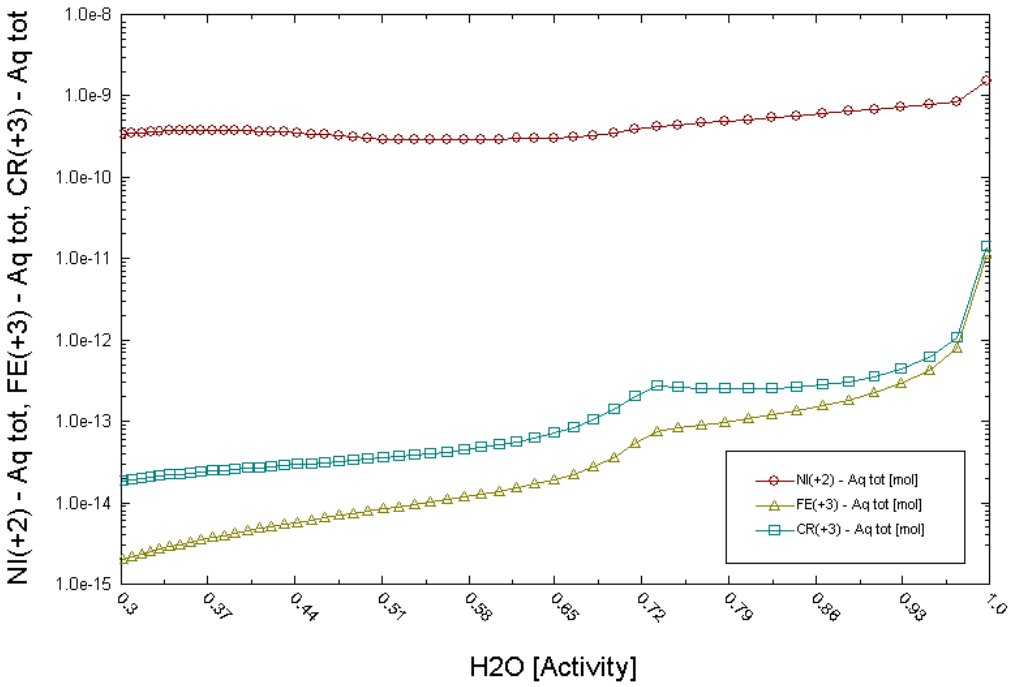
Porewater sample ESF-Thermalk-017/26.5-26.9/UC:



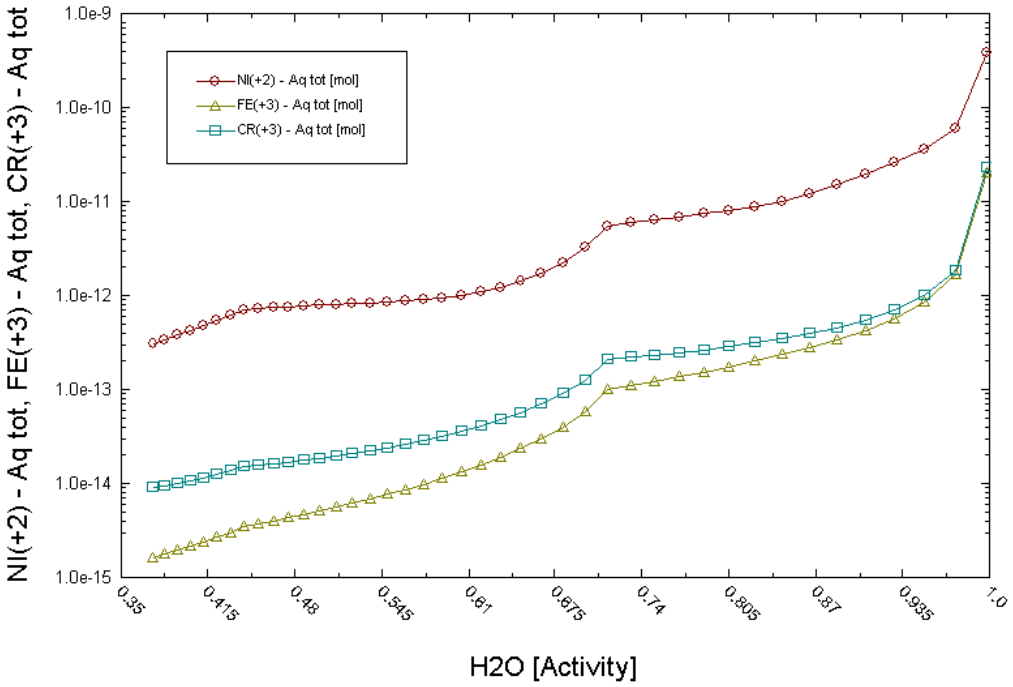
Porewater sample SD-9/1184.7-1184.8/UC:



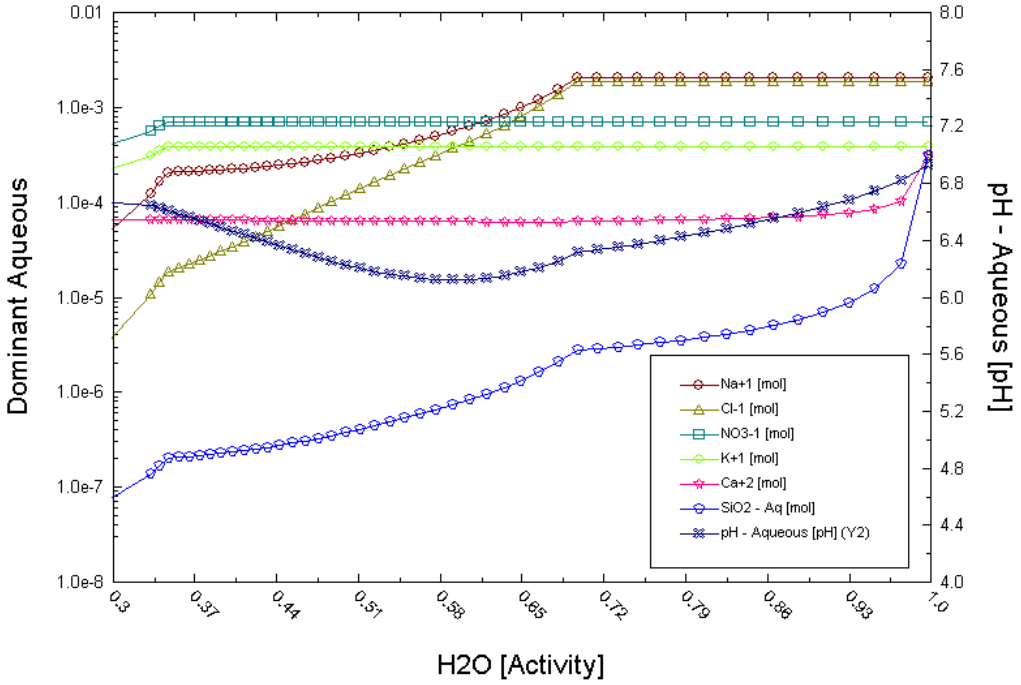
Porewater sample ESF-HD-PERM-3/34.8-35.1/Alcove 5:



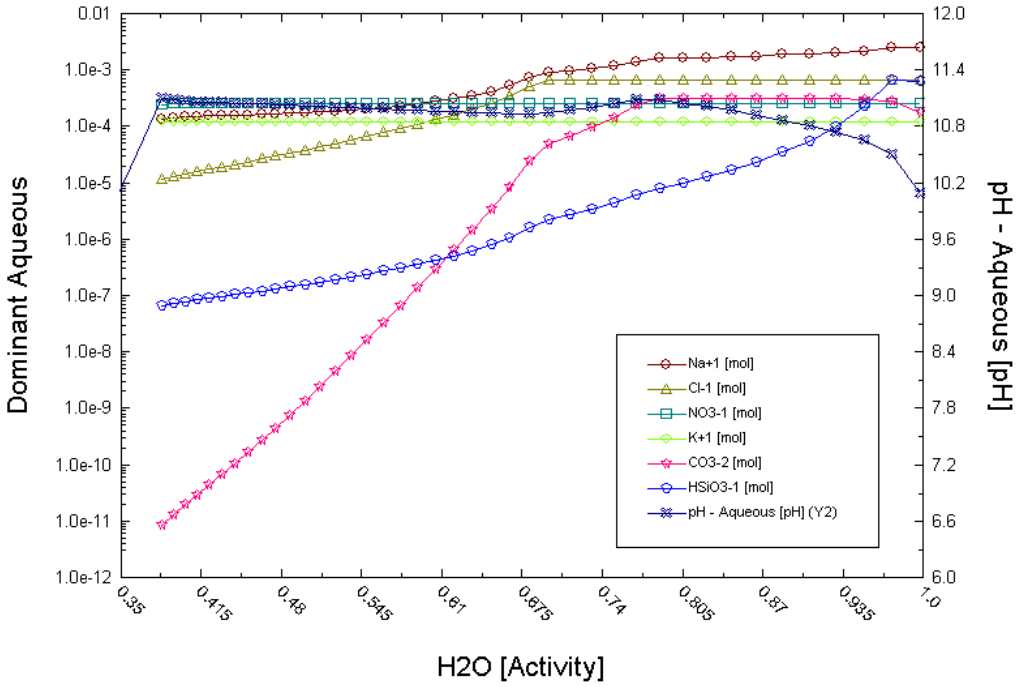
Porewater sample HD-PERM-3/56.7-57.1/UC:



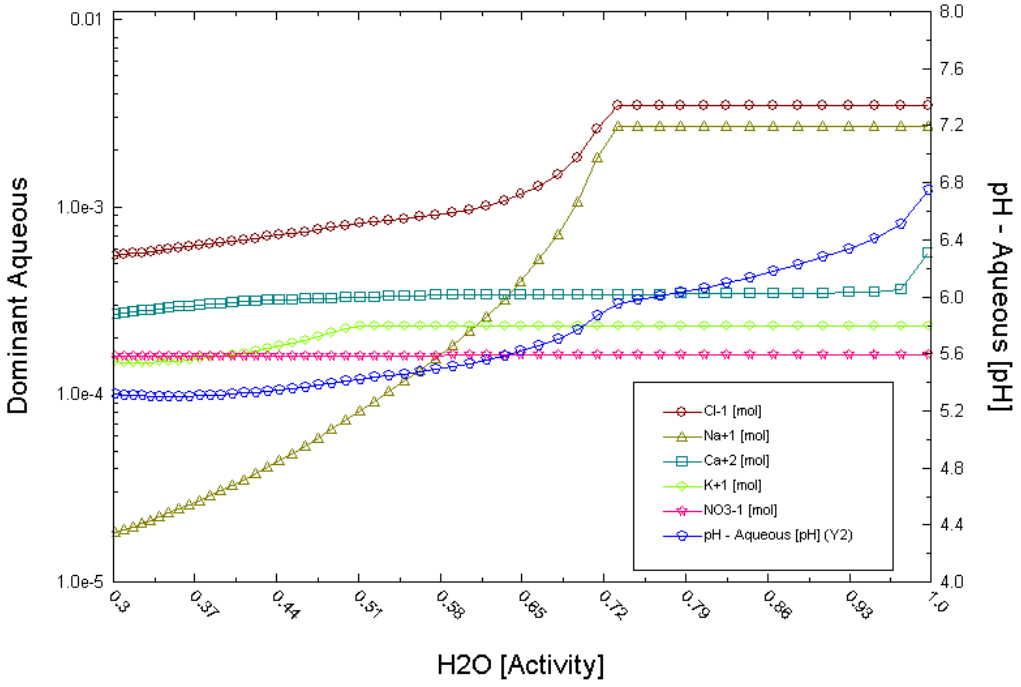
The following figures plot the pH and dominant aqueous species for porewater sample ESF-Thermalk-017/26.5-26.9/UC:



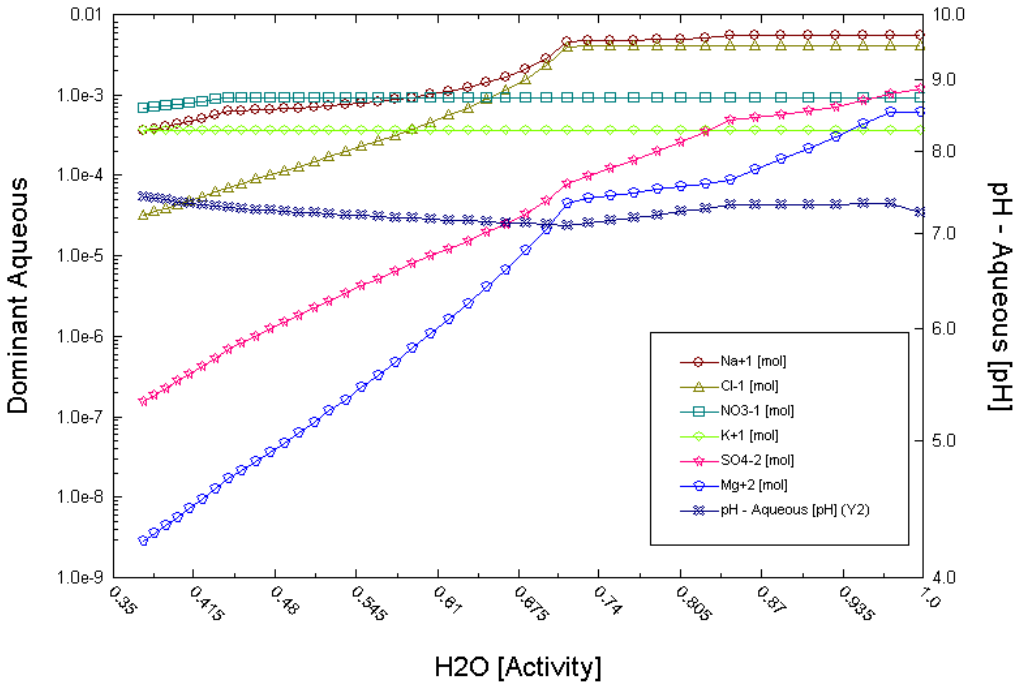
pH and dominant aqueous species for porewater sample SD-9/1184.7-1184.8/UC:



pH and dominant aqueous species for porewater sample ESF-HD-PERM-3/34.8-35.1/Alcove 5:



pH and dominant aqueous species for porewater sample HD-PERM-3/56.7-57.1/UC:



From: Helean, K. "Engineered Barrier System: Physical and Chemical Environment." ANL-EBS-MD-000033, Revision 06. Las Vegas, Nevada: Sandia National Laboratories. 2007.

SELECTION OF TSW PORE WATERS

Previously, the chemistry of the near field was evaluated using five starting waters, selected as being representative of the available pore-water analyses at the time. However, in recent years, additional analyses have become available, and, to ensure that the range of pore-water compositions was being adequately represented, all currently available TSw pore-water analyses (125) have been compiled and re-evaluated. This process is graphically depicted in Figure 6.6-1.

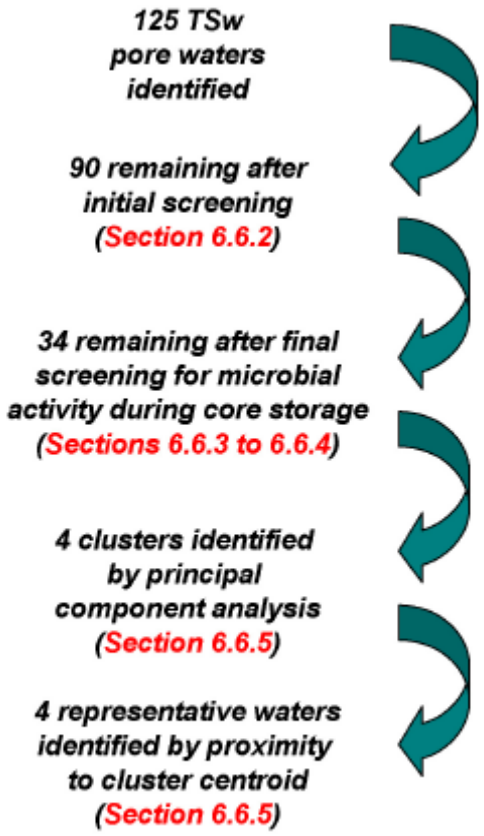


Figure 6.6-1. Diagram Showing the Flow of the Pore-Water Down-Selection Process

First, an initial screening of incomplete pore-water analyses and those not considered representative of current ambient conditions was carried out, reducing the total to 90 analyses. When the remaining analyses were examined, discrepancies in the data were identified and ultimately linked to biological processes occurring in the cores during core storage. Criteria for evaluating the degree of modification by microbial processes were developed and used to screen out affected waters, reducing the total to 34. The statistical method of principle component analysis was then used to determine the number of chemically distinct clusters represented by the remaining water analyses (4), and representative waters from each group were chosen by selecting those nearest to the cluster centroid. All waters identified as being minimally affected by microbial activity provide feeds to the P&CE models in the form of chloride:nitrate ratios sampled by TSPA; the four representative water compositions are used as starting water compositions for

EQ3/6 calculations of diluted and evaporated seepage water compositions within the drift, which are provided to TSPA by the P&CE abstraction models.

Table 6.6-3. Representative Waters for Each of the Four Water Groups Used in Developing NFC Model Starting Waters

Group	# Waters	Representative Water
1	21	SD-9/1184.7-1184.8/UC
2	7	ESF-THERMALK-017/26.5-26.9/UC
3	3	ESF-HD-PERM-3/34.8-35.1/Alcove 5
4	3	HD-PERM-3/56.7-57.1/UC

MessageFrom: Andre Anderko [aanderko@olisystems.com]
Sent: Thursday, May 08, 2008 3:55 PM
To: rpabalan@cnwra.swri.edu
Cc: 'Berthold'
Subject: RE: Corrosion Analyzer MSE vs H+

Bobby:

Yes, we used solubility data (primarily those of Ziemniak et al. from 1998) to parameterize the parameters for CrOOH in MSE. I am attaching a spreadsheet that shows the results of our calculations. We have both Cr(OH)3 and CrOOH in MSE. Cr(OH)3 is metastable but it precipitates primarily at lower temperatures. CrOOH is stable and is obtained primarily at higher temperatures. In the aqueous model, we have literature thermochemical properties for Cr2O3 (we did not derive them ourselves from solubility data).

Best regards,

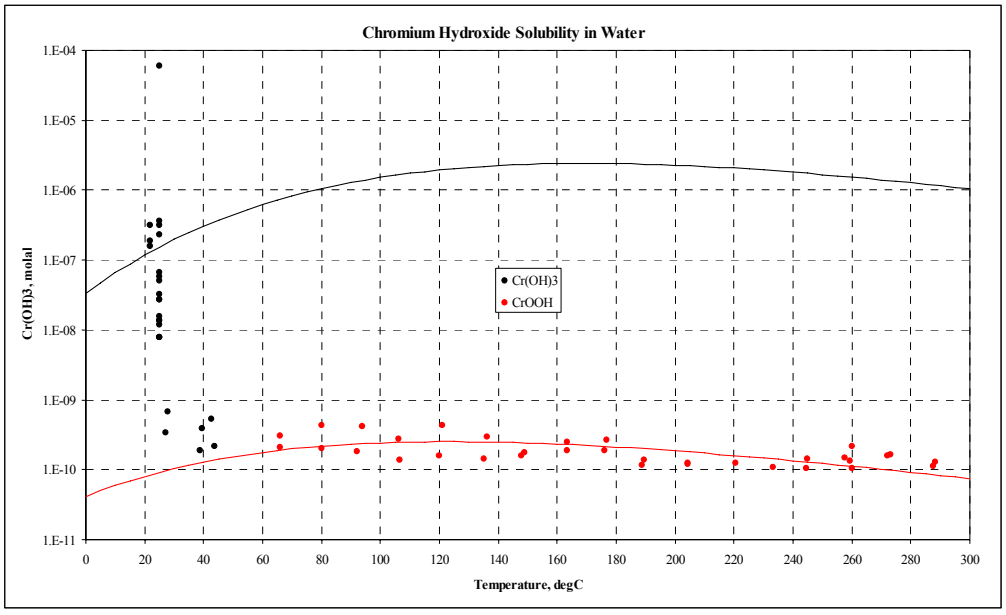
Andre

From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Thursday, May 08, 2008 3:50 PM
To: 'Andre Anderko'
Cc: 'Berthold'
Subject: RE: Corrosion Analyzer MSE vs H+

Andre,

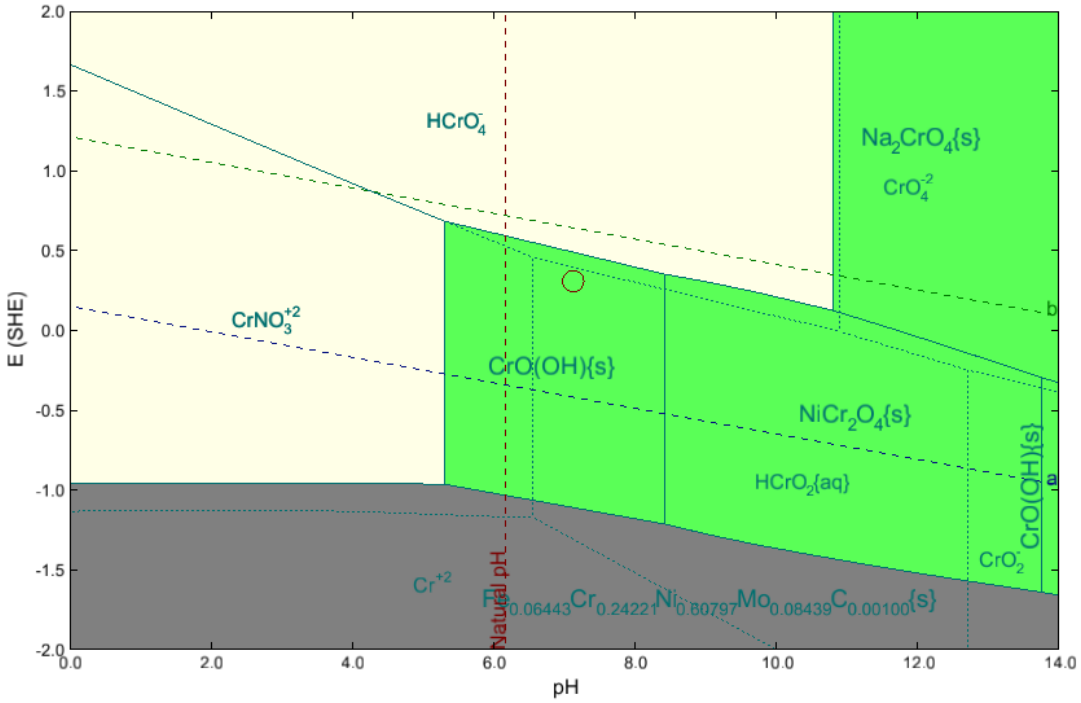
Just to follow up. When I use MSE, the chromium solid that is stable is CrO(OH), as opposed to Cr2O3 when I use the Aq. H+ model. Does it mean the MSE model was parameterized using solubility data for CrO(OH)?

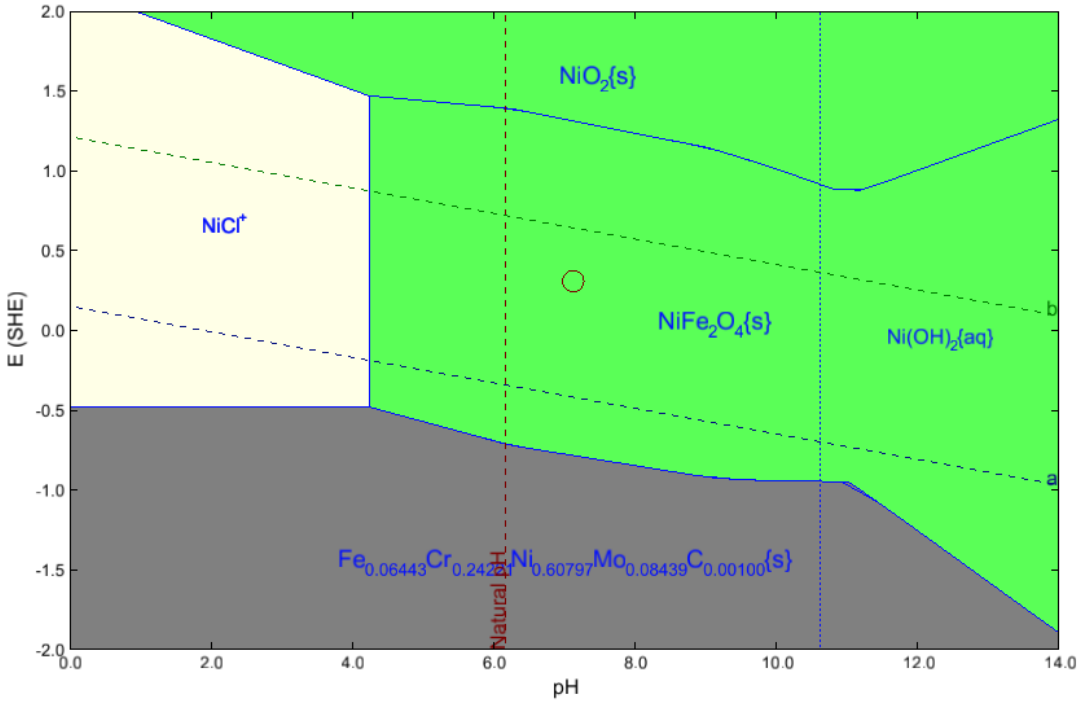
Thanks. -- Bobby

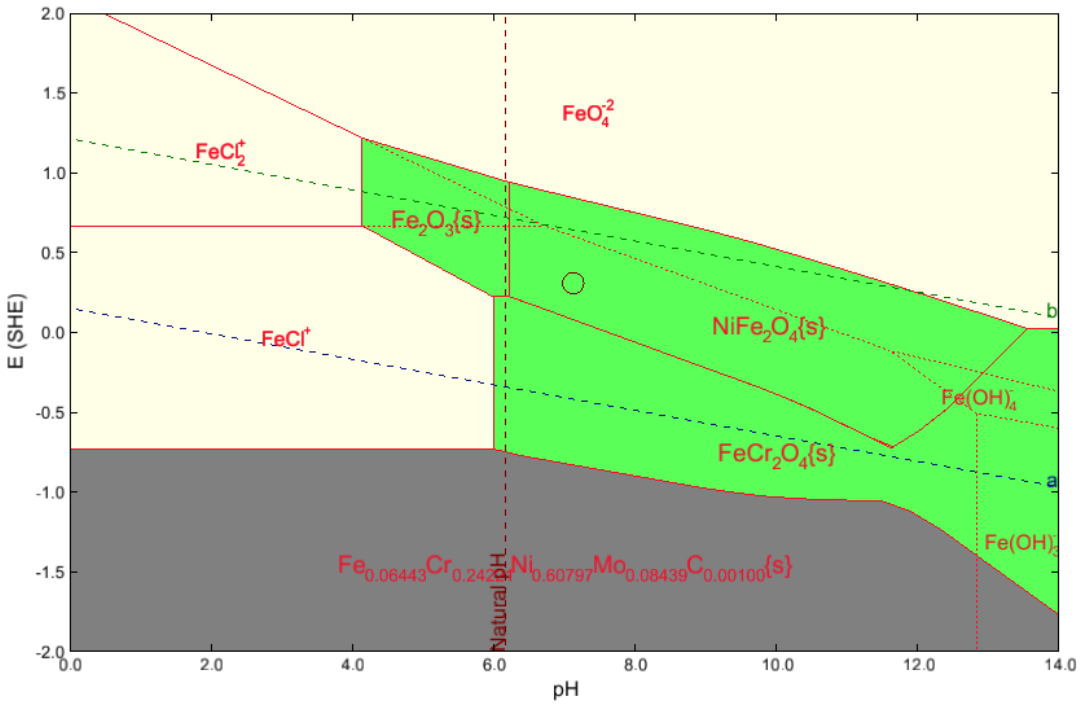


May 9, 2008

The following are stability diagrams of Alloy 22 at 130 °C in contact with a brine saturated with three salts NaCl, NaNO3, and KNO3. The diagrams were calculated using CorrosionAnalyzer Version 2.0.






E (SHE)
pH
FeO4-2
FeCl2+
Fe2O3(s)
NiFe2O4(s)
FeCl+
Fe(OH)4
FeCr2O4(s)
Fe(OH)2
Fe0.06443Cr0.24274Ni0.60797Mo0.08439C0.00100(s)
Natural pH
b
a

THERMODYNAMIC EVALUATION OF THE STABILITY OF ALLOY 22 PASSIVE OXIDE FILMS IN GEOLOGIC REPOSITORY ENVIRONMENTS

CorrosionAnalyzer Version 2.0 was used to calculate the following stability diagrams of Alloy 22 in contact with pure water at 25 °C. For clarity, the stability fields for the chromium and nickel subsystems are plotted separately. The shaded areas of the plots are where either the metal is stable or a stable oxide film can form. Figures 1(a) and 1(b) show the stability of chromium and nickel, respectively, in the Alloy 22 relative to the stability of water.

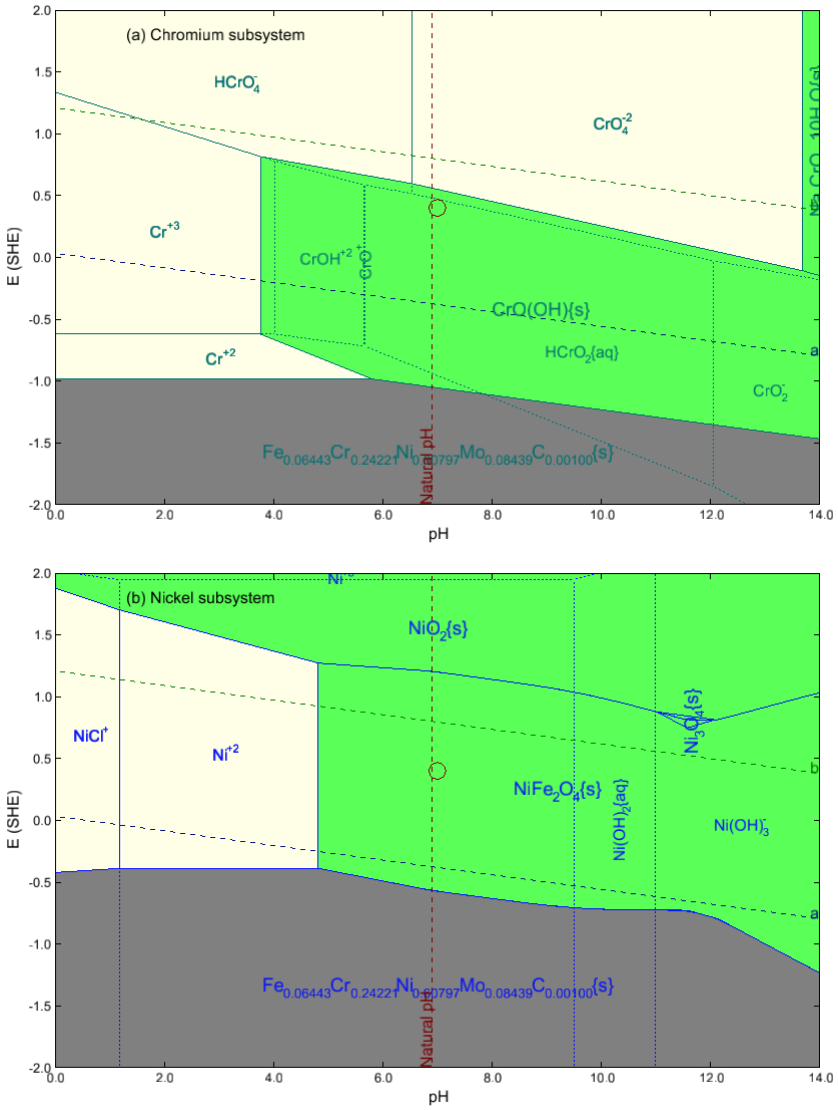


Figure 1. Stability Diagrams at 25 °C for (a) Chromium and (b) Nickel in Alloy 22 in Contact with Pure Water. CrO(OH) and $NiFe_2O_4$ Are Stable Over Wide Ranges of pH and Oxidation/Reduction Potential (E_{SHE}).

The above figures indicate that over a wide range of pH and oxidation/reduction potential, two solids, CrO(OH) and $NiFe_2O_4$ are stable. These solids possibly represent the passive film protecting Alloy 22 from corrosion.

As part of investigations into the long-term stability of passive films on Alloy 22, thermodynamic calculations were conducted on the solubility of CrO(OH) and $NiFe_2O_4$ under various physical and chemical conditions. Two scenarios relevant to a potential repository for high-level nuclear waste were investigated: (i) seepage scenario and (ii) dust deliquescence scenario. The former represents a situation in which percolating water above the repository seeps into the drift and contacts the Alloy 22 waste package material. The higher temperature of the waste package surface will cause evaporation of seepage water to occur, which will increase the ionic strength of the aqueous phase and result in precipitation of various minerals. This situation occurs when the drift wall temperature falls below the boiling point of water (96 °C at the elevation of the potential repository at Yucca Mountain, Nevada) such that percolating water is able to penetrate the "boiling isotherm" and enter the repository drift. The other scenario represents a situation in which salts present in dusts that deposited on the waste package surface deliquesces to form a brine phase. This situation can occur even at temperatures above the boiling point of water because some salt mixtures can deliquesce at higher temperatures.

Seepage Scenario

The first scenario was investigated using CorrosionAnalyzer Version 2.0 by calculating the solubilites of CrO(OH) and $NiFe_2O_4$ at 95 °C as a function of degree of evaporation of seepage water. Four water compositions were used to represent the compositions of seepage water that enters the repository drift. These four compositions, which are listed in Table 1, were selected by DOE to represent the more than 100 compositions determined for pore waters in the stratigraphic horizon where the potential Yucca Mountain repository is located. DOE used the four compositions to develop its near-field chemical model and evaluate the potential chemistry of water entering the repository drift. In this study, the degree of evaporation was varied by decreasing stepwise the relative humidity of the system over the range of 100 to 30 percent. With decreasing relative humidity, the ionic strength of the aqueous phase increases and various minerals precipitate. The increase in ionic strength, change in aqueous concentrations, and mineral precipitation with decreasing relative humidity are illustrated in Figure 2. The solubilities of CrO(OH) and $NiFe_2O_4$ were calculated at each stepwise change in relative humidity and corresponding change in water chemistry.

Table 1. Chemical Compositions (mg/L) of Four Pore Waters Used to Represent Seepage Water Chemistry. Values Taken From Helean (2007)

	Pore Water Identification			
	ESF-Thermalk-017/26.5-26.9/UC	SD-9/1184.7-1184.8/UC	HD-PERM-3/56.7-57.1/UC	ESF-HD-PERM-3/34.8-35.1/Alcove 5
Na^+	45	59	123	62
K^+	14.4	4.8	13.8	9
Mg^{2+}	7.9	0.7	16.7	17.4
Ca^{2+}	62	19	59.9	97
Cl^-	67	23	146	123
SO_4^{2-}	82	16	126	120
HCO_3^-	126	142	149	—
NO_3^-	44	16	57.4	10
F^-	1.4	2.2	1.3	0.76
SiO_2	52	42	—	75

The calculated solubilities of CrO(OH) and NiFe2O4 in the four water compositions are plotted in Figure 3 as a function of degree of evaporation. As shown in the figure, the solubilities are very low, consistent with negligible corrosion rates measured for Alloy 22 under similar temperatures and chemical conditions. The calculated values suggest these phases can form protective barriers to the corrosion of Alloy 22 in scenarios involving evaporation of seepage waters.

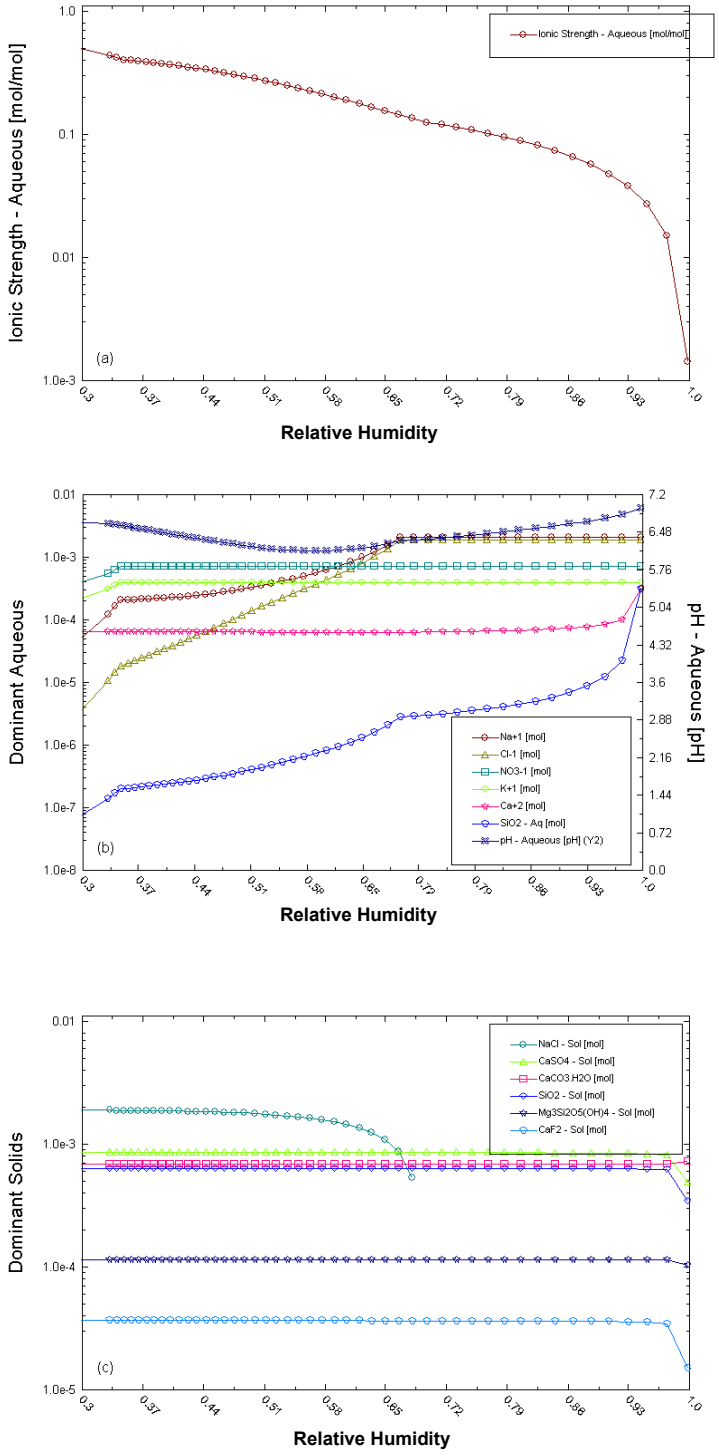


Figure 2. (a) Increase in Ionic Strength, (b) Change in pH and Concentration of Dominant Aqueous Species, and (c) Dominant Minerals That Precipitate Upon Evaporation at 95 °C of Initially Dilute Pore Water (Sample ESF-Thermalk-017/26.5-26.9/UC). Decreasing Amount of H_2O (Leftward on the X-Axis) Corresponds to Increasing Degree of Evaporation.

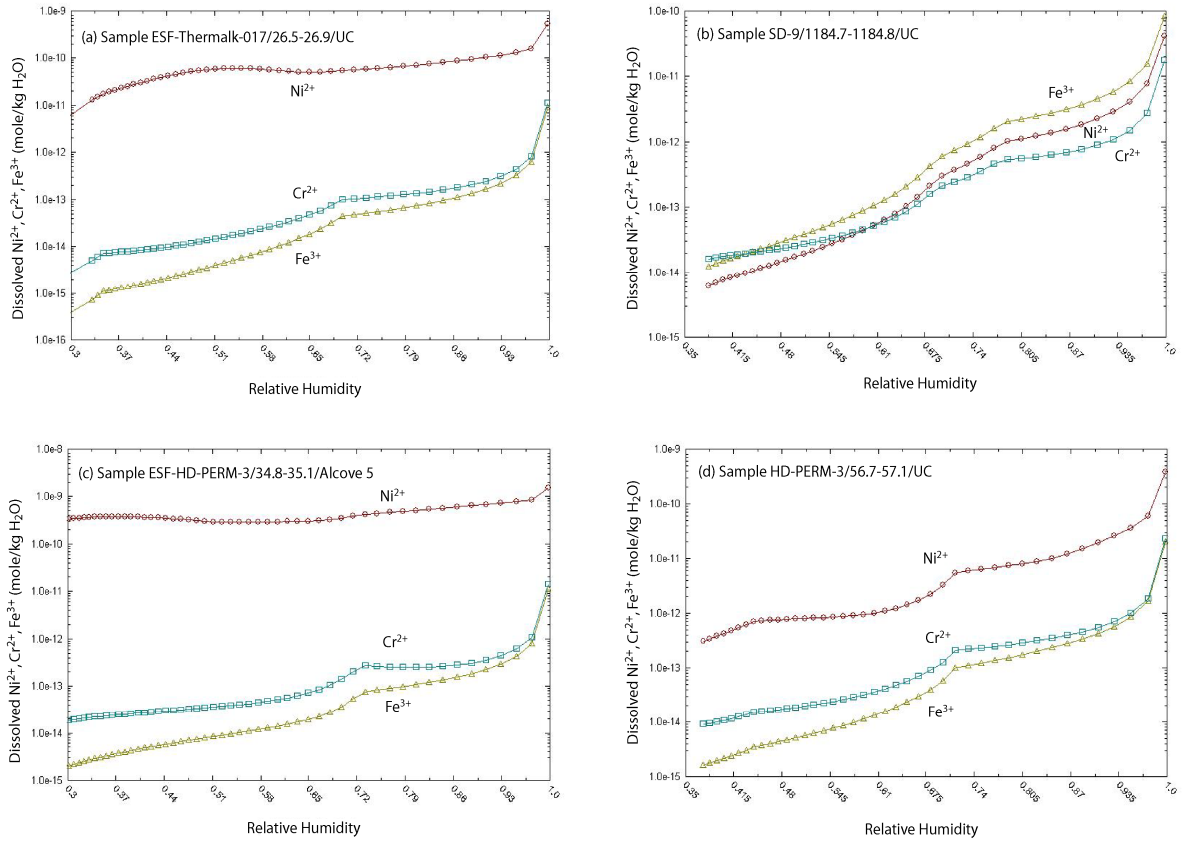


Figure 4. Calculated solubilities of CrO(OH) and $NiFe_2O_4$ at 95 °C in brines formed by evaporation of initially dilute seepage waters. Decreasing relative humidity (leftward on the x-axis) corresponds to increasing degree of evaporation.

Dust Deliquescence Scenario

Deliquescence is a process in which a soluble substance sorbs water vapor from the air to form a saturated aqueous solution. At the potential high-level waste repository at Yucca Mountain, Nevada, deposition of aerosols and dusts entrained in ventilation air and evaporation of groundwater seeping into the drifts of the potential repository could lead to the accumulation of hygroscopic salts on the waste package surface. The deliquescence of these salts, which would occur when the relative humidity in the environment is at or above the deliquescence relative humidity of the salt mixture, could form brines potentially corrosive to the waste package material. Formation of these brines could affect the performance of the waste package during the repository time period when the drift wall temperature is above the boiling point of water and seepage water is unlikely to enter the repository drift. During this time, corrosion of the Alloy 22 waste package material could be facilitated by the elevated temperature of the system if corrosive brine contacts the waste package surface.

To assess the stability of passive oxide films on Alloy 22 in the presence of dust deliquescence brines, CorrosionAnalyzer Version 2.0 was used to calculate the solubility of CrO(OH) and $NiFe_2O_4$ in contact with these brines. Of particular interest are brines that form from

deliquescence of $NaCl–NaNO_3–KNO_3$ salt mixtures because these have very low deliquescence relative humidity. These salt mixtures are considered by DOE to be salt assemblages that could control the deliquescence of dusts deposited inside the drift of the potential Yucca Mountain repository (BSC, 2005). Experiments conducted by DOE suggest that $NaCl–NaNO_3–KNO_3$ brines can form at temperatures exceeding 190 °C [374 °F] (BSC, 2005).

For this study, the calculation was done for a temperature of 130 °C and over the pH range 3.5 to 9.0. The temperature and pH range used in the calculation were selected to permit comparison with Alloy 22 corrosion rate data measured by Yang, et al. (2008) using a multielectrode array sensor. In that study, the corrosion rate of Alloy 22 was measured as a function of pH and the test temperature varied from 124 to 134 °C [255 to 273 °F]. In the thermodynamic calculation, the brine was specified to be saturated with the three salts NaCl, $NaNO_3$, and KNO_3, and also with the metal (hydr)oxides CrO(OH) and $NiFe_2O_4$. The pH was varied by addition of HCl or NaOH. At these conditions, the brine is very concentrated, with calculated concentrations of sodium, potassium, chloride and nitrate ions equal to 47, 59, 3, and 103 moles/kg H_2O, respectively.

The calculated solubilities are plotted in Fig. 6 as total dissolved concentrations of nickel, chromium, and iron versus pH. The figure shows that the dissolved nickel, chromium, and iron concentrations are relatively constant at pHs higher than 5.0. However, there is a steep increase in solubility with decreasing pH below a pH ~4.5. This trend in increased concentration with decreasing pH is consistent with the corrosion rates of Alloy 22 measured by Yang et al. (2008), which are shown in Fig. 7.

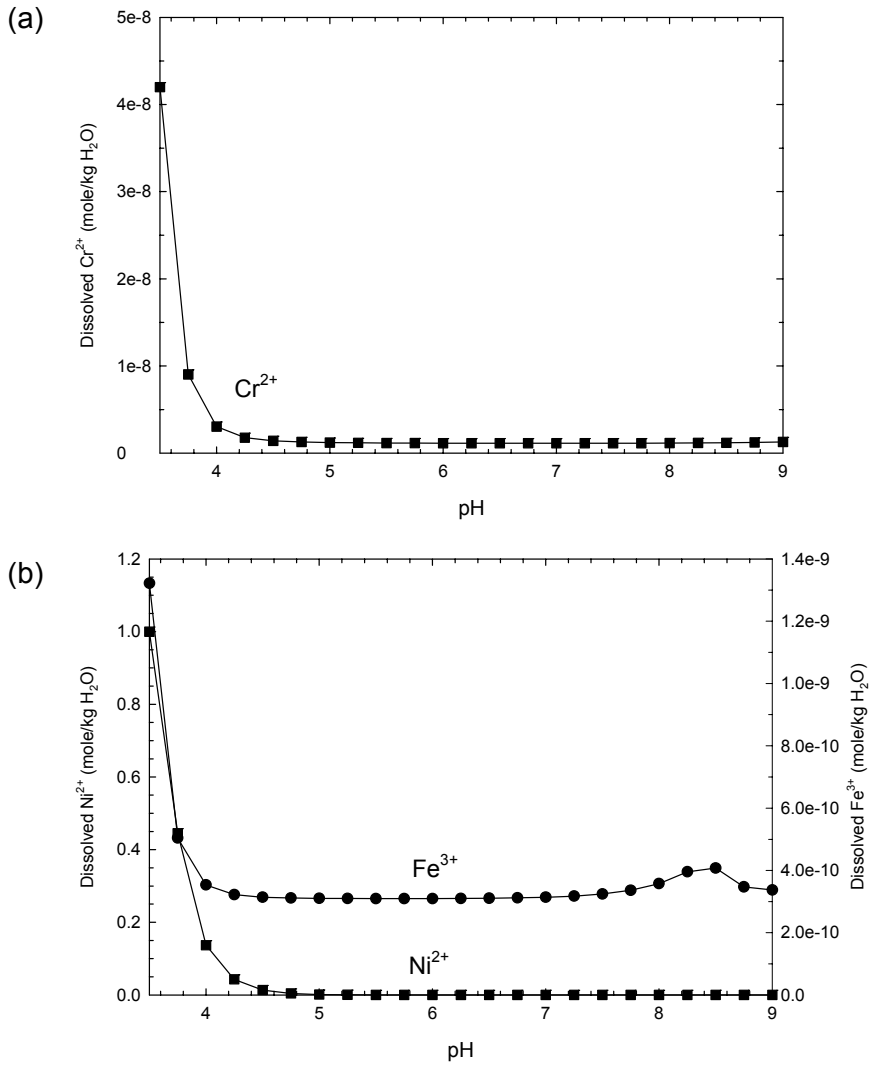


Figure 6. Calculated solubility of (a) CrO(OH) and (b) $NiFe_2O_4$ at 130 °C as a function of pH in brines saturated with NaCl, $NaNO_3$, and KNO_3.

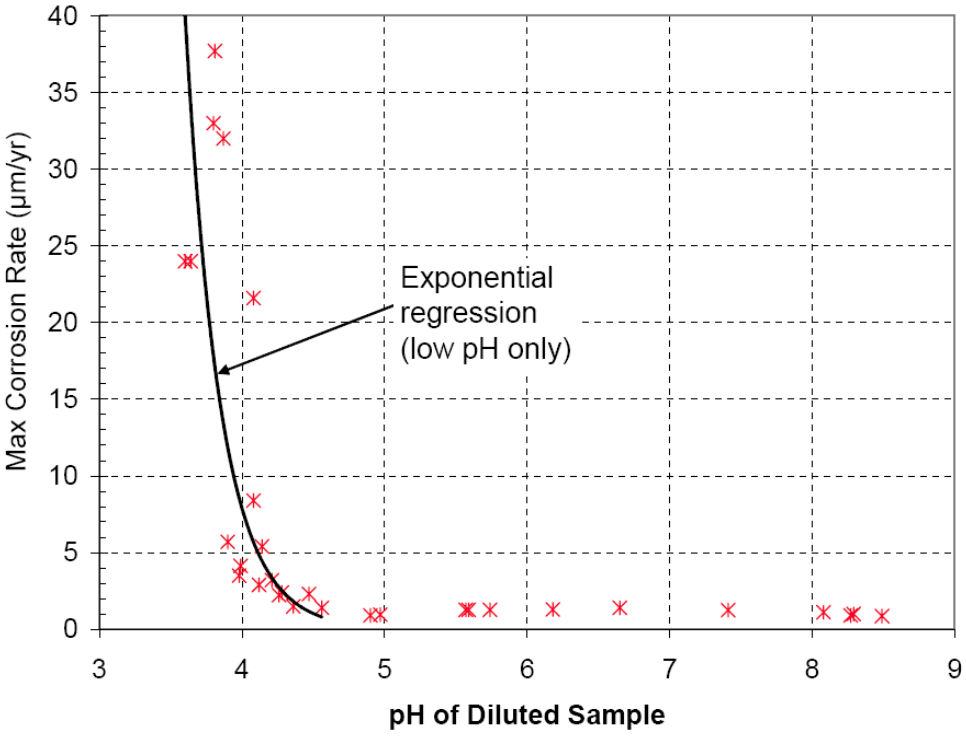
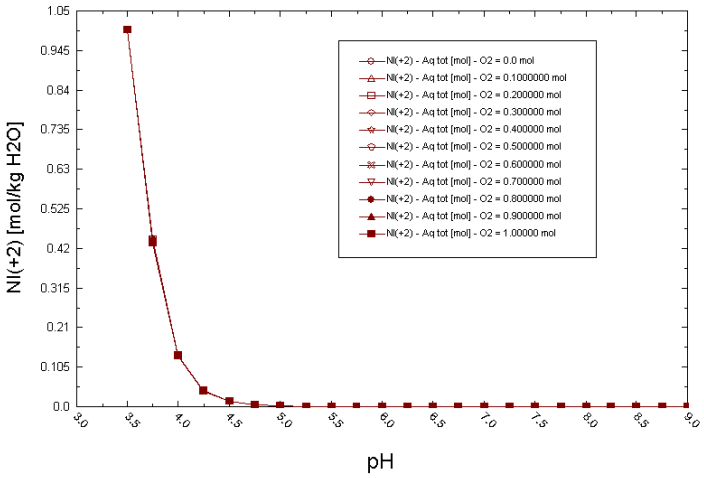
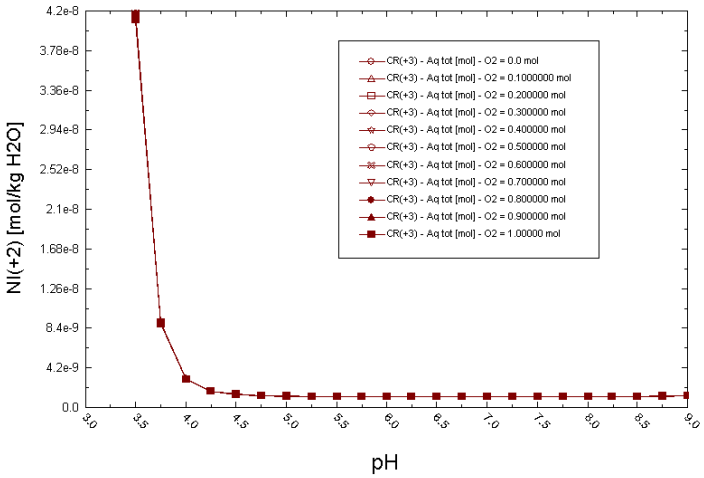


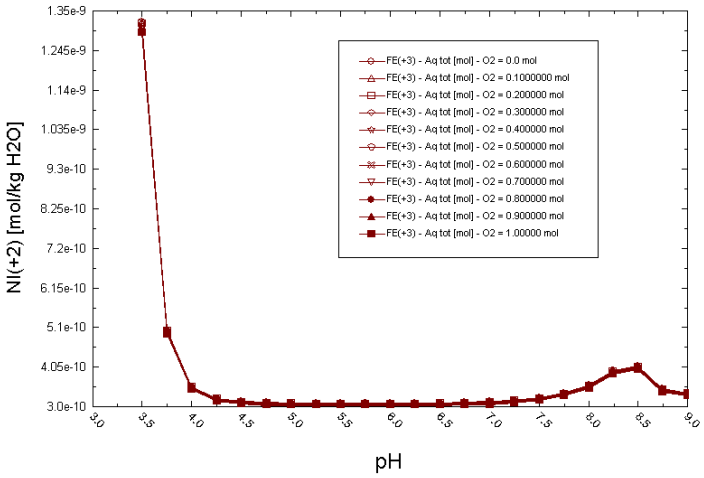
Figure 7. Relationship Between Corrosion Rates of the Alloy 22 Specimens Exposed to the Liquid Phase and the pH of the Diluted Samples From the Liquid Phase (Yang, et al., 2008)

May 12, 2008

To determine if the presence of oxygen will have an influence on the calculated solubility of CrO(OH) and NiFe2O4, a dual survey calculation (vs pH AND O2 amount) was done. The O2 amount was specified to range from 0 to 1 mole. The following are the calculated solubilities.

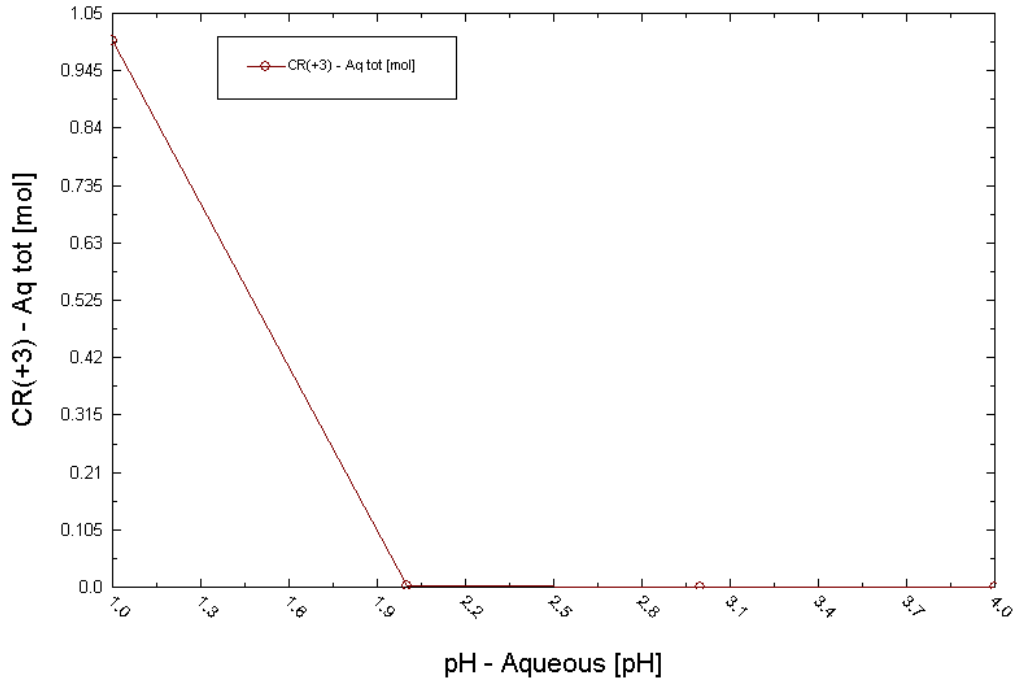




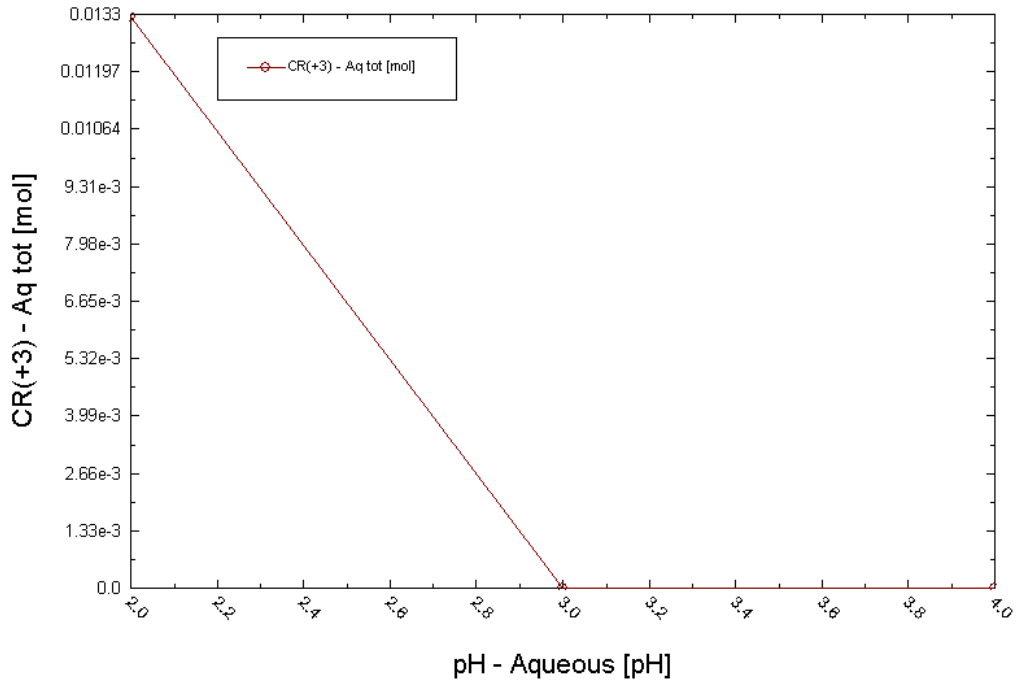


These figures indicate the addition of oxygen does not have a significant effect on the calculated solubility of CrO(OH) and NiFe2O4. The likely reason is the low solubility of oxygen brine solution, approximately 1.6×10^{-3} moles/kgH2O, based on the CorrosionAnalyzer Report.

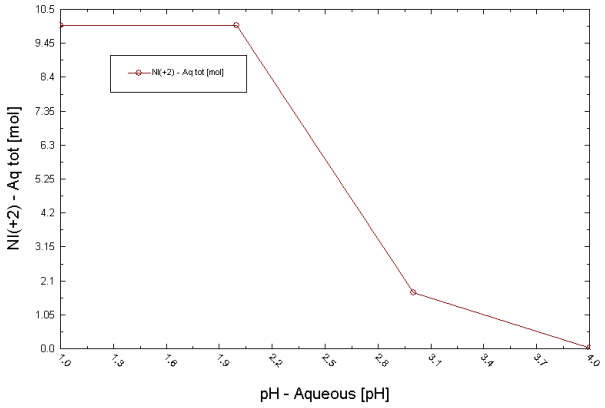
CrO(OH) solubility, 90 C, 1 m NaCl, HCl added

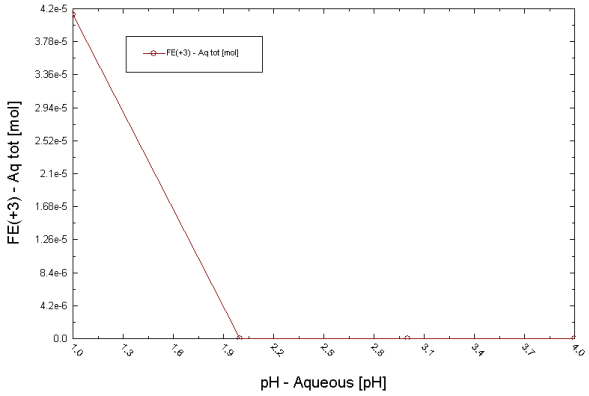


CrO(OH) solubility, 90 C, 1 m NaCl, HNO3 added

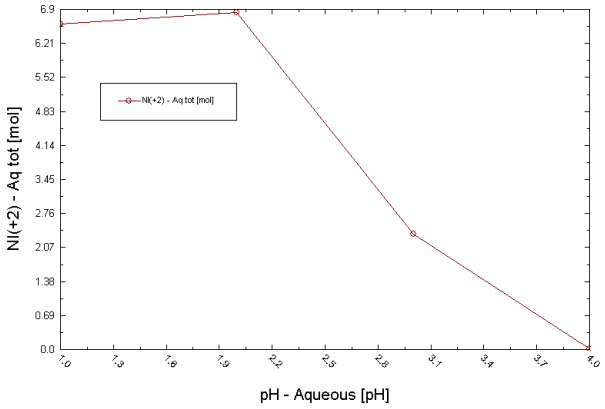


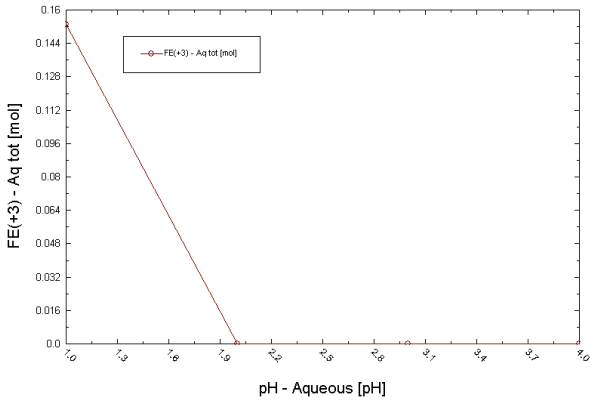
NiFe2O4 solubility; 90 C, HNO3 added



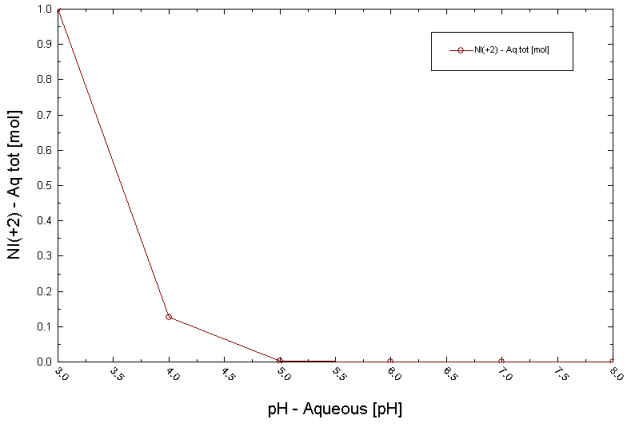


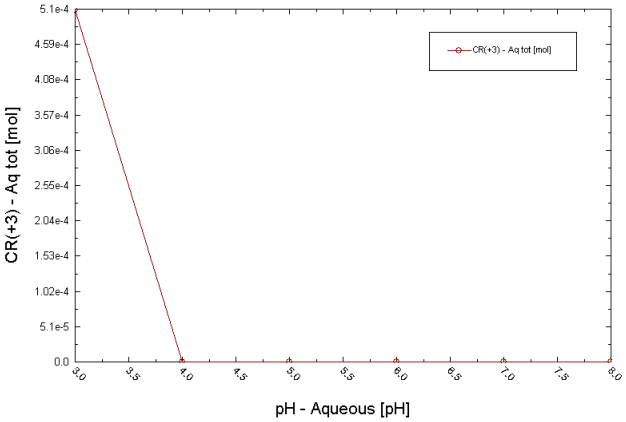
NiFe2O4 solubility; 90 C, HCl added

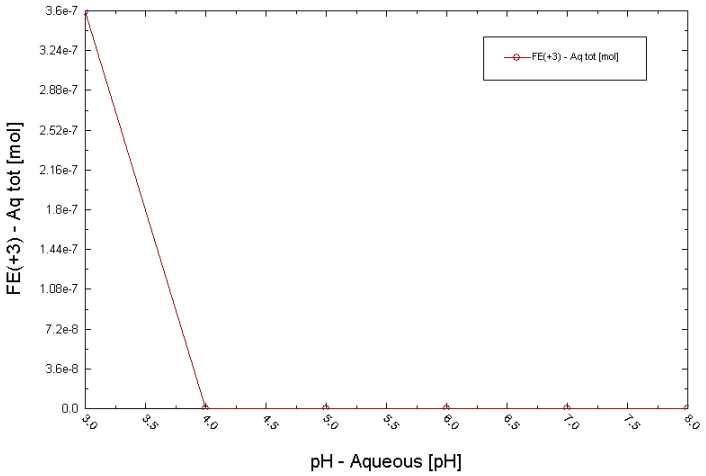




NiFe2O4 and CrO(OH) solubility in 18 m CaCl2 + 9 m Ca(NO3)2 at 155 C

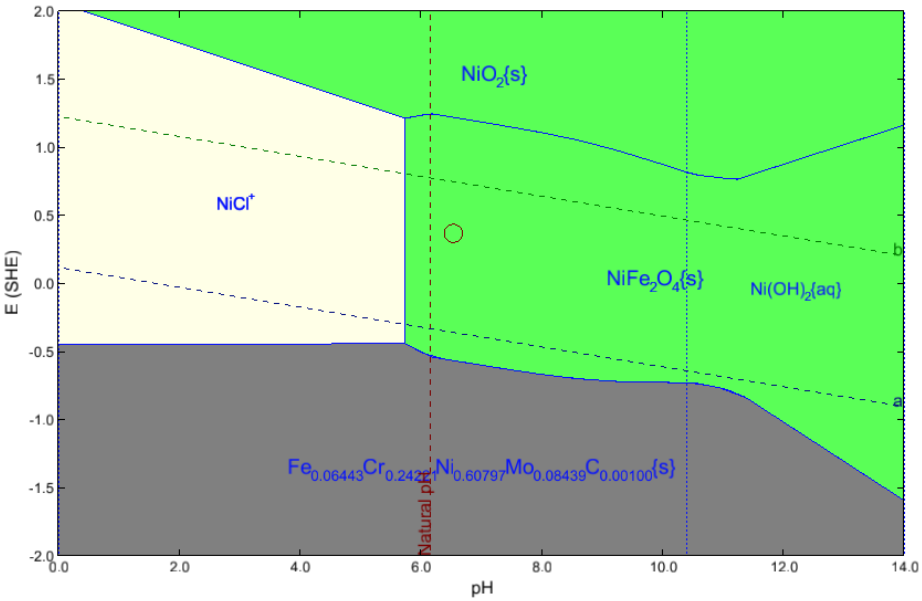


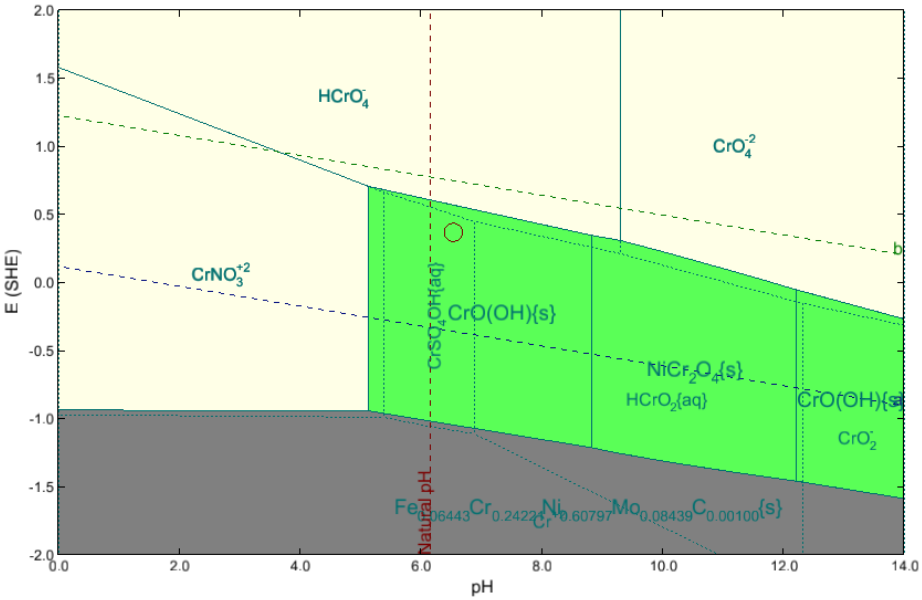


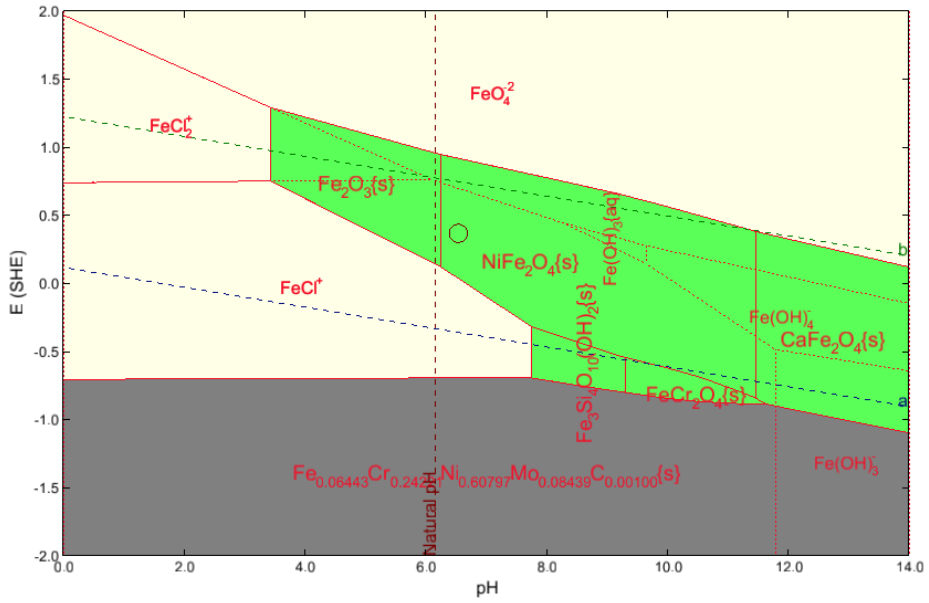

FE(+3) - Aq tot [mol]
3.6e-7
3.24e-7
2.88e-7
2.52e-7
2.16e-7
1.8e-7
1.44e-7
1.08e-7
7.2e-8
3.6e-8
0.0
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
pH - Aqueous [pH]

May 13, 2008

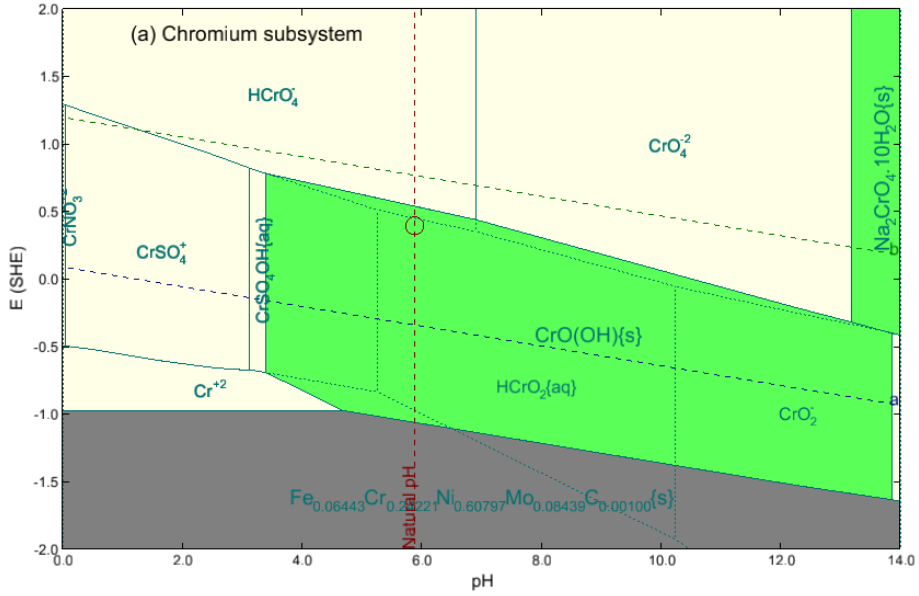
Stability diagram of Alloy 22 in contact with porewater ESF-Thermalk-017/26.5-26.9/UC; 95 C; P = 0.310224 atm

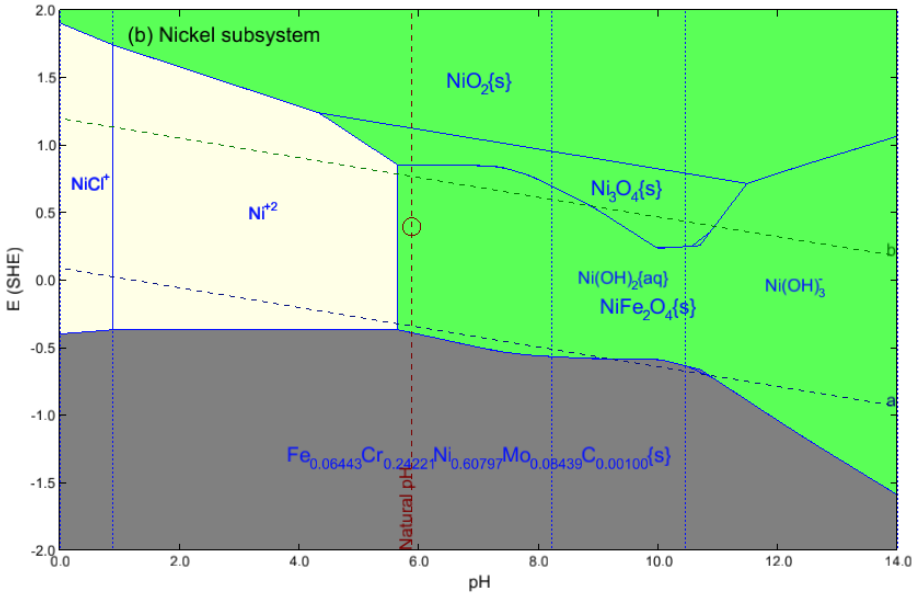


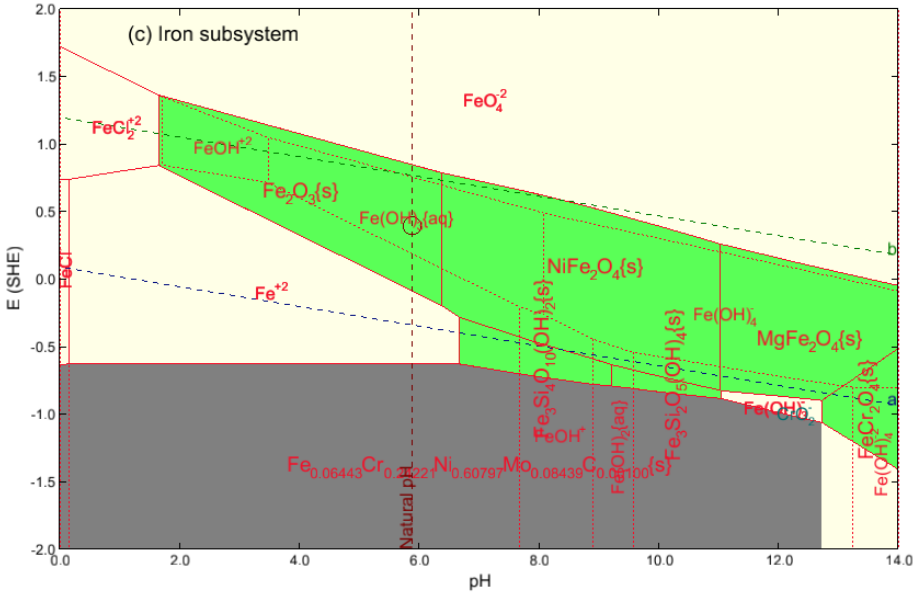




Stability diagram of Alloy 22 in contact with porewater ESF-Thermalk-017/26.5-26.9/UC; 95 C; P = 0.85 atm




(b) Nickel subsystem
NiO2{s}
NiCl+
Ni+2
Ni3O4{s}
Ni(OH)2{aq}
Ni(OH)3-
NiFe2O4{s}
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH


(c) Iron subsystem
FeO4-2
FeCl2+2
FeOH+2
Fe2O3{s}
Fe(OH)3{aq}
FeCl+
Fe+2
NiFe2O4{s}
Fe(OH)4-
MgFe2O4{s}
Fe3Si4O10(OH)2{s}
Fe3Si2O5(OH)4{s}
Fe(OH)3{aq}
FeOH+
FeCr2O4{s}
Fe(OH)4+
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH

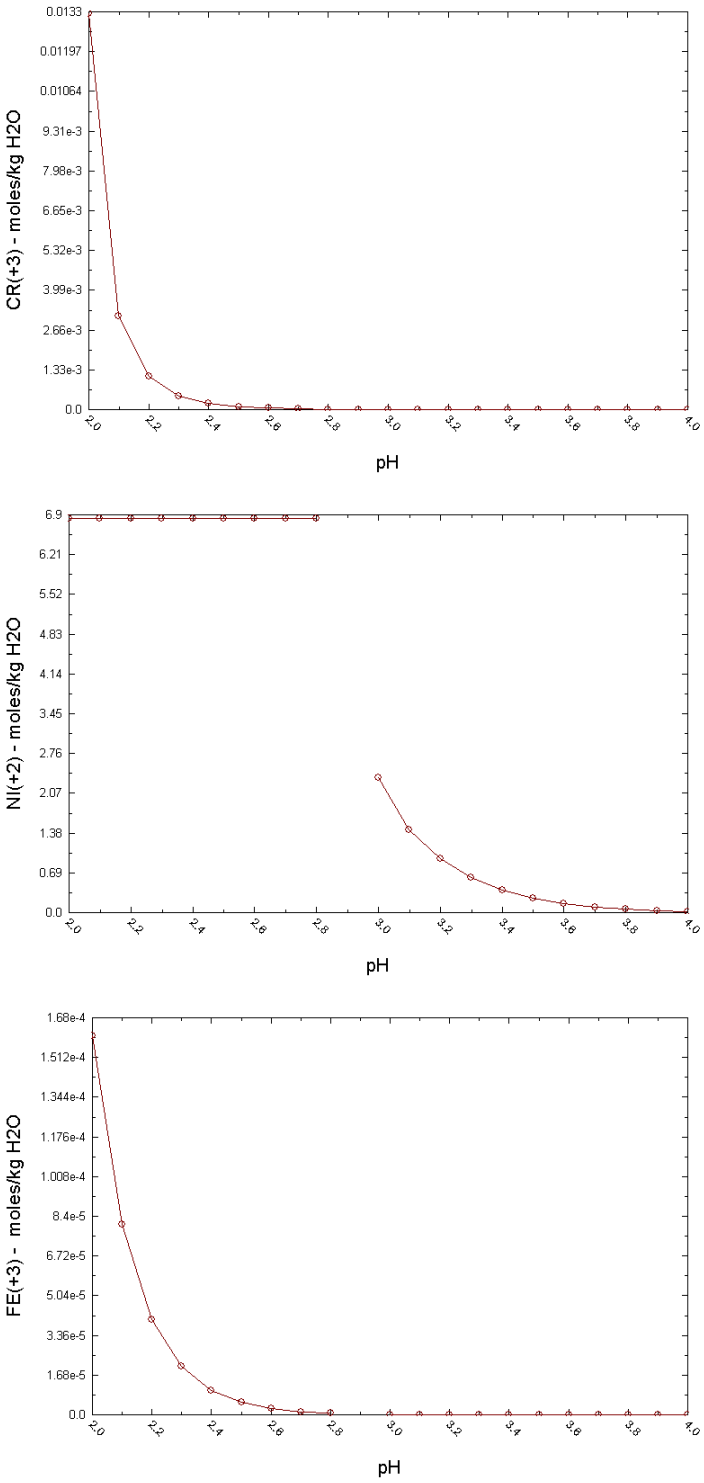
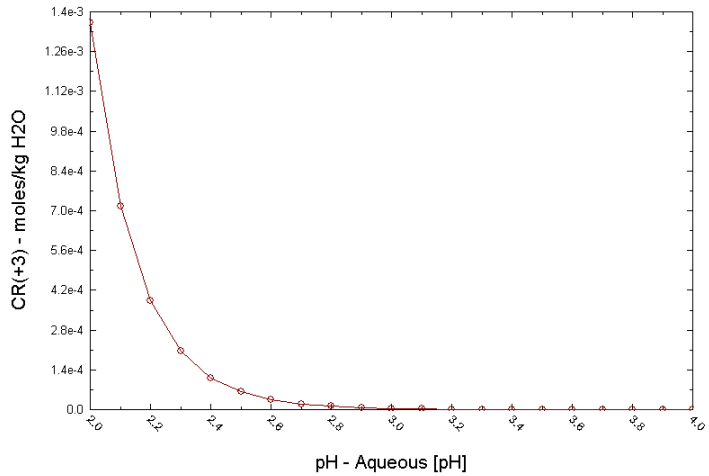


Figure X. Calculated solubilities at 90 °C [203 °F] of CrO(OH) [Fig. X(a); moles chromium per kg H_2O] and $NiFe_2O_4$ [Fig. X(b) and X(c); moles nickel and iron per kg H_2O] in 1 mole per kg H_2O NaCl with HNO_3 added to adjust the pH.



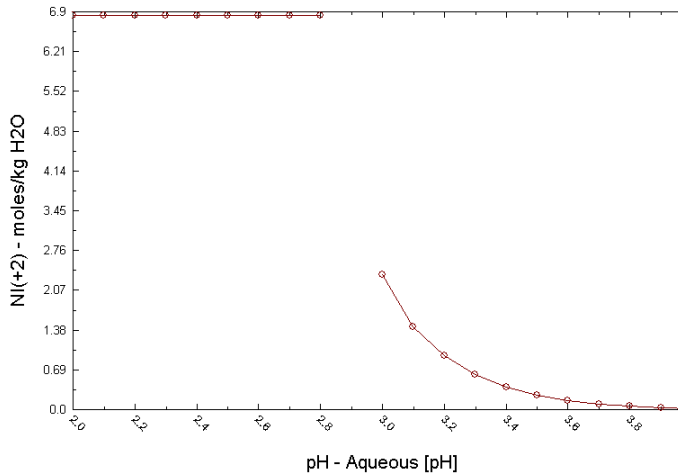
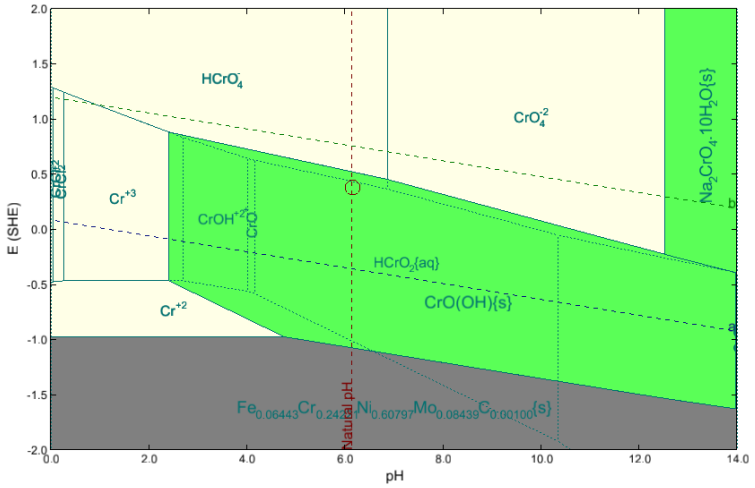
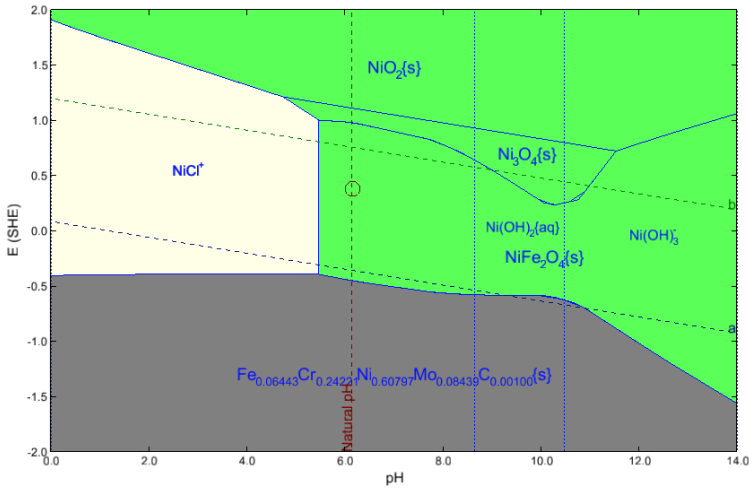
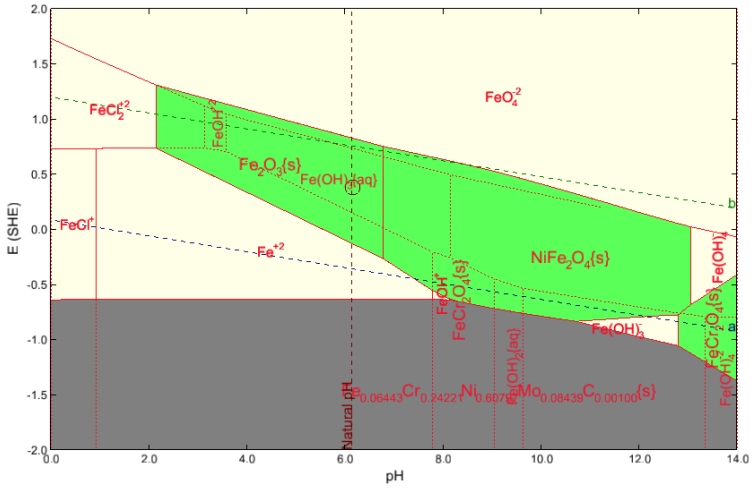


Figure Y. Calculated solubilities at 90 °C [203 °F] of CrO(OH) [Fig. X(a); moles chromium per kg H_2O] and H_2O] in 1 mole per kg H_2O NaCl with HCl added to adjust the pH.

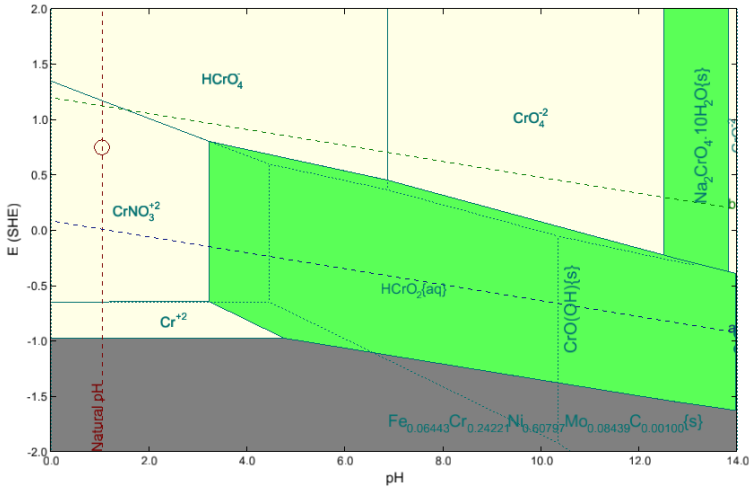
Pourbaix diagram of Alloy 22 in 1 m NaCl solution at 90 C:

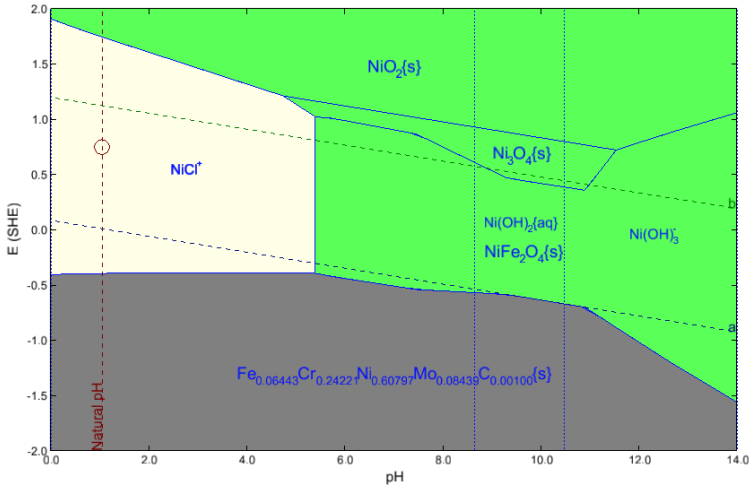


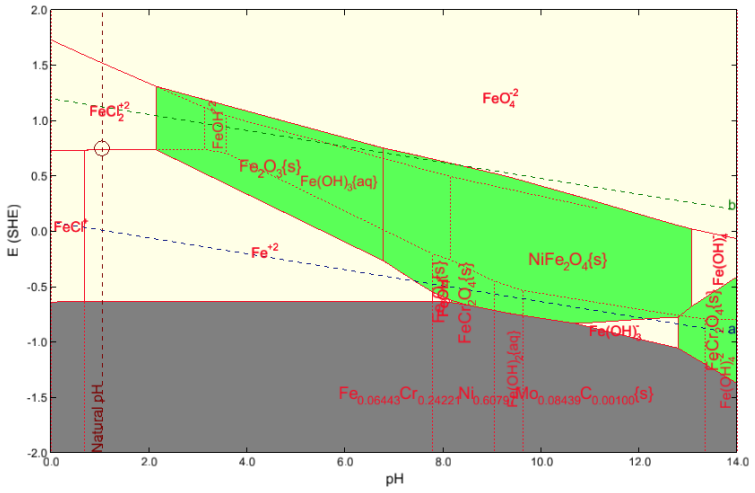

NiO2{s}
NiCl+
Ni3O4{s}
Ni(OH)2{aq}
Ni(OH)3-
NiFe2O4{s}
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH


FeO4-2
FeCl2+2
FeOH+
Fe2O3{s}
Fe(OH)2+aq
FeCl+
Fe+2
NiFe2O4{s}
FeOH+
FeCr2O4{s}
Fe(OH)2{aq}
Fe(OH)3-
Fe(OH)4
FeCr2O4{s}
Fe(OH)3
Fe0.06443Cr0.24221Ni0.60797Mo0.08439C0.00100{s}
Natural pH
E (SHE)
pH

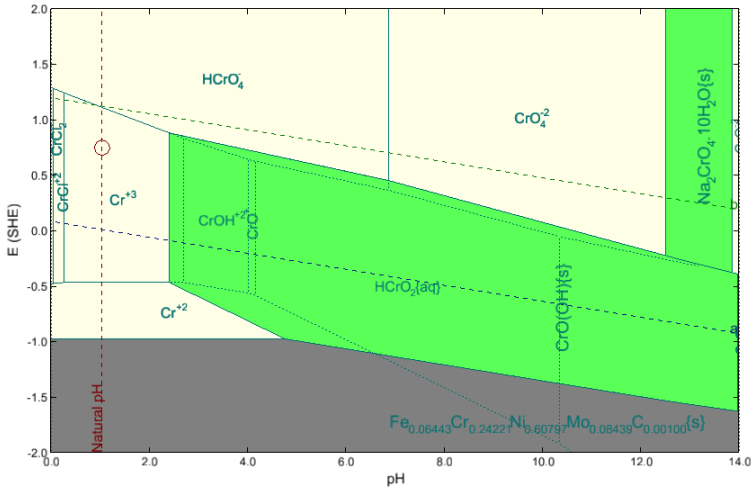
Pourbaix diagram of Alloy 22 in 1 m NaCl + 0.1 m HNO3 solution at 90 C:

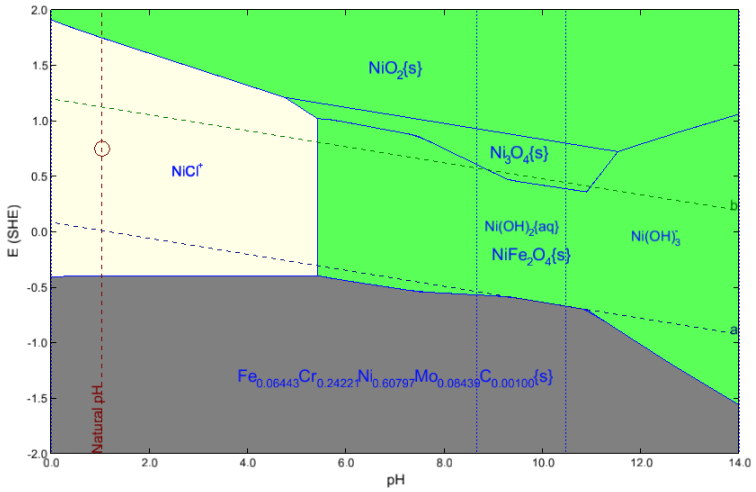


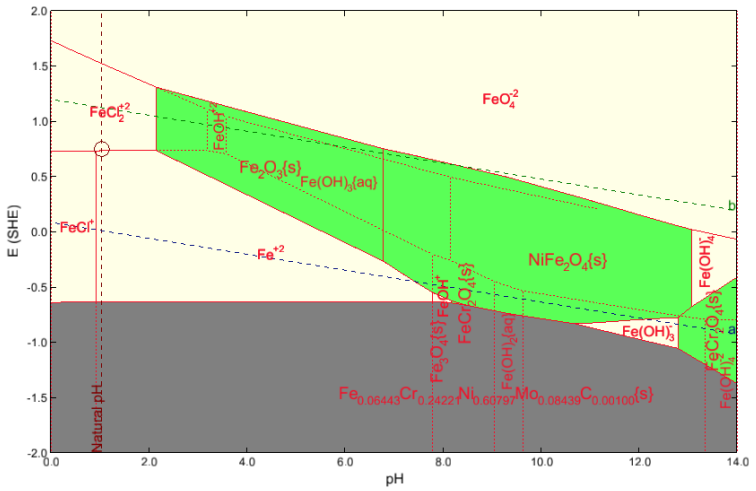




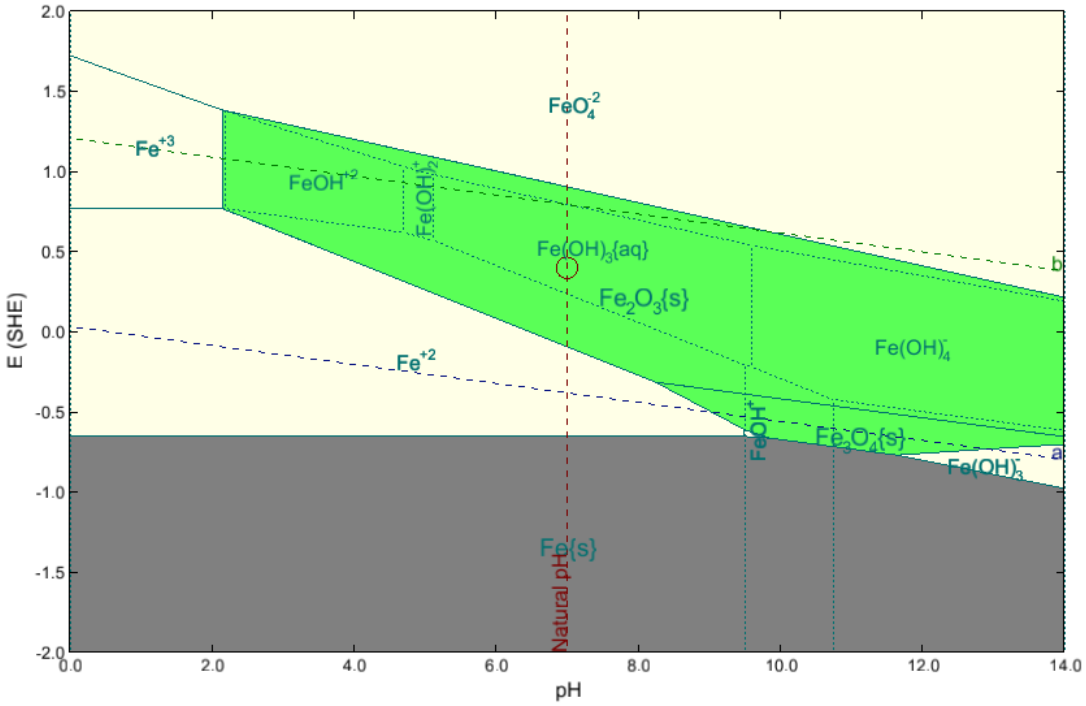
Pourbaix diagram of Alloy 22 in 1 m NaCl + 0.1 m HCl solution at 90 C:



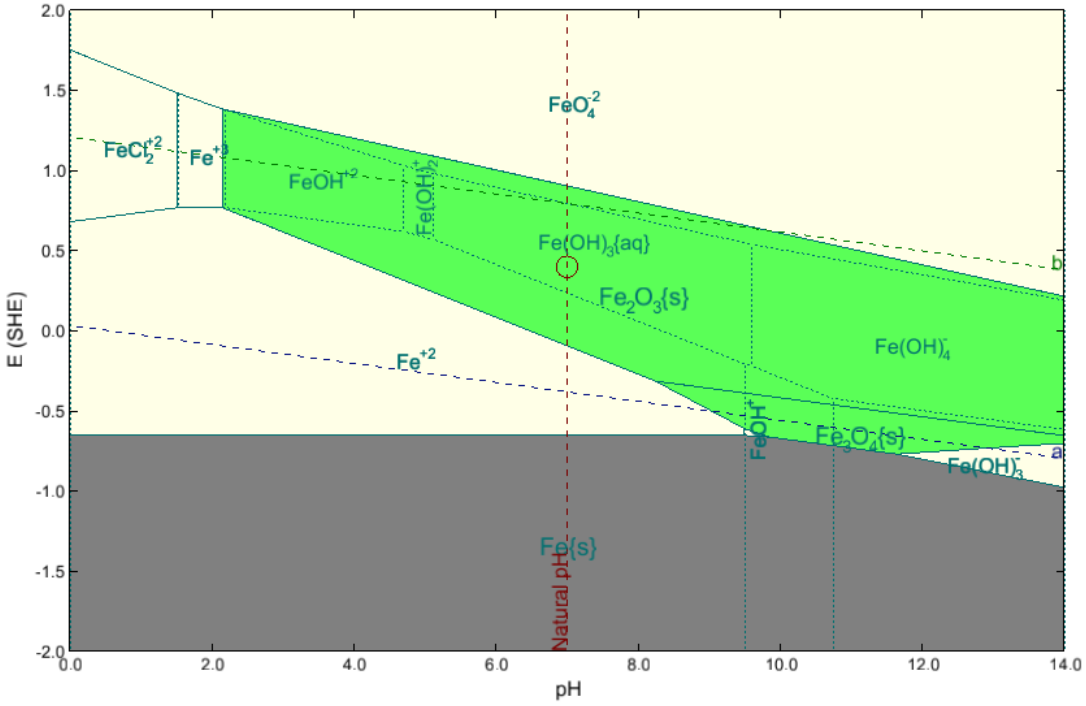




Fe – HNO3



Fe – HCl



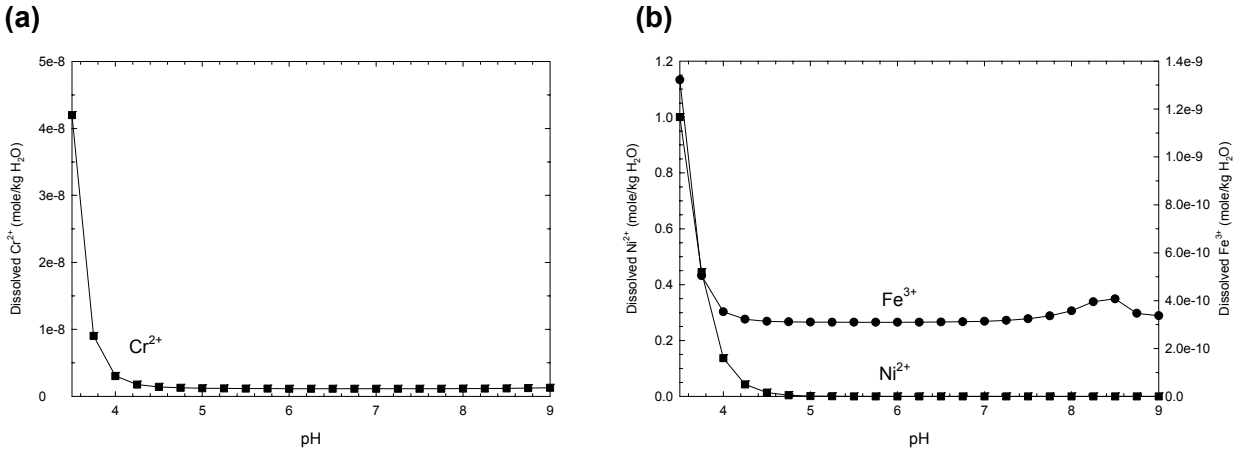


Figure 6. Calculated solubility of (a) CrO(OH) and (b) $NiFe_2O_4$ at 130 °C as a function of pH in brines saturated with NaCl, $NaNO_3$, and KNO_3.

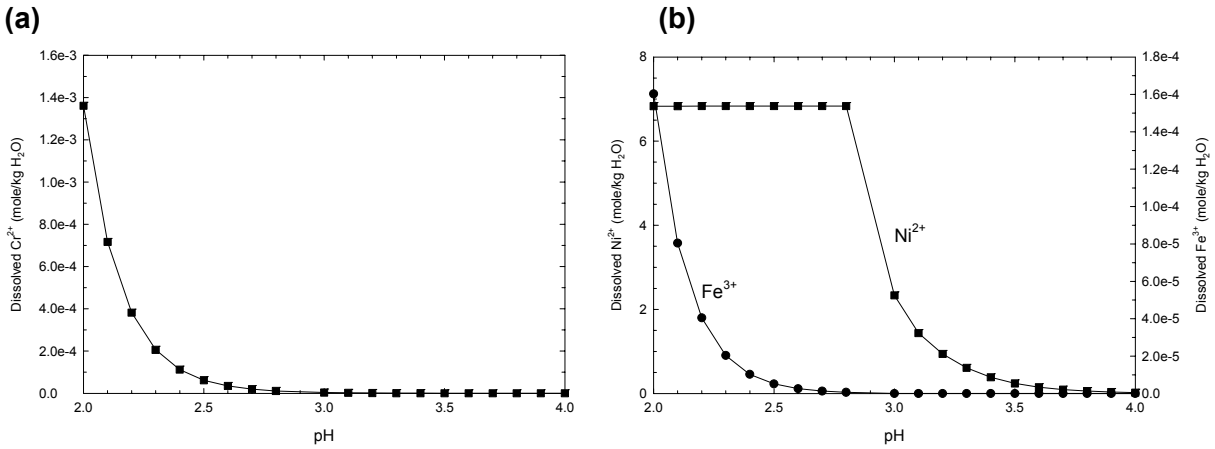


Figure 7. Calculated solubility of (a) CrO(OH) and (b) $NiFe_2O_4$ in 1 m NaCl solution with HCl added to adjust the pH.

June 11, 2008

The following table is from p. 2.3.5-173 of the DOE License Application:

Table 2.3.5-5. Representative Pore-Water Compositions for the Four Groups, Used as Inputs for the Near-Field Chemistry Model

Sample ID		SD-9/ 1184.7-1184.8/UC	ESF-THERMALK-017/ 26.5-26.9/UC	ESF-HD-PERM-3/ 34.8-35.1/Alcove 5	HD-PERM-3/ 56.7-57.1/UC
Lithostratigraphic Unit		Tptpll	Tptpul	Tptpmn	Tptpmn
Water designation		Gp1	Gp2	Gp3	Gp4
Members in Group		21	7	3	3
Parameter	Units	Values			
pH (meas.)	pH	8.2	7.7	8.31	—
Na^+	mg/L	59	45	62	123
K^+	mg/L	4.8	14.4	9	13.8
Mg^{2+}	mg/L	0.7	7.9	17.4	16.7
Ca^{2+}	mg/L	19	62	97	59.9
Cl^-	mg/L	23	67	123	146
SO_4^{2-}	mg/L	16	82	120	126
HCO_3^-	mg/L	142	126	—	149
NO_3^-	mg/L	16	44	10	57.4
F^-	mg/L	2.2	1.4	0.76	1.3
SiO_2(aq)	mg/L	42	52	75	—

Source: SNL 2007b, Tables 4.1-3, 6.6-3.

The following was taken from page 2.3.5-39 of the DOE License Application:

2.3.5.3.3.2.2 Starting Pore-Water Compositions

Prior to using the representative pore-water compositions described in Section 2.3.5.3.2.2.1, the compositions were charge balanced using the EQ3/6 thermodynamic speciation and solubility code. This was accomplished by adjusting the H^+ concentrations while fixing the bicarbonate concentration to be in equilibrium with a partial pressure of CO_2 of 10^{-3} bars, the typical ambient partial pressure throughout the Topopah Spring Tuff. Charge-balancing is required prior to using the waters for thermodynamic modeling. It was also necessary because one of the four starting waters, the HD-PERM-3 sample from Alcove 5 (SNL 2007b, Table 4.1-3), did not have a measured value for bicarbonate. Aluminum concentrations were not measured for the pore waters, and were estimated by adjusting aluminum concentration to be in equilibrium with alkali feldspar ($Na_{0.51}K_{0.46}Ca_{0.03}Al_{1.03}Si_{2.97}O_8$, Section 2.3.5.3.3.2.5), the most abundant aluminosilicate in the tuff. This resulted in slight supersaturation with respect to several aluminosilicates, but this was deemed preferable to *a priori* assuming equilibrium with any alteration minerals. In the succeeding equilibration step, trace amounts of stellerite, the most supersaturated phase, precipitated. This reduced the aluminum concentrations slightly but had no significant effect on other components in solution. For the Group 4 representative water, the aqueous silica concentration was not measured, and was calculated assuming equilibrium with amorphous silica. A second equilibration step at the starting temperature was used to precipitate out any minerals that saturated in the original calculation (SNL 2007b, Section 6.3.2.3).

GWB React Version 6.0.3 was used to charge balance on H+ the compositions given in Table 2.3.5-5 of the DOE LA. Log fCO2(g) was fixed at -3.0. The React input for Group-1 water is as follows:

```
React> show
      Temperature is 25 C
      Thermo dataset:  C:\Programs\Gwb-6.0\Gtdata\thermo.com.V8.R6+.dat
      Working directory:  d:\temp
      Options: Debye-Huckel

      Basis is:
       H2O                      1 free kg
       Na+                     59 mg/l
       K+                     4.8 mg/l
       Mg++                    .7 mg/l
       Ca++                    19 mg/l
       Cl-                    23 mg/l
       SO4--                   16 mg/l
       CO2(g)  (swapped for HCO3-)    -3 log fugacity
       NO3-  (swapped for NH3(aq))    16 mg/l
       F-                     2.2 mg/l
       SiO2(aq)                42 mg/l
       H+                     charge balance
       O2(g)  (swapped for O2(aq))    .7 fugacity
        No reactants specified.
```

The following is the React output for Group-1 water:

```
Step #     0          Xi = 0.0000
       Temperature =  25.0 C    Pressure =  1.013 bars
       pH =  8.136            log fO2 =   -0.155
       Eh =   0.7455 volts      pe =  12.6020
       Ionic strength      =    0.004296
       Activity of water   =    0.999977
       Solvent mass        =    1.000000 kg
       Solution mass       =    1.000358 kg
       Solution density    =    1.013    g/cm3
       Chlorinity          =    0.000649 molal
       Dissolved solids    =         358 mg/kg sol'n
       Rock mass           =    0.000000 kg
       Carbonate alkalinity=      116.71 mg/kg as CaCO3

                    moles       moles        grams         cm3
Reactants           remaining     reacted       reacted       reacted
--------------------------------------------------------------------------------
 CO2(g)            -- fixed fugacity buffer --

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
--------------------------------------------------------------------------------
 Na+                 0.002556        58.73      0.9318       -2.6232
 HCO3-               0.002253       137.4       0.9318       -2.6779
 O2(aq)              0.0008847       28.30      1.0000       -3.0532
 SiO2(aq)            0.0006867       41.24      1.0000       -3.1633
 Cl-                0.0006485       22.98      0.9305       -3.2194
 Ca++                0.0004497       18.02      0.7611       -3.4656
 NO3-                0.0002576       15.97      0.9305       -3.6204
 SO4--               0.0001585       15.22      0.7529       -3.9232
 K+                 0.0001227        4.794      0.9305       -3.9426
 F-                 0.0001155        2.194      0.9311       -3.9683
 CO2(aq)             3.397e-005       1.494      1.0000       -4.4689
 Mg++                2.731e-005       0.6635     0.7688       -4.6779
 CO3--               1.783e-005       1.069      0.7550       -4.8710
 HSiO3-              1.124e-005       0.8659     0.9318       -4.9800
 CaCO3(aq)           9.784e-006       0.9789     1.0000       -5.0095
 CaHCO3+             8.588e-006       0.8679     0.9318       -5.0968
 NaHCO3(aq)          7.129e-006       0.5987     1.0000       -5.1470
 CaSO4(aq)           5.276e-006       0.7180     1.0000       -5.2777
 NaSO4-              2.015e-006       0.2398     0.9318       -5.7264
 OH-                1.485e-006      0.02524     0.9311       -5.8594
 NaHSiO3(aq)         1.110e-006       0.1110     1.0000       -5.9547
 MgSO4(aq)           6.465e-007      0.07779     1.0000       -6.1894
 MgHCO3+             5.135e-007      0.04380     0.9318       -6.3201
 CaNO3+              4.413e-007      0.04503     0.9318       -6.3859
 MgCO3(aq)           2.692e-007      0.02269     1.0000       -6.5700
 NaCl(aq)            2.401e-007      0.01403     1.0000       -6.6196
 CaF+                1.899e-007      0.01121     0.9318       -6.7522
 NaCO3-              1.124e-007      0.009329    0.9318       -6.9798
 KSO4-               1.108e-007      0.01497     0.9318       -6.9862
 MgF+                5.456e-008      0.002362    0.9318       -7.2938
 CaCl+               4.468e-008      0.003373    0.9318       -7.3806
 NaF(aq)             2.576e-008      0.001081    1.0000       -7.5891
  (only species > 1e-8 molal listed)

 Mineral saturation states
                log Q/K                      log Q/K
--------------------------------------------------------------------------------
 Talc            0.9892s/sat   Cristobalite(bet  -0.1580
 Quartz          0.8360s/sat   SiO2(am)          -0.4497
 Tridymite       0.6645s/sat   Monohydrocalcite  -0.6902
 Chalcedony      0.5648s/sat   Dolomite-dis      -1.2858
 Cristobalite(alp  0.2855s/sat   Fluorite        -1.3652
 Dolomite-ord    0.2586s/sat   Magnesite         -1.5137
 Dolomite        0.2586s/sat   Chrysotile        -2.6714
 Calcite         0.1435s/sat   Diopside          -2.8915
 Coesite         0.0260s/sat   Enstatite         -2.8966
 Aragonite      -0.0009        Gypsum            -2.9065
 Ice            -0.1387        Tremolite         -2.9635
  (only minerals with log Q/K > -3 listed)

 Gases              fugacity     log fug.
--------------------------------------------------
 O2(g)               0.7000      -0.155
 H2O(g)              0.02598     -1.585
 CO2(g)              0.001000    -3.000
 HF(g)              6.073e-014   -13.217
 HCl(g)             2.185e-018   -17.661
 NO2(g)             4.365e-020   -19.360
 N2(g)              3.698e-021   -20.432
 NO(g)              3.497e-026   -25.456
 Cl2(g)             5.791e-028   -27.237
 SiF4(g)            4.110e-037   -36.386
 H2(g)              3.350e-042   -41.475
 CO(g)              1.046e-048   -47.980
 SO2(g)             4.010e-057   -56.397
 NH3(g)             2.842e-070   -69.546
 Na(g)              2.581e-075   -74.588
 K(g)               2.371e-077   -76.625
 F2(g)              3.513e-082   -81.454
 Mg(g)              7.425e-130   -129.129
 H2S(g)             3.722e-145   -144.429
 CH4(g)             1.004e-146   -145.998
 Ca(g)              1.797e-151   -150.745
 C(g)               2.933e-190   -189.533
 Si(g)              8.691e-221   -220.061
 S2(g)              2.754e-232   -231.560
 C2H4(g)            1.773e-239   -238.751

                              In fluid              Sorbed          Kd
Original basis total moles    moles      mg/kg      moles      mg/kg      L/kg
--------------------------------------------------------------------------------
 Ca++          0.000474   0.000474      19.0
 Cl-           0.000649   0.000649      23.0
 F-            0.000116   0.000116      2.20
 H+           -0.000266  -0.000266     -0.268
 H2O             55.5       55.5  1.00e+006
 HCO3-          0.00233    0.00233      142.
 K+            0.000123   0.000123     4.80
 Mg++          2.88e-005  2.88e-005    0.700
 NH3(aq)        0.000258   0.000258     4.39
 Na+            0.00257    0.00257     59.0
 O2(aq)         0.00140    0.00140     44.8
 SO4--          0.000167   0.000167    16.0
 SiO2(aq)       0.000699   0.000699    42.0

 Elemental composition          In fluid              Sorbed
              total moles      moles      mg/kg      moles      mg/kg
--------------------------------------------------------------------------------
 Calcium        0.0004741    0.0004741     18.99
 Carbon         0.002331     0.002331      27.99
 Chlorine       0.0006488    0.0006488     22.99
 Fluorine       0.0001158    0.0001158     2.199
 Hydrogen         111.0        111.0   1.119e+005
 Magnesium      2.880e-005   2.880e-005    0.6997
 Nitrogen       0.0002580    0.0002580     3.613
 Oxygen           55.52        55.52   8.880e+005
 Potassium      0.0001228    0.0001228     4.798
 Silicon        0.0006990    0.0006990     19.63
 Sodium         0.002566     0.002566      58.98
 Sulfur         0.0001666    0.0001666     5.339


      Step #     0          Xi = 0.0000
      Temperature =  25.0 C    Pressure =  1.013 bars
      pH =  8.105            log fO2 =   -0.155
      Eh =   0.7473 volts      pe =  12.6323
      Ionic strength      =    0.004041
      Activity of water   =    0.999977
      Solvent mass        =    1.000002 kg
      Solution mass       =    1.000310 kg
      Solution density    =    1.013    g/cm3
      Chlorinity          =    0.000649 molal
      Dissolved solids    =         309 mg/kg sol'n
      Rock mass           =    0.000045 kg
      Carbonate alkalinity=      108.49 mg/kg as CaCO3

                   moles       moles        grams         cm3
Reactants          remaining     reacted       reacted       reacted
```

CO2(g) -- fixed fugacity buffer --

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	8.286e-005	-4.082	0.008294	0.003060
Dolomite	3.606e-006	-5.443	0.0006649	0.0002321
Quartz	0.0005972	-3.224	0.03588	0.01355
(total)			0.04484	0.01684

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.002557	58.77	0.9336	-2.6221
HCO3-	0.002097	127.9	0.9336	-2.7083
O2(aq)	0.0008847	28.30	1.0000	-3.0532
Cl-	0.0006485	22.98	0.9323	-3.2185
Ca++	0.0003690	14.78	0.7667	-3.5484
NO3-	0.0002577	15.97	0.9323	-3.6193
SO4--	0.0001594	15.31	0.7589	-3.9173
K+	0.0001227	4.794	0.9323	-3.9417
F-	0.0001156	2.195	0.9330	-3.9673
SiO2(aq)	0.0001002	6.016	1.0000	-3.9993
CO2(aq)	3.397e-005	1.495	1.0000	-4.4689
Mg++	2.393e-005	0.5815	0.7740	-4.7323
CO3--	1.538e-005	0.9227	0.7609	-4.9317
CaCO3(aq)	7.031e-006	0.7035	1.0000	-5.1530
NaHCO3(aq)	6.664e-006	0.5597	1.0000	-5.1763
CaHCO3+	6.605e-006	0.6676	0.9336	-5.2099
CaSO4(aq)	4.420e-006	0.6015	1.0000	-5.3546
NaSO4-	2.044e-006	0.2432	0.9336	-5.7194
HSiO3-	1.525e-006	0.1176	0.9336	-5.8465
OH-	1.382e-006	0.02349	0.9330	-5.8898
MgSO4(aq)	5.782e-007	0.06958	1.0000	-6.2379
MgHCO3+	4.217e-007	0.03597	0.9336	-6.4048
CaNO3+	3.649e-007	0.03723	0.9336	-6.4677
NaCl(aq)	2.412e-007	0.01409	1.0000	-6.6176
MgCO3(aq)	2.065e-007	0.01740	1.0000	-6.6851
CaF+	1.570e-007	0.009272	0.9336	-6.8340
NaHSiO3(aq)	1.513e-007	0.01514	1.0000	-6.8201
KSO4-	1.123e-007	0.01517	0.9336	-6.9795
NaCO3-	9.782e-008	0.008116	0.9336	-7.0394
MgF+	4.816e-008	0.002085	0.9336	-7.3472
CaCl+	3.693e-008	0.002788	0.9336	-7.4625
NaF(aq)	2.588e-008	0.001086	1.0000	-7.5870

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	0.0000 sat	Coesite	-0.8100
Quartz	0.0000 sat	Monohydrocalcite	-0.8337
Dolomite	0.0000 sat	Cristobalite(bet	-0.9940
Calcite	0.0000 sat	SiO2(am)	-1.2857
Ice	-0.1387	Fluorite	-1.4460
Aragonite	-0.1444	Dolomite-dis	-1.5444
Tridymite	-0.1715	Magnesite	-1.6288
Chalcedony	-0.2712	Talc	-2.7003
Cristobalite(alp	-0.5505	Gypsum	-2.9834

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	6.528e-014	-13.185
HCl(g)	2.348e-018	-17.629
NO2(g)	4.692e-020	-19.329
N2(g)	4.273e-021	-20.369
NO(g)	3.759e-026	-25.425
Cl2(g)	6.687e-028	-27.175
SiF4(g)	8.004e-038	-37.097
H2(g)	3.350e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	4.675e-057	-56.330
NH3(g)	3.055e-070	-69.515
Na(g)	2.413e-075	-74.617
K(g)	2.215e-077	-76.655
F2(g)	4.059e-082	-81.392
Mg(g)	5.696e-130	-129.244
H2S(g)	4.339e-145	-144.363
CH4(g)	1.004e-146	-145.998
Ca(g)	1.292e-151	-150.889
C(g)	2.933e-190	-189.533
Si(g)	1.268e-221	-220.897
S2(g)	3.742e-232	-231.427
C2H4(g)	1.773e-239	-238.751

	In fluid	Sorbed		Kd
Original basis total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000474	0.000388	15.5		
Cl-	0.000649	0.000649	23.0		
F-	0.000116	0.000116	2.20		
H+	-0.000340	-0.000250	-0.252		
H2O	55.5	55.5	1.00e+006		
HCO3-	0.00226	0.00217	132.		
K+	0.000123	0.000123	4.80		
Mg++	2.88e-005	2.52e-005	0.612		
NH3(aq)	0.000258	0.000258	4.39		
Na+	0.00257	0.00257	59.0		
O2(aq)	0.00140	0.00140	44.8		
SO4--	0.000167	0.000167	16.0		
SiO2(aq)	0.000699	0.000102	6.12		

Elemental composition	In fluid		Sorbed	
total moles	moles	mg/kg	moles	mg/kg
Calcium	0.0004741	0.0003876	15.53	
Carbon	0.002257	0.002167	26.02	
Chlorine	0.0006488	0.0006488	22.99	
Fluorine	0.0001158	0.0001158	2.199	
Hydrogen	111.0	111.0	1.119e+005	
Magnesium	2.880e-005	2.519e-005	0.6122	
Nitrogen	0.0002580	0.0002580	3.613	
Oxygen	55.52	55.52	8.880e+005	
Potassium	0.0001228	0.0001228	4.799	
Silicon	0.0006990	0.0001018	2.859	
Sodium	0.002566	0.002566	58.98	
Sulfur	0.0001666	0.0001666	5.339	

For Group-2 water, the React input is shown below:

React> show

Temperature is 25 C
Thermo dataset: C:\Programs\Gwb-6.0\Gtdata\thermo.com.V8.R6+.dat
Working directory: d:\temp
Options: Debye-Huckel

Basis is:

H2O	1 free kg
Na+	45 mg/l
K+	14.4 mg/l
Mg++	7.9 mg/l
Ca++	62 mg/l
Cl-	67 mg/l
SO4--	82 mg/l
CO2(g) (swapped for HCO3-)	-3 log fugacity
NO3- (swapped for NH3(aq))	44 mg/l
F-	1.4 mg/l
SiO2(aq)	52 mg/l
H+	charge balance
O2(g) (swapped for O2(aq))	.7 fugacity

Reactants:

Fix fugacity of CO2(g)

The React output for Group-2 water is the following:

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.977 log fO2 = -0.155
Eh = 0.7548 volts pe = 12.7604
Ionic strength = 0.008310
Activity of water = 0.999933
Solvent mass = 1.000000 kg
Solution mass = 1.000512 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001890 molal
Dissolved solids = 512 mg/kg sol'n
Rock mass = 0.000000 kg
Carbonate alkalinity= 84.47 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.001946	44.71	0.9093	-2.7522
Cl-	0.001889	66.92	0.9069	-2.7663
HCO3-	0.001603	97.77	0.9093	-2.8363
Ca++	0.001444	57.86	0.6955	-2.9980
O2(aq)	0.0008847	28.29	1.0000	-3.0532
SiO2(aq)	0.0008548	51.33	1.0000	-3.0681
SO4--	0.0007517	72.17	0.6821	-3.2901
NO3-	0.0007061	43.76	0.9069	-3.1936
K+	0.0003669	14.34	0.9069	-3.4779
Mg++	0.0002922	7.098	0.7078	-3.6844
F-	7.299e-005	1.386	0.9081	-4.1786
CaSO4(aq)	6.652e-005	9.051	1.0000	-4.1770
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
MgSO4(aq)	2.736e-005	3.292	1.0000	-4.5629
CaHCO3+	1.793e-005	1.812	0.9093	-4.7876
CaCO3(aq)	1.384e-005	1.385	1.0000	-4.8587
HSiO3-	9.953e-006	0.7669	0.9093	-5.0433
CO3--	9.467e-006	0.5678	0.6855	-5.1878
NaSO4-	6.592e-006	0.7843	0.9093	-5.2223
NaHCO3(aq)	3.678e-006	0.3088	1.0000	-5.4344
MgHCO3+	3.600e-006	0.3070	0.9093	-5.4850
CaNO3+	3.546e-006	0.3618	0.9093	-5.4916
KSO4-	1.422e-006	0.1921	0.9093	-5.8885
MgCO3(aq)	1.278e-006	0.1077	1.0000	-5.8933
OH-	1.057e-006	0.01797	0.9081	-6.0178
NaHSiO3(aq)	7.128e-007	0.07130	1.0000	-6.1470
NaCl(aq)	5.065e-007	0.02958	1.0000	-6.2955
CaCl+	3.814e-007	0.02879	0.9093	-6.4599
CaF+	3.518e-007	0.02078	0.9093	-6.4949
MgF+	3.393e-007	0.01469	0.9093	-6.5106
MgCl+	2.855e-007	0.01705	0.9093	-6.5856
NaCO3-	4.128e-008	0.003424	0.9093	-7.4256
KCl(aq)	1.825e-008	0.001360	1.0000	-7.7388
CaOH+	1.481e-008	0.0008450	0.9093	-7.8707
NaF(aq)	1.179e-008	0.0004949	1.0000	-7.9284
H+	1.146e-008	1.154e-005	0.9197	-7.9773

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	7.4569s/sat	Ice	-0.1387
Talc	3.3997s/sat	SiO2(am)	-0.3545
Tremolite	1.4822s/sat	Chrysotile	-0.4512
Dolomite-ord	1.0861s/sat	Dolomite-dis	-0.4583
Dolomite	1.0861s/sat	Monohydrocalcite	-0.5394
Quartz	0.9312s/sat	Magnesite	-0.8370
Tridymite	0.7597s/sat	Fluorite	-1.3182
Chalcedony	0.6600s/sat	Gypsum	-1.8059

Cristobalite(alp 0.3807s/sat Diopside -1.8738
Calcite 0.2943s/sat Anhydrite -1.9817
Sepiolite 0.2278s/sat Enstatite -2.1249
Aragonite 0.1499s/sat Bassanite -2.6267
Coesite 0.1212s/sat Sellaite -2.6574
Cristobalite(bet -0.0628 CaSO4:0.5H2O(bet -2.7948
(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	5.388e-014	-13.269
HCl(g)	8.931e-018	-17.049
NO2(g)	1.679e-019	-18.775
N2(g)	5.474e-020	-19.262
NO(g)	1.345e-025	-24.871
Cl2(g)	9.679e-027	-26.014
SiF4(g)	3.172e-037	-36.499
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	3.573e-056	-55.447
NH3(g)	1.093e-069	-68.961
Na(g)	1.332e-075	-74.876
K(g)	4.799e-077	-76.319
F2(g)	2.766e-082	-81.558
Mg(g)	3.527e-129	-128.453
H2S(g)	3.316e-144	-143.479
CH4(g)	1.004e-146	-145.998
Ca(g)	2.543e-151	-150.595
C(g)	2.933e-190	-189.533
Si(g)	1.082e-220	-219.966
S2(g)	2.186e-230	-229.660
C2H4(g)	1.773e-239	-238.751

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Ca++	0.00155	0.00155	62.0			
Cl-	0.00189	0.00189	67.0			
F-	7.37e-005	7.37e-005	1.40			
H+	-0.000712	-0.000712	-0.717			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00169	0.00169	103.			
K+	0.000368	0.000368	14.4			
Mg++	0.000325	0.000325	7.90			
NH3(aq)	0.000710	0.000710	12.1			
Na+	0.00196	0.00196	45.0			
O2(aq)	0.00230	0.00230	73.7			
SO4--	0.000854	0.000854	82.0			
SiO2(aq)	0.000865	0.000865	52.0			

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Calcium	0.001547	0.001547	61.97		
Carbon	0.001687	0.001687	20.25		
Chlorine	0.001890	0.001890	66.97		
Fluorine	7.369e-005	7.369e-005	1.399		
Hydrogen	111.0	111.0	1.118e+005		
Magnesium	0.0003250	0.0003250	7.896		
Nitrogen	0.0007096	0.0007096	9.934		
Oxygen	55.52	55.52	8.879e+005		
Potassium	0.0003683	0.0003683	14.39		
Silicon	0.0008655	0.0008655	24.29		
Sodium	0.001957	0.001957	44.98		
Sulfur	0.0008536	0.0008536	27.36		

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.785 log fO2 = -0.155
Eh = 0.7662 volts pe = 12.9526
Ionic strength = 0.007473
Activity of water = 0.999933
Solvent mass = 1.000005 kg
Solution mass = 1.000424 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001890 molal
Dissolved solids = 419 mg/kg sol'n
Rock mass = 0.000075 kg
Carbonate alkalinity= 54.21 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Dolomite	0.0001574	-3.803	0.02903	0.01013
Quartz	0.0007645	-3.117	0.04593	0.01734
(total)		0.07496	0.02748	

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.001948	44.76	0.9133	-2.7499
Cl-	0.001889	66.94	0.9111	-2.7642
Ca++	0.001306	52.33	0.7067	-3.0347
HCO3-	0.001025	62.54	0.9133	-3.0285
O2(aq)	0.0008847	28.30	1.0000	-3.0532
SO4--	0.0007669	73.64	0.6943	-3.2737
NO3-	0.0007064	43.78	0.9111	-3.1914
K+	0.0003668	14.34	0.9111	-3.4760
Mg++	0.0001509	3.667	0.7182	-3.9650
SiO2(aq)	0.0001002	6.016	1.0000	-3.9993
F-	7.317e-005	1.390	0.9122	-4.1755
CaSO4(aq)	6.348e-005	8.639	1.0000	-4.1973
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
MgSO4(aq)	1.489e-005	1.792	1.0000	-4.8271
CaHCO3+	1.054e-005	1.065	0.9133	-5.0165
NaSO4-	6.851e-006	0.8153	0.9133	-5.2036
CaCO3(aq)	5.251e-006	0.5253	1.0000	-5.2798
CO3--	3.840e-006	0.2303	0.6975	-5.5722
CaNO3+	3.260e-006	0.3327	0.9133	-5.5261
NaHCO3(aq)	2.375e-006	0.1994	1.0000	-5.6243
KSO4-	1.477e-006	0.1995	0.9133	-5.8701
MgHCO3+	1.207e-006	0.1029	0.9133	-5.9578
HSiO3-	7.459e-007	0.05748	0.9133	-6.1667
OH-	6.759e-007	0.01149	0.9122	-6.2100
NaCl(aq)	5.115e-007	0.02988	1.0000	-6.2911
CaCl+	3.506e-007	0.02647	0.9133	-6.4945
CaF+	3.242e-007	0.01915	0.9133	-6.5286
MgCO3(aq)	2.765e-007	0.02330	1.0000	-6.5583
MgF+	1.783e-007	0.007719	0.9133	-6.7882
MgCl+	1.497e-007	0.008942	0.9133	-6.8642
NaHSiO3(aq)	5.394e-008	0.005396	1.0000	-7.2681
KCl(aq)	1.841e-008	0.001372	1.0000	-7.7348
H+	1.777e-008	1.791e-005	0.9228	-7.7851
NaCO3-	1.705e-008	0.001414	0.9133	-7.8077
NaF(aq)	1.194e-008	0.0005011	1.0000	-7.9230

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	0.0000	sat	Cristobalite(bet -0.9940
Dolomite	0.0000	sat	SiO2(am) -1.2857
Quartz	0.0000	sat	Fluorite -1.3488
Calcite	-0.1268		Magnesite -1.5020
Ice	-0.1387		Dolomite-dis -1.5444
Tridymite	-0.1715		Gypsum -1.8262
Aragonite	-0.2712		Anhydrite -2.0020
Chalcedony	-0.2712		Talc -2.3199
Cristobalite(alp	-0.5505		Bassanite -2.6470
Coesite	-0.8100		CaSO4:0.5H2O(bet -2.8151
Monohydrocalcite	-0.9605		Sellaite -2.9318

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	8.448e-014	-13.073
HCl(g)	1.397e-017	-16.855
NO2(g)	2.627e-019	-18.581

N2(g)	1.340e-019	-18.873
NO(g)	2.105e-025	-24.677
Cl2(g)	2.368e-026	-25.626
SiF4(g)	2.245e-037	-36.649
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	8.992e-056	-55.046
NH3(g)	1.711e-069	-68.767
Na(g)	8.600e-076	-75.065
K(g)	3.097e-077	-76.509
F2(g)	6.798e-082	-81.168
Mg(g)	7.628e-130	-129.118
H2S(g)	8.345e-144	-143.079
CH4(g)	1.004e-146	-145.998
Ca(g)	9.645e-152	-151.016
C(g)	2.933e-190	-189.533
Si(g)	1.268e-221	-220.897
S2(g)	1.384e-229	-228.859
C2H4(g)	1.773e-239	-238.751

	In fluid	Sorbed	Kd	
Original basis total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.00155	0.00139	55.7		
Cl-	0.00189	0.00189	67.0		
F-	7.37e-005	7.37e-005	1.40		

H+	-0.00100	-0.000686	-0.692
H2O	55.5	55.5	1.00e+006
HCO3-	0.00140	0.00108	66.0
K+	0.000368	0.000368	14.4
Mg++	0.000325	0.000168	4.07
NH3(aq)	0.000710	0.000710	12.1
Na+	0.00196	0.00196	45.0
O2(aq)	0.00230	0.00230	73.7
SO4--	0.000854	0.000854	82.0
SiO2(aq)	0.000865	0.000101	6.06

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.001547	0.001390	55.67		
Carbon	0.001398	0.001083	13.00		
Chlorine	0.001890	0.001890	66.97		
Fluorine	7.369e-005	7.369e-005	1.399		
Hydrogen	111.0	111.0	1.118e+005		
Magnesium	0.0003250	0.0001676	4.072		
Nitrogen	0.0007096	0.0007096	9.935		
Oxygen	55.52	55.52	8.879e+005		
Potassium	0.0003683	0.0003683	14.39		
Silicon	0.0008655	0.0001010	2.834		
Sodium	0.001957	0.001957	44.98		
Sulfur	0.0008536	0.0008536	27.36		

For Group-3 water, the React input is as follows:

React> show

Temperature is 25 C
Thermo dataset: C:\Programs\Gwb-6.0\Gtdata\thermo.com.V8.R6+.dat
Working directory: d:\temp
Options: Debye-Huckel

Basis is:

H2O	1 free kg
Na+	62 mg/l
K+	9 mg/l
Mg++	17.4 mg/l
Ca++	97 mg/l
Cl-	123 mg/l
SO4--	120 mg/l
CO2(g) (swapped for HCO3-)	-3 log fugacity
NO3- (swapped for NH3(aq))	10 mg/l
F-	.76 mg/l
SiO2(aq)	75 mg/l
H+	charge balance
O2(g) (swapped for O2(aq))	.7 fugacity

Reactants:

Fix fugacity of CO2(g)

The React output for Group-3 water is as follows:

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 8.204 log fO2 = -0.155
Eh = 0.7414 volts pe = 12.5336
Ionic strength = 0.012495
Activity of water = 0.999878
Solvent mass = 1.000000 kg
Solution mass = 1.000727 kg

Solution density = 1.013 g/cm3
Chlorinity = 0.003469 molal
Dissolved solids = 727 mg/kg sol'n
Rock mass = 0.000000 kg
Carbonate alkalinity= 147.41 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted

CO2(g) -- fixed fugacity buffer --

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.003466	122.8	0.8892	-2.5111
HCO3-	0.002753	167.8	0.8926	-2.6096
Na+	0.002673	61.41	0.8926	-2.6223
Ca++	0.002196	87.96	0.6504	-2.8451
SiO2(aq)	0.001222	73.34	1.0000	-2.9131
SO4--	0.001044	100.2	0.6326	-3.1803
O2(aq)	0.0008847	28.29	1.0000	-3.0532
Mg++	0.0006239	15.15	0.6665	-3.3811
K+	0.0002290	8.948	0.8892	-3.6911
NO3-	0.0001601	9.922	0.8892	-3.8465
CaSO4(aq)	0.0001218	16.57	1.0000	-3.9143
MgSO4(aq)	7.085e-005	8.522	1.0000	-4.1496
CaCO3(aq)	5.593e-005	5.594	1.0000	-4.2524
CaHCO3+	4.378e-005	4.423	0.8926	-4.4080
F-	3.936e-005	0.7472	0.8910	-4.4551
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
CO3--	2.893e-005	1.735	0.6372	-4.7343
HSiO3-	2.442e-005	1.881	0.8926	-4.6616
MgHCO3+	1.243e-005	1.060	0.8926	-4.9550
NaSO4-	1.166e-005	1.387	0.8926	-4.9826
NaHCO3(aq)	8.360e-006	0.7018	1.0000	-5.0778
MgCO3(aq)	7.303e-006	0.6153	1.0000	-5.1365
NaHSiO3(aq)	2.315e-006	0.2315	1.0000	-5.6354
OH-	1.816e-006	0.03086	0.8910	-5.7911
NaCl(aq)	1.229e-006	0.07177	1.0000	-5.9104
CaNO3+	1.142e-006	0.1165	0.8926	-5.9916
KSO4-	1.142e-006	0.1542	0.8926	-5.9918
MgCl+	1.052e-006	0.06285	0.8926	-6.0271
CaCl+	9.941e-007	0.07503	0.8926	-6.0519
MgF+	3.677e-007	0.01591	0.8926	-6.4838
CaF+	2.696e-007	0.01592	0.8926	-6.6186
NaCO3-	1.611e-007	0.01336	0.8926	-6.8422
CaOH+	3.616e-008	0.002063	0.8926	-7.4911
KCl(aq)	2.010e-008	0.001497	1.0000	-7.6968

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	49.0543s/sat	Monohydrocalcite	0.0669s/sat
Tremolite	7.7192s/sat	Magnesite	-0.0802
Talc	6.2902s/sat	Ice	-0.1388
Sepiolite	4.1851s/sat	SiO2(am)	-0.1995
Dolomite-ord	2.4492s/sat	Diopside	-0.2006
Dolomite	2.4492s/sat	Huntite	-0.9115
Chrysotile	2.1293s/sat	Enstatite	-1.2130
Anthophyllite	1.0876s/sat	Gypsum	-1.5432
Quartz	1.0862s/sat	Fluorite	-1.7184
Tridymite	0.9147s/sat	Anhydrite	-1.7190
Dolomite-dis	0.9048s/sat	Bassanite	-2.3639
Calcite	0.9006s/sat	CaSO4:0.5H2O(bet	-2.5320
Chalcedony	0.8150s/sat	Lansfordite	-2.6278
Aragonite	0.7562s/sat	Okenite	-2.6450
Cristobalite(alp	0.5357s/sat	Nesquehonite	-2.7823
Coesite	0.2762s/sat	Sellaite	-2.9070
Cristobalite(bet	0.0922s/sat		

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02597	-1.585
CO2(g)	0.001000	-3.000
HF(g)	1.691e-014	-13.772
HCl(g)	9.535e-018	-17.021
NO2(g)	2.216e-020	-19.655
N2(g)	9.529e-022	-21.021
NO(g)	1.775e-026	-25.751
Cl2(g)	1.103e-026	-25.957
SiF4(g)	4.399e-039	-38.357
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	1.620e-056	-55.791
NH3(g)	1.442e-070	-69.841
Na(g)	3.027e-075	-74.519
K(g)	4.952e-077	-76.305
F2(g)	2.725e-083	-82.565
Mg(g)	2.015e-128	-127.696
H2S(g)	1.503e-144	-143.823
CH4(g)	1.004e-146	-145.998
Ca(g)	1.027e-150	-149.988
C(g)	2.933e-190	-189.533
Si(g)	1.546e-220	-219.811
S2(g)	4.492e-231	-230.348
C2H4(g)	1.773e-239	-238.751

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Ca++	0.00242	0.00242	96.9			
Cl-	0.00347	0.00347	123.			
F-	4.00e-005	4.00e-005	0.759			
H+	-0.000248	-0.000248	-0.250			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00294	0.00294	179.			
K+	0.000230	0.000230	8.99			
Mg++	0.000716	0.000716	17.4			
NH3(aq)	0.000161	0.000161	2.74			
Na+	0.00270	0.00270	62.0			
O2(aq)	0.00121	0.00121	38.6			
SO4--	0.00125	0.00125	120.			
SiO2(aq)	0.00125	0.00125	74.9			

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Calcium	0.002420	0.002420	96.93		
Carbon	0.002943	0.002943	35.33		
Chlorine	0.003469	0.003469	122.9		
Fluorine	4.000e-005	4.000e-005	0.7594		
Hydrogen	111.0	111.0	1.118e+005		
Magnesium	0.0007159	0.0007159	17.39		
Nitrogen	0.0001613	0.0001613	2.257		
Oxygen	55.53	55.53	8.878e+005		
Potassium	0.0002302	0.0002302	8.993		
Silicon	0.001248	0.001248	35.03		
Sodium	0.002697	0.002697	61.95		
Sulfur	0.001249	0.001249	40.03		

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.743 log fO2 = -0.155
Eh = 0.7687 volts pe = 12.9947
Ionic strength = 0.009884
Activity of water = 0.999878
Solvent mass = 1.000017 kg
Solution mass = 1.000524 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.003469 molal
Dissolved solids = 506 mg/kg sol'n
Rock mass = 0.000164 kg
Carbonate alkalinity= 50.15 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Dolomite	0.0005130	-3.290	0.09460	0.03302
Quartz	0.001147	-2.940	0.06894	0.02603
(total)		0.1635	0.05905	

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	0.003467	122.8	0.8997	-2.5060
Na+	0.002680	61.57	0.9025	-2.6165
Ca++	0.001774	71.07	0.6767	-2.9206
SO4--	0.001099	105.5	0.6615	-3.1384

HCO3-	0.0009417	57.43	0.9025	-3.0706
O2(aq)	0.0008847	28.29	1.0000	-3.0532
K+	0.0002289	8.945	0.8997	-3.6862
Mg++	0.0001779	4.322	0.6905	-3.9106
NO3-	0.0001603	9.935	0.8997	-3.8409
CaSO4(aq)	0.0001128	15.34	1.0000	-3.9479
SiO2(aq)	0.0001002	6.015	1.0000	-3.9993
F-	3.966e-005	0.7530	0.9011	-4.4469
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
MgSO4(aq)	2.305e-005	2.773	1.0000	-4.6373
NaSO4-	1.287e-005	1.532	0.9025	-4.9348
CaHCO3+	1.259e-005	1.272	0.9025	-4.9445
CaCO3(aq)	5.624e-006	0.5626	1.0000	-5.2499
CO3--	3.315e-006	0.1988	0.6655	-5.6564
NaHCO3(aq)	2.931e-006	0.2461	1.0000	-5.5330
NaCl(aq)	1.261e-006	0.07363	1.0000	-5.8994
KSO4-	1.258e-006	0.1699	0.9025	-5.9450
MgHCO3+	1.256e-006	0.1071	0.9025	-5.9456
CaNO3+	9.617e-007	0.09812	0.9025	-6.0615
CaCl+	8.364e-007	0.06314	0.9025	-6.1222
HSiO3-	6.850e-007	0.05278	0.9025	-6.2088
OH-	6.210e-007	0.01056	0.9011	-6.2521
MgCl+	3.112e-007	0.01859	0.9025	-6.5515
MgCO3(aq)	2.581e-007	0.02175	1.0000	-6.5882
CaF+	2.284e-007	0.01349	0.9025	-6.6858
MgF+	1.095e-007	0.004739	0.9025	-7.0052
NaHSiO3(aq)	6.655e-008	0.006658	1.0000	-7.1768
KCl(aq)	2.057e-008	0.001533	1.0000	-7.6868
H+	1.976e-008	1.991e-005	0.9144	-7.7430
NaCO3-	1.932e-008	0.001603	0.9025	-7.7585
CaOH+	1.040e-008	0.0005932	0.9025	-8.0276

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	0.0000 sat	Cristobalite(bet	-0.9940
Dolomite	0.0000 sat	SiO2(am)	-1.2857
Quartz	0.0000 sat	Magnesite	-1.5319
Calcite	-0.0969	Dolomite-dis	-1.5444
Ice	-0.1388	Gypsum	-1.5768
Tridymite	-0.1715	Anhydrite	-1.7526
Aragonite	-0.2413	Fluorite	-1.7774
Chalcedony	-0.2712	Bassanite	-2.3975
Cristobalite(alp	-0.5505	Talc	-2.4096
Coesite	-0.8100	CaSO4:0.5H2O(bet	-2.5656
Monohydrocalcite	-0.9307		

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02597	-1.585
CO2(g)	0.001000	-3.000
HF(g)	4.983e-014	-13.303
HCl(g)	2.790e-017	-16.554
NO2(g)	6.488e-020	-19.188
N2(g)	8.171e-021	-20.088
Cl2(g)	9.443e-026	-25.025
NO(g)	5.197e-026	-25.284
SiF4(g)	2.718e-038	-37.566
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	1.491e-055	-54.827
NH3(g)	4.224e-070	-69.374
Na(g)	1.061e-075	-74.974
K(g)	1.732e-077	-76.761
F2(g)	2.365e-082	-81.626
Mg(g)	7.121e-130	-129.147
H2S(g)	1.384e-143	-142.859
CH4(g)	1.004e-146	-145.998
Ca(g)	1.033e-151	-150.986
C(g)	2.933e-190	-189.533
Si(g)	1.268e-221	-220.897
S2(g)	3.806e-229	-228.419
C2H4(g)	1.773e-239	-238.751

	In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.00242	0.00191	76.4			
Cl-	0.00347	0.00347	123.			
F-	4.00e-005	4.00e-005	0.760			
H+	-0.00116	-0.000138	-0.139			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00203	0.00100	61.1			
K+	0.000230	0.000230	9.00			
Mg++	0.000716	0.000203	4.93			
NH3(aq)	0.000161	0.000161	2.75			
Na+	0.00270	0.00270	62.0			
O2(aq)	0.00121	0.00121	38.6			
SO4--	0.00125	0.00125	120.			
SiO2(aq)	0.00125	0.000101	6.06			

Elemental composition	In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Calcium	0.002420	0.001907	76.40		
Carbon	0.002028	0.001002	12.03		
Chlorine	0.003469	0.003469	122.9		
Fluorine	4.000e-005	4.000e-005	0.7596		
Hydrogen	111.0	111.0	1.118e+005		
Magnesium	0.0007159	0.0002029	4.929		
Nitrogen	0.0001613	0.0001613	2.258		
Oxygen	55.53	55.52	8.878e+005		
Potassium	0.0002302	0.0002302	8.995		
Silicon	0.001248	0.0001009	2.833		
Sodium	0.002697	0.002697	61.97		
Sulfur	0.001249	0.001249	40.04		

For Group-4 water, the React input is as follows:

React> show

Temperature is 25 C

Thermo dataset: C:\Programs\Gwb-6.0\Gtdata\thermo.com.V8.R6+.dat

Working directory: d:\temp

Options: Debye-Huckel

Basis is:

H2O	1 free kg
Na+	123 mg/l
K+	13.8 mg/l
Mg++	16.7 mg/l

Ca++ 59.9 mg/l
Cl- 146 mg/l
SO4-- 126 mg/l
CO2(g) (swapped for HCO3-) -3 log fugacity
NO3- (swapped for NH3(aq)) 57.4 mg/l
F- 1.3 mg/l
H+ charge balance
O2(g) (swapped for O2(aq)) .7 fugacity
Reactants:
Fix fugacity of CO2(g)

The React output for Group-4 water is as follows:

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 8.105 log fO2 = -0.155
Eh = 0.7473 volts pe = 12.6323
Ionic strength = 0.012735
Activity of water = 0.999855
Solvent mass = 1.000000 kg
Solution mass = 1.000719 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.004118 molal
Dissolved solids = 718 mg/kg sol'n
Rock mass = 0.000000 kg
Carbonate alkalinity= 116.11 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.005309	122.0	0.8918	-2.3247
Cl-	0.004113	145.7	0.8884	-2.4372
HCO3-	0.002195	133.8	0.8918	-2.7083
Ca++	0.001365	54.65	0.6482	-3.0533
SO4--	0.001130	108.5	0.6302	-3.1473
NO3-	0.0009217	57.11	0.8884	-3.0868
O2(aq)	0.0008847	28.29	1.0000	-3.0532
Mg++	0.0005983	14.53	0.6645	-3.4006
K+	0.0003510	13.71	0.8884	-3.5061
CaSO4(aq)	8.137e-005	11.07	1.0000	-4.0895
MgSO4(aq)	7.309e-005	8.791	1.0000	-4.1362
F-	6.751e-005	1.282	0.8901	-4.2212
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
NaSO4-	2.499e-005	2.973	0.8918	-4.6520
CaCO3(aq)	2.198e-005	2.199	1.0000	-4.6579
CaHCO3+	2.162e-005	2.184	0.8918	-4.7149
CO3--	1.843e-005	1.105	0.6349	-4.9317
NaHCO3(aq)	1.322e-005	1.109	1.0000	-4.8789
MgHCO3+	9.475e-006	0.8079	0.8918	-5.0731
MgCO3(aq)	4.432e-006	0.3734	1.0000	-5.3534
CaNO3+	4.070e-006	0.4152	0.8918	-5.4402
NaCl(aq)	2.891e-006	0.1688	1.0000	-5.5389
KSO4-	1.888e-006	0.2550	0.8918	-5.7738
OH-	1.448e-006	0.02461	0.8901	-5.8898
MgCl+	1.194e-006	0.07131	0.8918	-5.9727
CaCl+	7.305e-007	0.05513	0.8918	-6.1861
MgF+	6.031e-007	0.02610	0.8918	-6.2694
CaF+	2.864e-007	0.01691	0.8918	-6.5928
NaCO3-	2.031e-007	0.01684	0.8918	-6.7420
KCl(aq)	3.649e-008	0.002718	1.0000	-7.4379
NaF(aq)	2.861e-008	0.001200	1.0000	-7.5435
CaOH+	1.785e-008	0.001018	0.8918	-7.7980

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	1.8268s/sat	Gypsum	-1.7184
Dolomite	1.8268s/sat	Anhydrite	-1.8942
Calcite	0.4951s/sat	Huntite	-1.9676
Aragonite	0.3507s/sat	Sellaite	-2.4587
Dolomite-dis	0.2824s/sat	Bassanite	-2.5391
Ice	-0.1388	CaSO4:0.5H2O(bet	-2.7072
Magnesite	-0.2971	Lansfordite	-2.8447
Monohydrocalcite	-0.3387	Nesquehonite	-2.9991
Fluorite	-1.4587		

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02597	-1.585
CO2(g)	0.001000	-3.000
HF(g)	3.638e-014	-13.439
HCl(g)	1.419e-017	-16.848
NO2(g)	1.599e-019	-18.796
N2(g)	4.963e-020	-19.304
NO(g)	1.281e-025	-24.892
Cl2(g)	2.443e-026	-25.612
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	2.753e-056	-55.560
NH3(g)	1.041e-069	-68.983
Na(g)	4.785e-075	-74.320
K(g)	6.041e-077	-76.219
F2(g)	1.261e-082	-81.899
Mg(g)	1.223e-128	-127.913
H2S(g)	2.555e-144	-143.593
CH4(g)	1.004e-146	-145.998
Ca(g)	4.038e-151	-150.394
C(g)	2.933e-190	-189.533
S2(g)	1.298e-230	-229.887
C2H4(g)	1.773e-239	-238.751

Original basis	In fluid total moles	Sorbed moles	Kd mg/kg	moles	mg/kg	L/kg
Ca++	0.00149	0.00149	59.9			
Cl-	0.00412	0.00412	146.			
F-	6.84e-005	6.84e-005	1.30			
H+	-0.000938	-0.000938	-0.945			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00232	0.00232	141.			
K+	0.000353	0.000353	13.8			
Mg++	0.000687	0.000687	16.7			
NH3(aq)	0.000926	0.000926	15.8			
Na+	0.00535	0.00535	123.			
O2(aq)	0.00274	0.00274	87.5			
SO4--	0.00131	0.00131	126.			

Elemental composition	In fluid total moles	moles	mg/kg	Sorbed moles	mg/kg

Calcium	0.001495	0.001495	59.86
Carbon	0.002318	0.002318	27.83
Chlorine	0.004118	0.004118	145.9
Fluorine	6.843e-005	6.843e-005	1.299
Hydrogen	111.0	111.0	1.118e+005
Magnesium	0.0006871	0.0006871	16.69
Nitrogen	0.0009257	0.0009257	12.96
Oxygen	55.53	55.53	8.877e+005
Potassium	0.0003530	0.0003530	13.79
Sodium	0.005350	0.005350	122.9
Sulfur	0.001312	0.001312	42.03

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.743 log fO2 = -0.155
Eh = 0.7687 volts pe = 12.9946
Ionic strength = 0.010983
Activity of water = 0.999855
Solvent mass = 1.000012 kg
Solution mass = 1.000628 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.004118 molal
Dissolved solids = 616 mg/kg sol'n
Rock mass = 0.000062 kg
Carbonate alkalinity= 50.22 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Dolomite	0.0003385	-3.470	0.06243	0.02179
(total)			0.06243	0.02179

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.005315	122.1	0.8981	-2.3212
Cl-	0.004114	145.8	0.8951	-2.4339
SO4--	0.001172	112.5	0.6487	-3.1189
Ca++	0.001071	42.90	0.6650	-3.1474
HCO3-	0.0009464	57.71	0.8981	-3.0706
NO3-	0.0009224	57.16	0.8951	-3.0832
O2(aq)	0.0008847	28.29	1.0000	-3.0532
K+	0.0003509	13.71	0.8951	-3.5029
Mg++	0.0003044	7.395	0.6798	-3.6841
CaSO4(aq)	6.996e-005	9.518	1.0000	-4.1552
F-	6.785e-005	1.288	0.8967	-4.2158
MgSO4(aq)	4.062e-005	4.886	1.0000	-4.3913
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
NaSO4-	2.670e-005	3.177	0.8981	-4.6201
CaHCO3+	7.506e-006	0.7583	0.8981	-5.1713
NaHCO3(aq)	5.785e-006	0.4857	1.0000	-5.2377
CO3--	3.379e-006	0.2027	0.6529	-5.6563
CaCO3(aq)	3.337e-006	0.3338	1.0000	-5.4766
CaNO3+	3.282e-006	0.3348	0.8981	-5.5305
NaCl(aq)	2.937e-006	0.1716	1.0000	-5.5320
MgHCO3+	2.126e-006	0.1813	0.8981	-5.7190
KSO4-	2.016e-006	0.2723	0.8981	-5.7422
OH-	6.241e-007	0.01061	0.8967	-6.2521
MgCl+	6.220e-007	0.03715	0.8981	-6.2529
CaCl+	5.886e-007	0.04443	0.8981	-6.2768
MgCO3(aq)	4.350e-007	0.03665	1.0000	-6.3615
MgF+	3.156e-007	0.01366	0.8981	-6.5475
CaF+	2.318e-007	0.01369	0.8981	-6.6815
NaCO3-	3.833e-008	0.003179	0.8981	-7.4631
KCl(aq)	3.703e-008	0.002759	1.0000	-7.4314
NaF(aq)	2.920e-008	0.001225	1.0000	-7.5346
H+	1.983e-008	1.998e-005	0.9111	-7.7431

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite	0.0000 sat	Fluorite	-1.5420
Dolomite-ord	0.0000 sat	Dolomite-dis	-1.5444
Ice	-0.1388	Gypsum	-1.7841
Calcite	-0.3236	Anhydrite	-1.9599
Aragonite	-0.4680	Bassanite	-2.6048
Monohydrocalcite	-1.1573	Sellaite	-2.7315
Magnesite	-1.3052	CaSO4:0.5H2O(bet	-2.7729

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

Gases	fugacity	log fug.
O2(g)	0.7000	-0.155
H2O(g)	0.02597	-1.585
CO2(g)	0.001000	-3.000
HF(g)	8.482e-014	-13.072
HCl(g)	3.293e-017	-16.482
NO2(g)	3.713e-019	-18.430
N2(g)	2.677e-019	-18.572
NO(g)	2.975e-025	-24.527
Cl2(g)	1.316e-025	-24.881
H2(g)	3.349e-042	-41.475
CO(g)	1.046e-048	-47.980
SO2(g)	1.559e-055	-54.807
NH3(g)	2.418e-069	-68.617
Na(g)	2.095e-075	-74.679
K(g)	2.642e-077	-76.578
F2(g)	6.854e-082	-81.164
Mg(g)	1.200e-129	-128.921
H2S(g)	1.447e-143	-142.840
CH4(g)	1.004e-146	-145.998
Ca(g)	6.131e-152	-151.212
C(g)	2.933e-190	-189.533
S2(g)	4.161e-229	-228.381
C2H4(g)	1.773e-239	-238.751

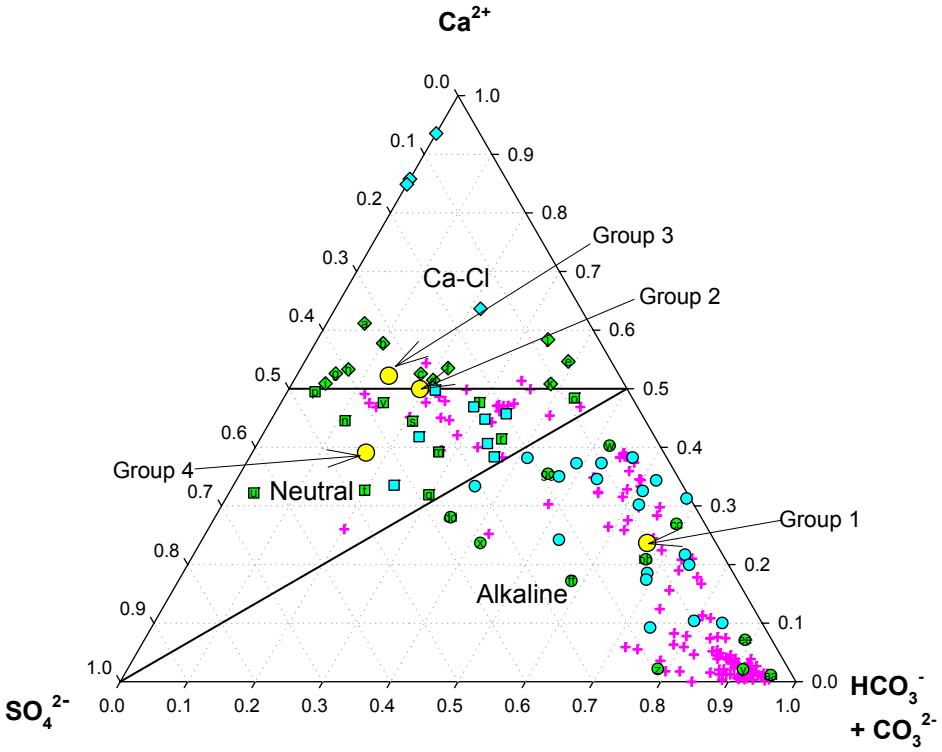
Original basis	In fluid total moles	Sorbed moles	Kd mg/kg	moles	mg/kg	L/kg
Ca++	0.00149	0.00116	46.3			
Cl-	0.00412	0.00412	146.			
F-	6.84e-005	6.84e-005	1.30			
H+	-0.00158	-0.000900	-0.906			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00168	0.00100	61.2			
K+	0.000353	0.000353	13.8			
Mg++	0.000687	0.000349	8.47			
NH3(aq)	0.000926	0.000926	15.8			
Na+	0.00535	0.00535	123.			
O2(aq)	0.00274	0.00274	87.5			
SO4--	0.00131	0.00131	126.			

Elemental composition	In fluid total moles	moles	mg/kg	Sorbed moles	mg/kg
Calcium	0.001495	0.001156	46.30		
Carbon	0.001680	0.001003	12.04		
Chlorine	0.004118	0.004118	145.9		
Fluorine	6.843e-005	6.843e-005	1.299		
Hydrogen	111.0	111.0	1.118e+005		
Magnesium	0.0006871	0.0003486	8.466		
Nitrogen	0.0009257	0.0009257	12.96		
Oxygen	55.52	55.52	8.878e+005		
Potassium	0.0003530	0.0003530	13.79		
Sodium	0.005350	0.005350	122.9		
Sulfur	0.001312	0.001312	42.03		

The following is a summary of the React results for Groups 1 to 4 waters:

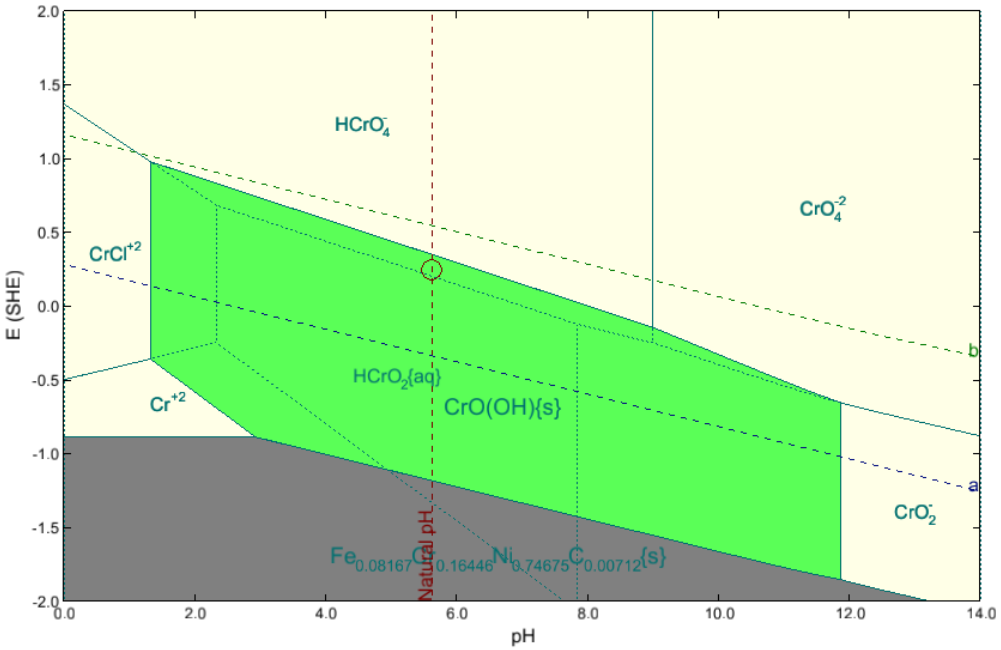
	Group 1 water		Group 2 water		Group 3 water		Group 4 water	
Original basis	moles	mg/kg	moles	mg/kg	moles	mg/kg	moles	mg/kg
Ca++	0.00039	15.5	0.00139	55.7	0.00191	76.4	0.00116	46.3
Cl-	0.00065	23	0.00189	67	0.00347	123	0.00412	146
F-	0.00012	2.2	7.37E-05	1.4	4.00E-05	0.76	6.84E-05	1.3
H+	-0.0003	-0.252	-0.0007	-0.692	-0.0001	-0.139	-0.0009	-0.906
H2O	55.5	1.00E+06	55.5	1.00E+06	55.5	9.99E+05	55.5	9.99E+05
HCO3-	0.00217	132	0.00108	66	0.001	61.1	0.001	61.2
K+	0.00012	4.8	0.00037	14.4	0.00023	9	0.00035	13.8
Mg++	2.52E-05	0.612	0.00017	4.07	0.0002	4.93	0.00035	8.47
NH3(aq)	0.00026	4.39	0.00071	12.1	0.00016	2.75	0.00093	15.8
Na+	0.00257	59	0.00196	45	0.0027	62	0.00535	123
O2(aq)	0.0014	44.8	0.0023	73.7	0.00121	38.6	0.00274	87.5
SO4--	0.00017	16	0.00085	82	0.00125	120	0.00131	126
SiO2(aq)	0.0001	6.12	0.0001	6.06	0.0001	6.06	—	—

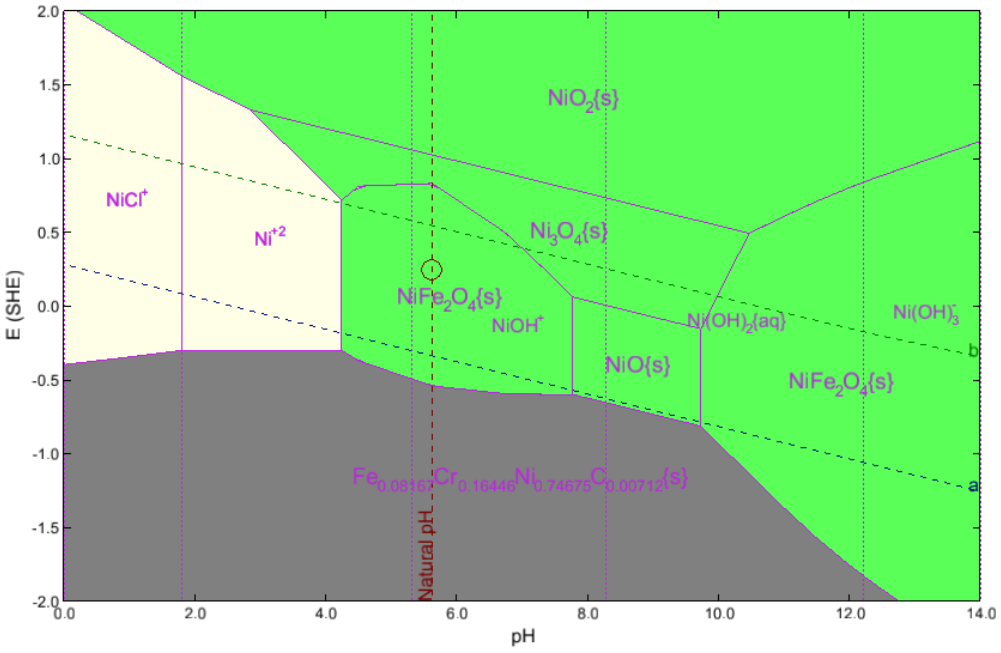
The following figure is a ternary Ca^{2+}–SO_4^{2-}–carbonate diagram showing the composition of Groups 1, 2, 3, and 4 waters, compared with YM unsaturated zone porewater compositions from Yang et al. (1996, 1998, 2003), and compositions of water sampled from the Drift Scale Test (see page 11 of this notebook).

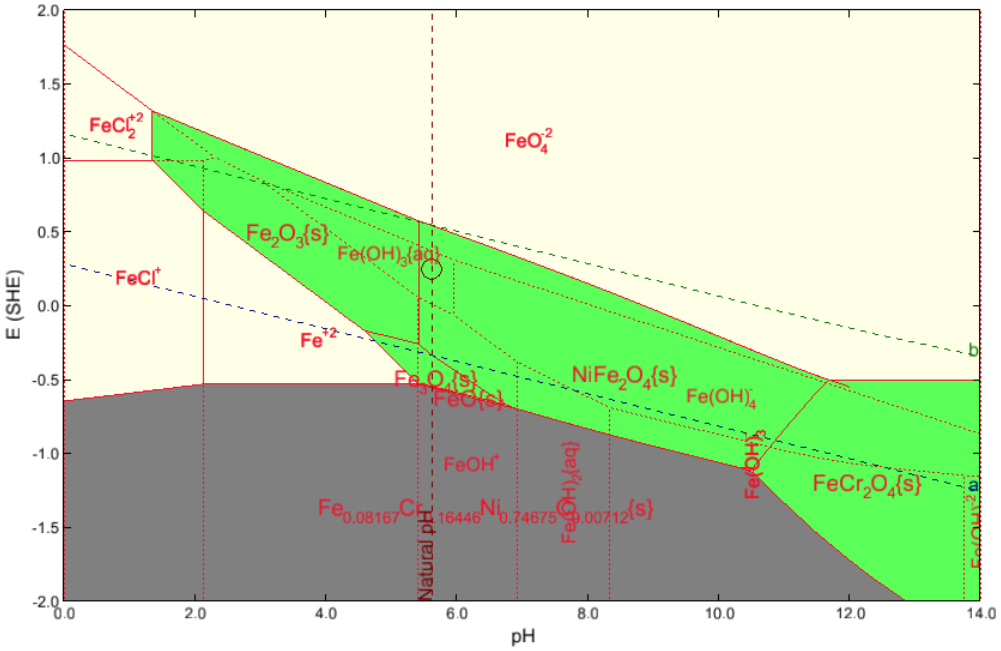


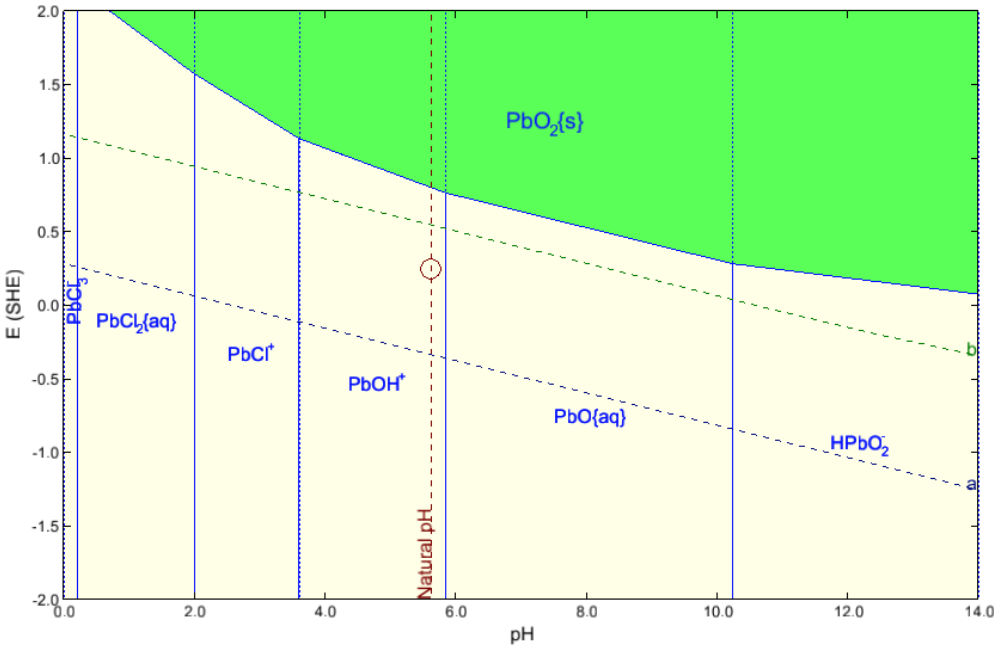
July 28, 2008

The following are the stability diagrams (chromium, nickel, and iron fields) of Alloy 600 at 280 °C and 65 bar in contact with pure water. The diagrams were calculated using CorrosionAnalyzer Version 2.0.

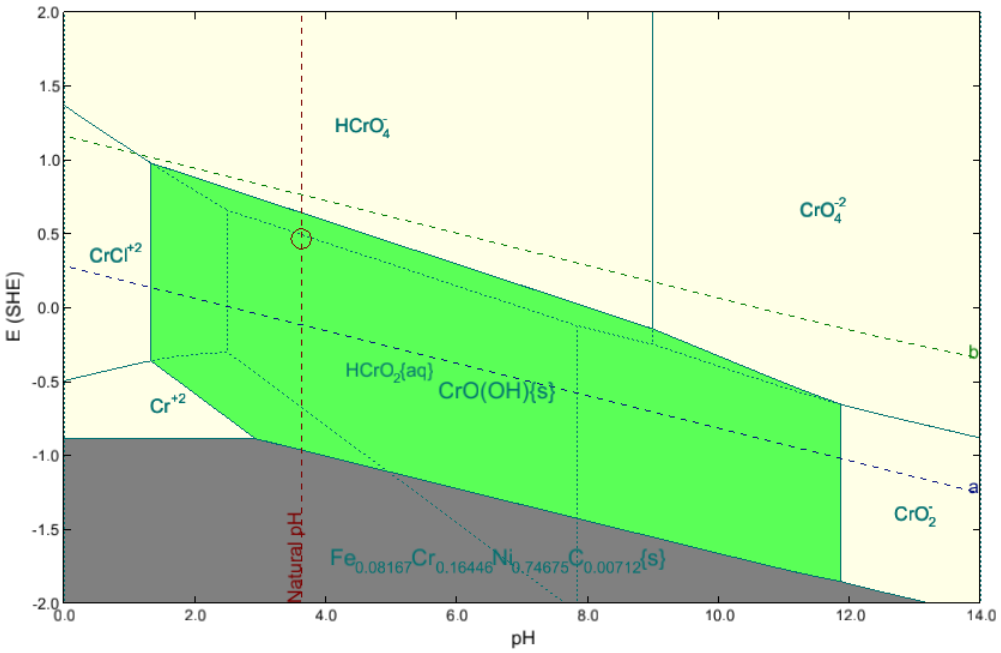


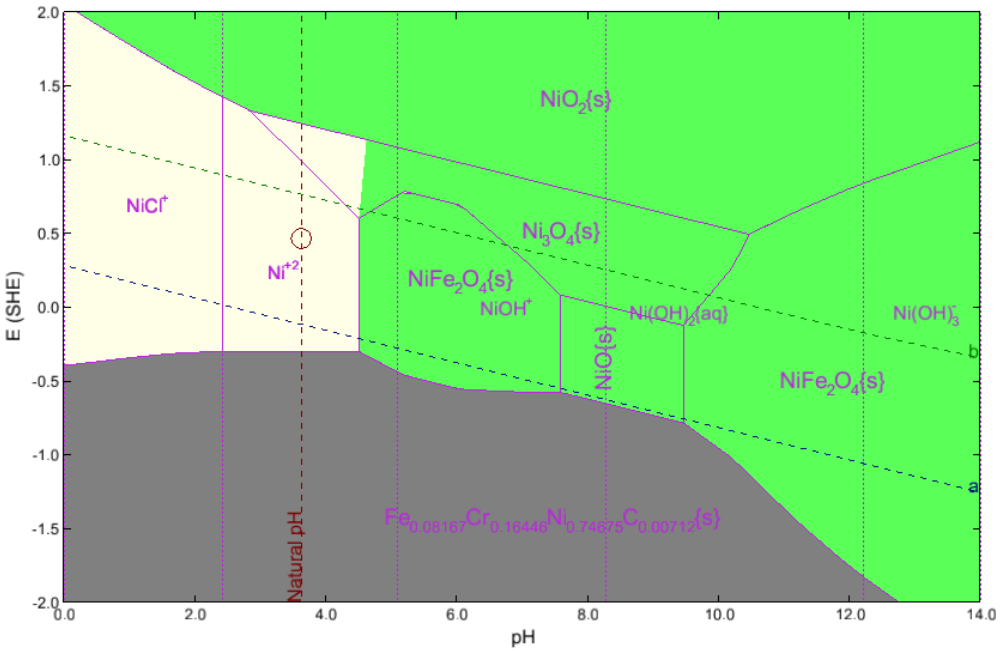


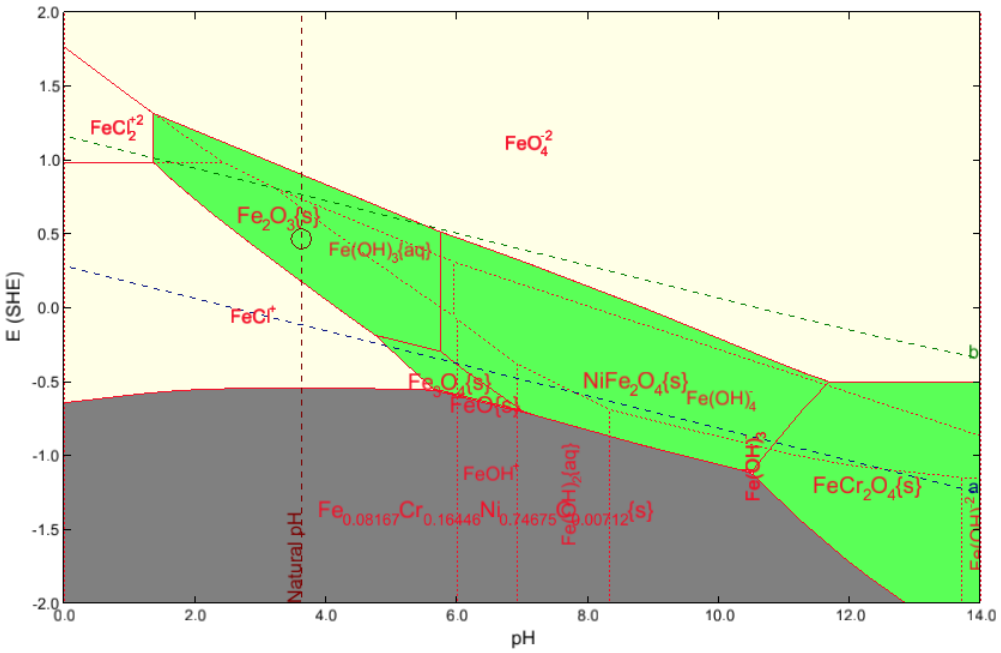

E (SHE)
pH
FeCl2+2
FeO4-2
Fe2O3{s}
Fe(OH)3{aq}
FeCl+
Fe+2
Fe3O4{s}
FeO{s}
NiFe2O4{s}
Fe(OH)-4
FeOH+
Fe(OH)2{aq}
Fe(OH)3
FeCr2O4{s}
Fe0.08167Cr1.16446Ni0.74675O4.00712{s}
Natural pH
a
b

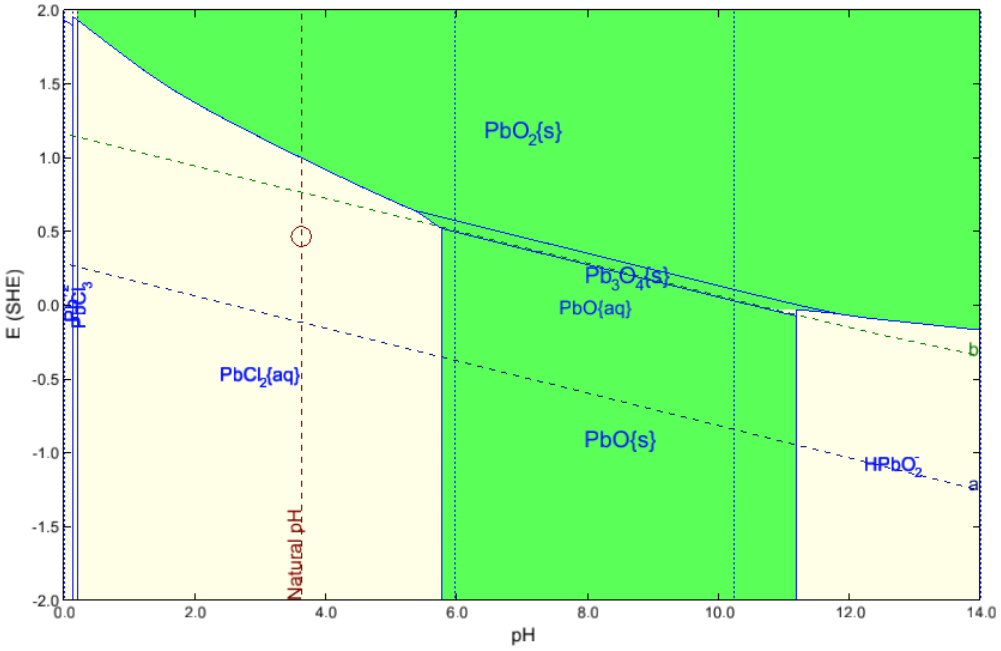

E (SHE)
pH
PbO2{s}
PbCl5-
PbCl2{aq}
PbCl+
PbOH+
PbO{aq}
HPbO2-
Natural pH
a
b

The following are the stability diagrams (lead, chromium, nickel, and iron fields) of Alloy 600 at 280 °C and 65 bar in contact with 0.0333 m $PbCl_2$ solution (6900 ppm Pb).



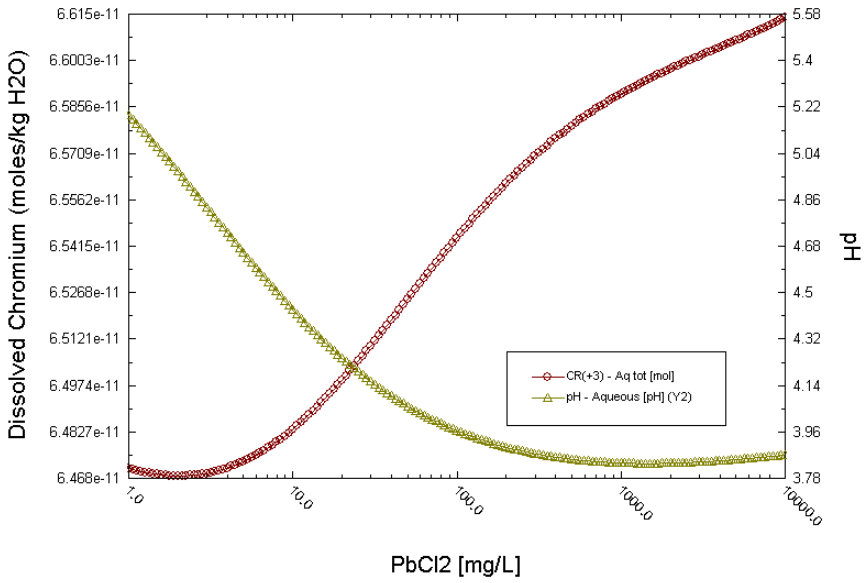


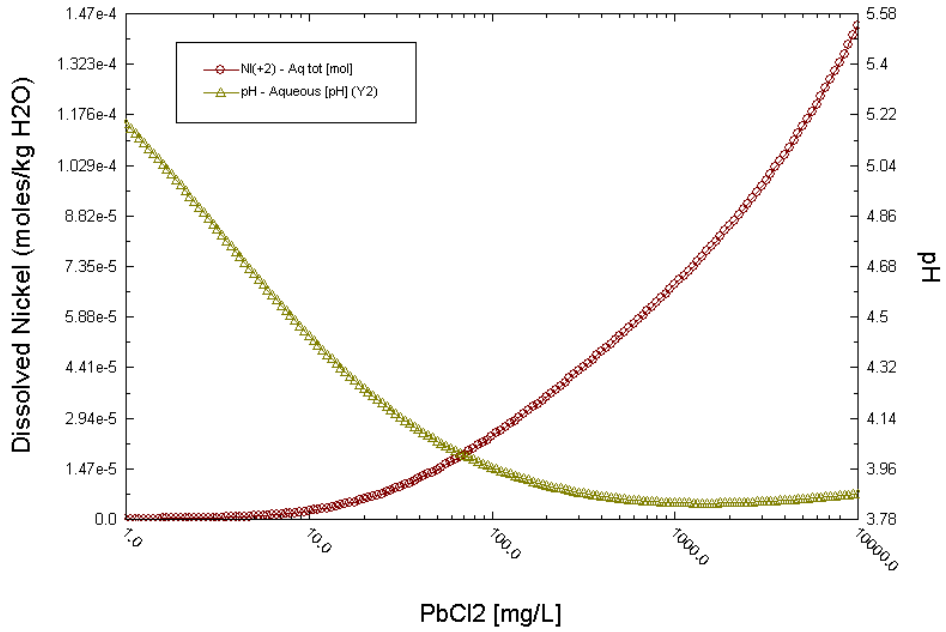


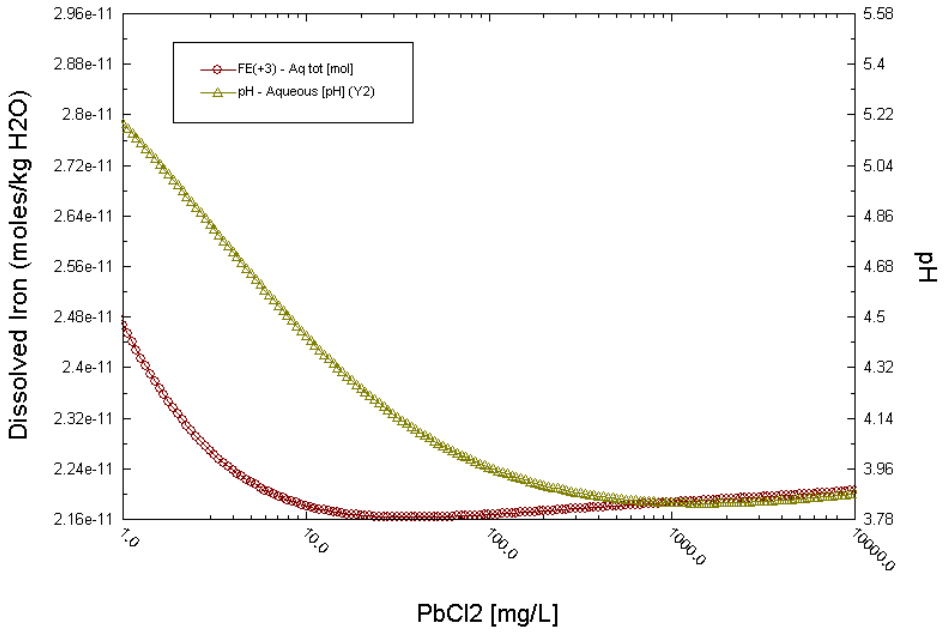


The above figures indicate that over a wide range of pH and oxidation/reduction potential, two solids, CrO(OH) and $NiFe_2O_4$ are stable. These solids possibly represent the passive film protecting Alloy 600 from corrosion. In the presence of 0.0333 m PbCl2, PbO(s) also is stable over a wide range of pH.

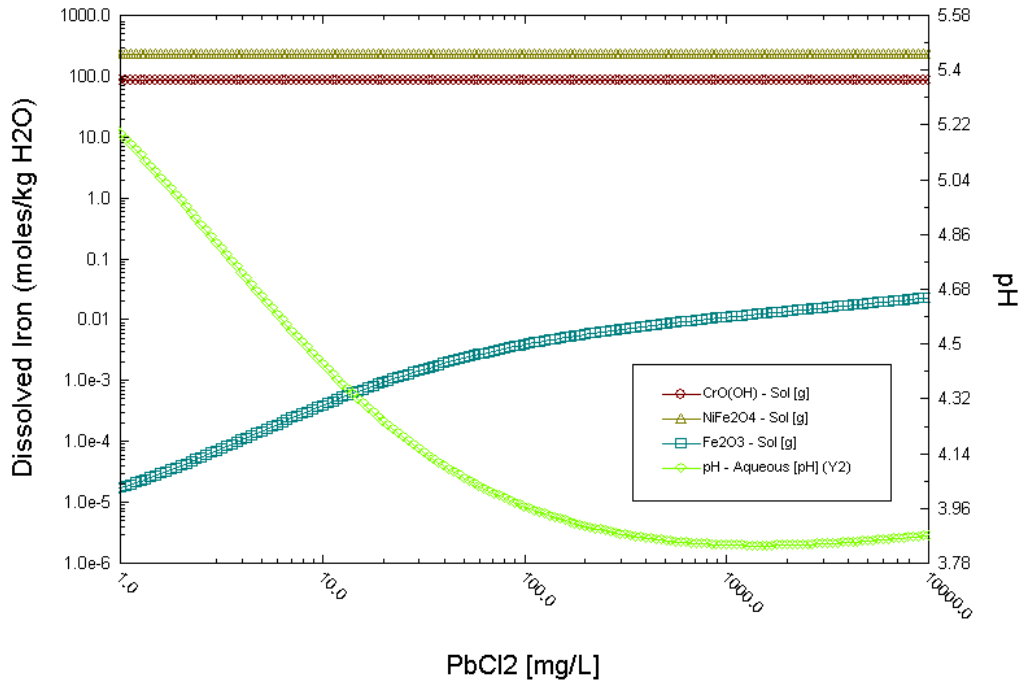
CorrosionAnalyzer Version 2 was used to calculate the solubility of CrO(OH) and $NiFe_2O_4$ at 280 °C and 65 bar as a function of $PbCl_2$ added to the system. The calculated pH and concentrations of chromium, nickel, and iron are shown below:







The following are the dominant solids present in the system:



Calculated solubility of CrO(OH) and NiFe2O4 at 280 °C and 65 bar:

The calculations were done using CorrosionAnalyzer (MSE aqueous model; Corrosion database included). In the calculations, the pH at 280 °C was fixed at the values indicated below. In contrast, in the experiments reported by Sakai et al. (1992), the pH was adjusted at 25 °C and the solubility of Alloy 600 was measured at 280 °C.

1. 0.0333 molal $PbCl_2$ (6900 ppm Pb) solution with pH fixed at 3.0 (adjusted with HCl):

1.56490e-10 mole/kg H2O	8.13685E-06 ppm	Cr^{3+}
0.0212535 mole/kg H2O	1.2476E+03 ppm	Ni^{2+}
1.14253e-10 mole/kg H2O	6.3807E-06 ppm	Fe^{3+}

2. 0.01834 molal $PbCl_2$ (3800 ppm Pb) solution with pH fixed at 4.5 (adjusted with NaOH):

9.21685e-11 mole/kg H2O	4.79239E-06 ppm	Cr^{3+}
7.88598e-6 mole/kg H2O	4.6291E-01 ppm	Ni^{2+}
3.14070e-11 mole/kg H2O	1.7540E-06 ppm	Fe^{3+}

3. 1.448E-3 molal $PbCl_2$ (300 ppm Pb) solution with pH fixed at 7.0 (adjusted with NaOH):

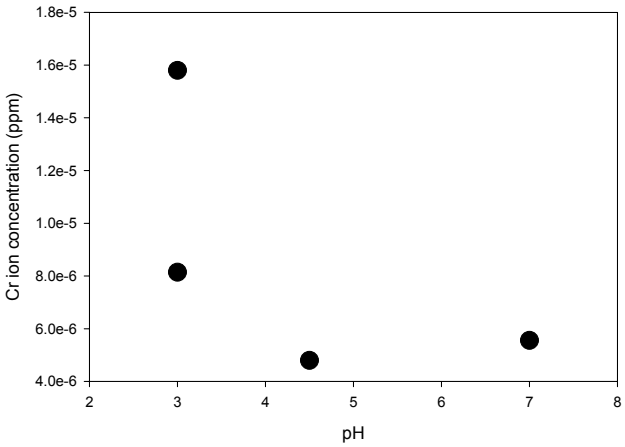
1.06818e-10 mole/kg H2O	5.55411E-06 ppm	Cr^{3+}
1.19470e-9 mole/kg H2O	7.0129E-05 ppm	Ni^{2+}
4.04027e-10 mole/kg H2O	2.2564E-05 ppm	Fe^{3+}

4. 0.2413 molal $PbCl_2$ (50 g/L Pb) solution with pH fixed at 3.0 (adjusted with HCl):

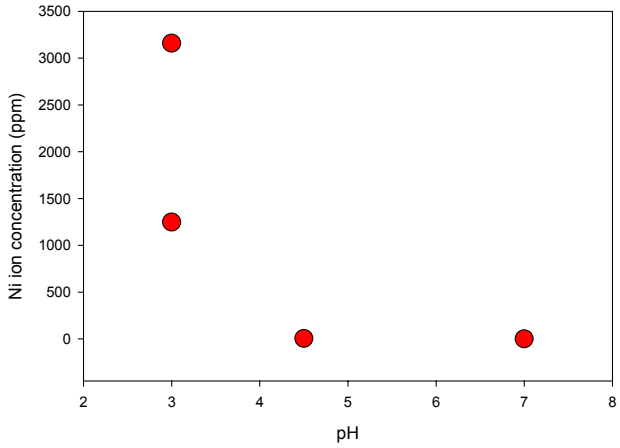
3.05E-10 mole/kg H2O	1.58E-05 ppm	Cr^{3+}
0.053898 mole/kg H2O	3.16E+03 ppm	Ni^{2+}
3.29E-10 mole/kg H2O	1.84E-05 ppm	Fe^{3+}

The calculated dissolved concentrations of chromium, nickel, and iron at 280 °C versus the pH measured at 25 °C are shown in the following page.

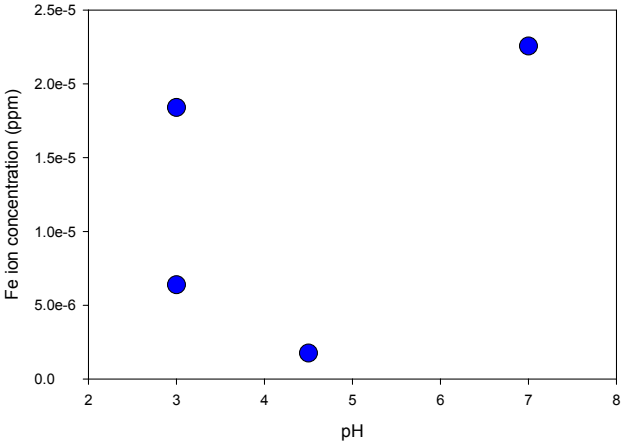
Dissolved Chromium Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



Dissolved Nickel Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)

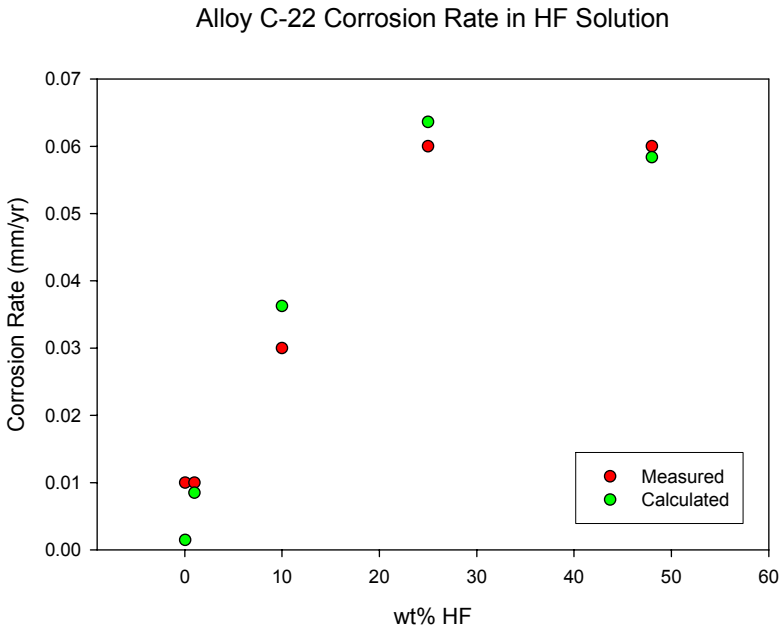


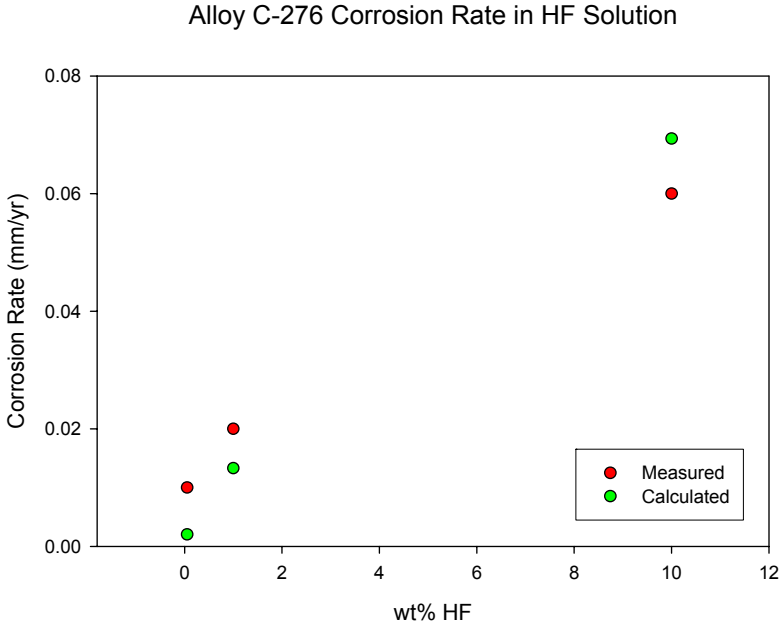
Dissolved Iron Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



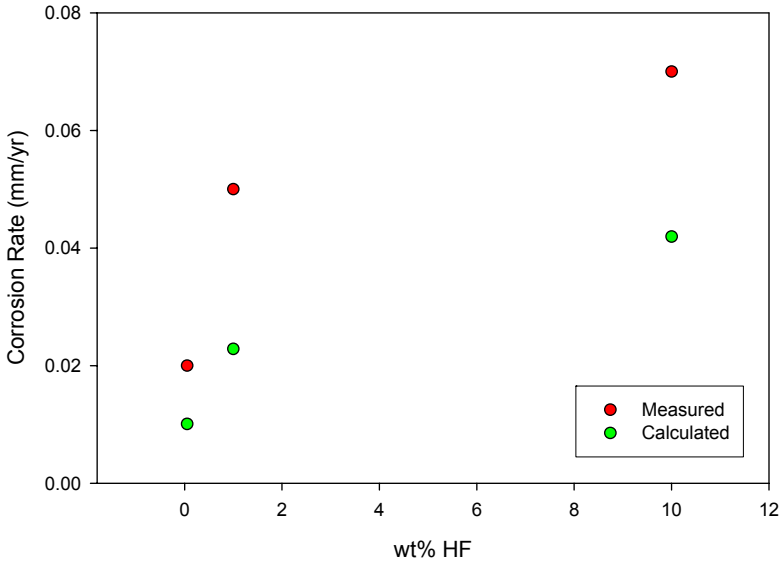
July 30, 2008

General corrosion rate of various alloys in HF solutions at 24 °C were calculated using CorrosionAnalyzer Version 2.0 (aqueous H+ model). The calculated values are compared to values measured by Pawel (1994) in the following figures:

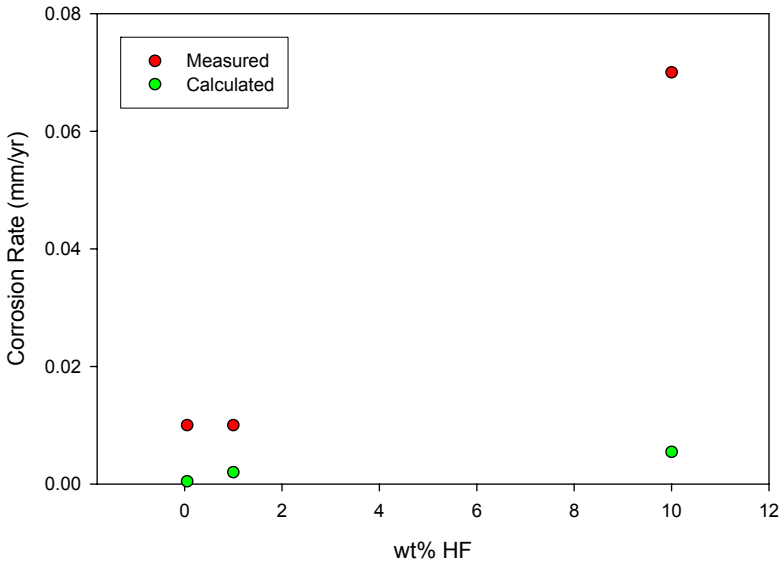


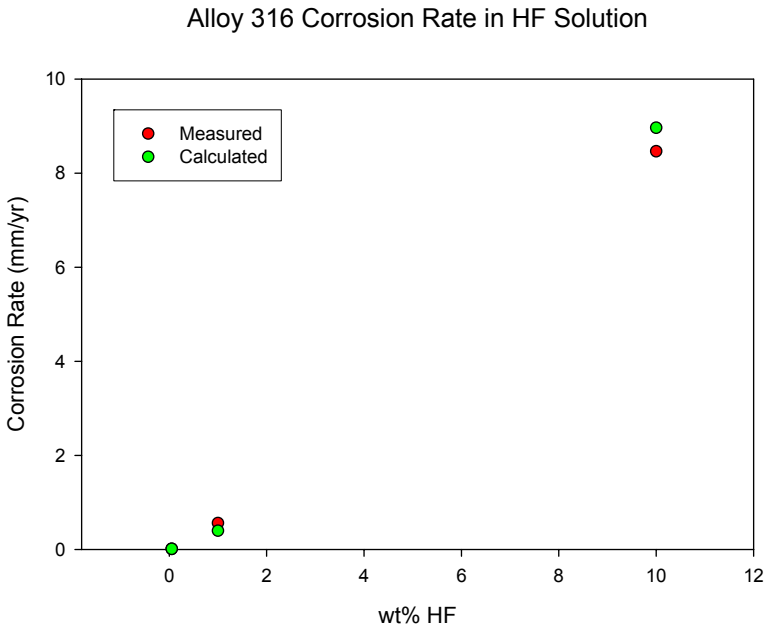


Alloy 600 Corrosion Rate in HF Solution

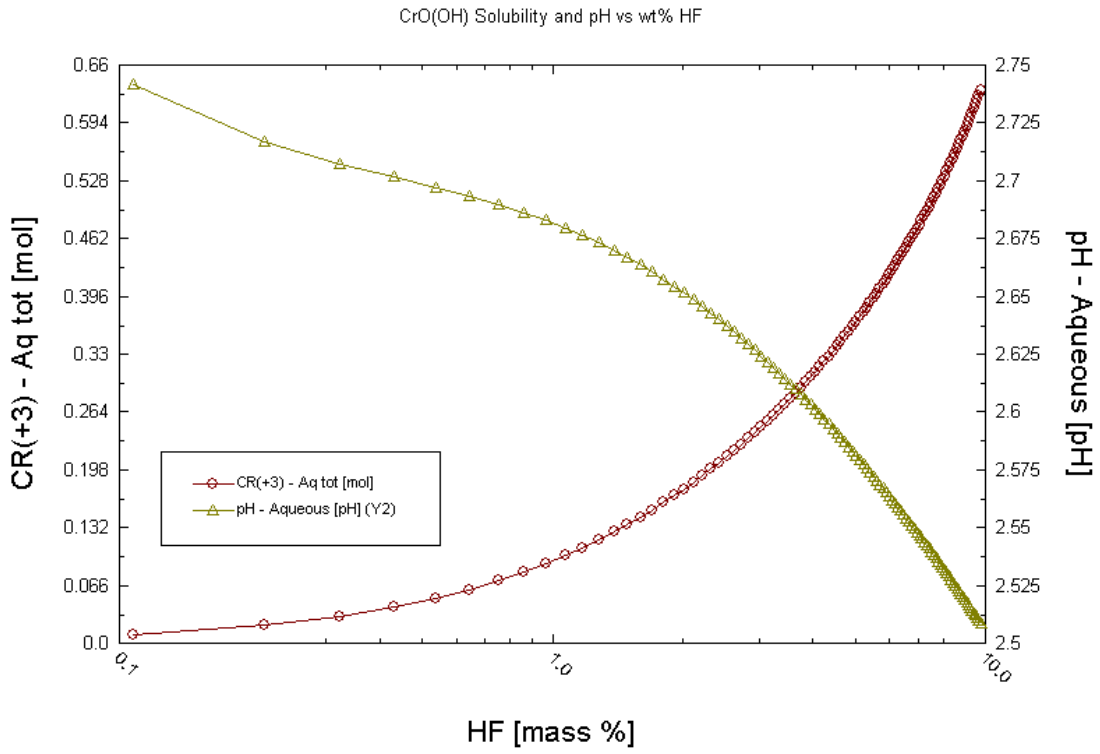


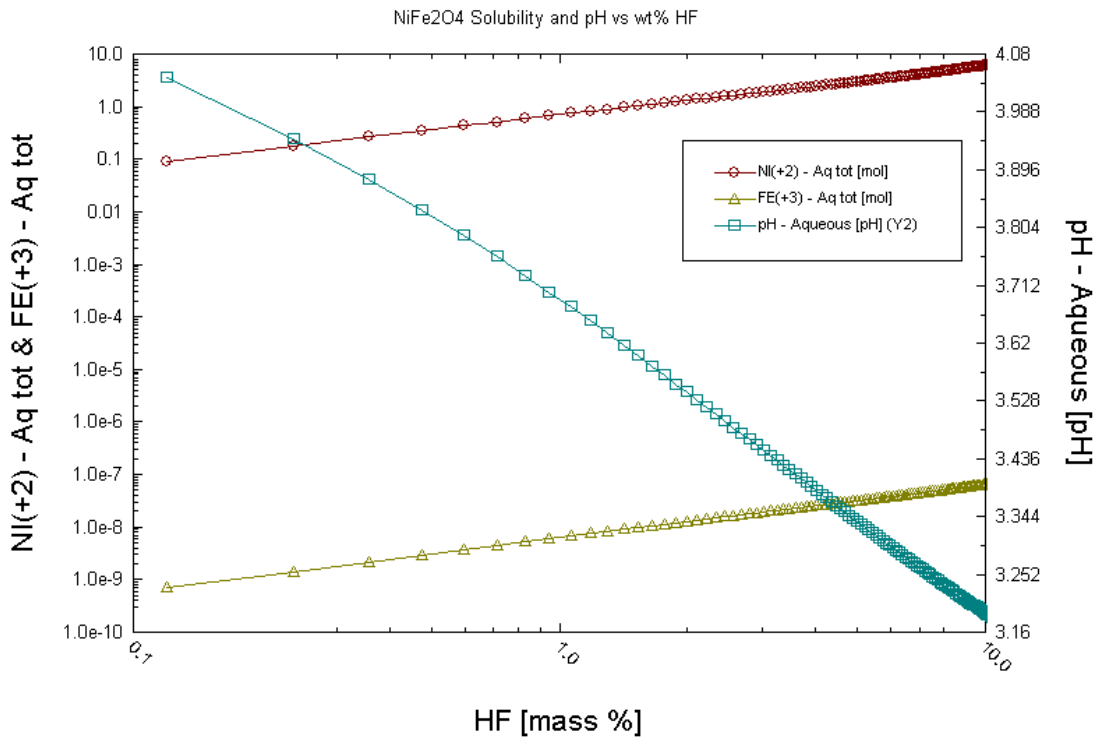
Alloy 825 Corrosion Rate in HF Solution





Calculated solubility of CrO(OH) and NiFe2O4 (possible oxide films on the surface of Alloy C-22) at 24 °C in HF solutions calculated using CorrosionAnalyzer Version 2.0:




NiFe2O4 Solubility and pH vs wt% HF
Ni(+2) - Aq tot & FE(+3) - Aq tot
pH - Aqueous [pH]
HF [mass %]
Ni(+2) - Aq tot [mol]
FE(+3) - Aq tot [mol]
pH - Aqueous [pH] (Y2)
10.0
1.0
0.1
0.01
1.0e-3
1.0e-4
1.0e-5
1.0e-6
1.0e-7
1.0e-8
1.0e-9
1.0e-10
4.08
3.988
3.896
3.804
3.712
3.62
3.528
3.436
3.344
3.252
3.16
0.1
1.0
10.0

To mimick the Sakai et al. (1992) experiments more closely, the pH of the $PbCl_2$ solutions was adjusted at 25 °C, and a stream was generated of the equilibrated $PbCl_2$ solution at the gixed pH was created. Subsequently, the solubility of CrO(OH) and NiFe2O4 was calculated at 280 °C and 65 bar. The calculated dissolved metal concentrations and pH are given below:

1. 0.0333 molal $PbCl_2$ (6900 ppm Pb) solution with pH fixed at 3.0 at 25 °C (adjusted with HCl); Calculated pH = 3.60 at 280 °C; pH measured after the test (at 25 °C) by Sakai et al. (1992) = 3.03.

9.5783E-11 moles/kg H2O	4.9803E-06 ppm	Cr^{3+}
5.8996E-04 moles/kg H2O	3.4631E+01 ppm	Ni^{2+}
3.2459E-11 moles/kg H2O	1.8127E-06 ppm	Fe^{3+}

2. 0.01834 molal $PbCl_2$ (3800 ppm Pb) solution with pH fixed at 4.5 at 25 °C (adjusted with NaOH); Calculated pH = 3.92 at 280 °C; pH measured after the test (at 25 °C) by Sakai et al. (1992) = 3.08.

9.3414E-11 moles/kg H2O	4.8572E-06 ppm	Cr^{3+}
1.0454E-04 moles/kg H2O	6.1367E+00 ppm	Ni^{2+}
3.1051E-11 moles/kg H2O	1.7341E-06 ppm	Fe^{3+}

3. 1.448E-3 molal $PbCl_2$ (300 ppm Pb) solution with pH fixed at 7.0 at 25 °C (adjusted with NaOH); Calculated pH = 5.16 at 280 °C; pH measured after the test (at 25 °C) by Sakai et al. (1992) = 3.40.

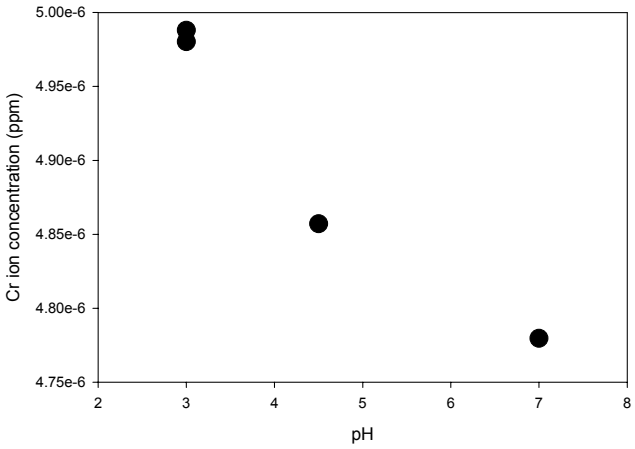
9.1924E-11 moles/kg H2O	4.7797E-06 ppm	Cr^{3+}
2.5214E-07 moles/kg H2O	1.4801E-02 ppm	Ni^{2+}
3.5254E-11 moles/kg H2O	1.9689E-06 ppm	Fe^{3+}

4. 0.2413 molal $PbCl_2$ (50 g/L Pb) solution with pH fixed at 3.0 at 25 °C (adjusted with HCl); Calculated pH = 3.75 at 280 °C; pH measured after the test (at 25 °C) by Sakai et al. (1992) = 3.71.

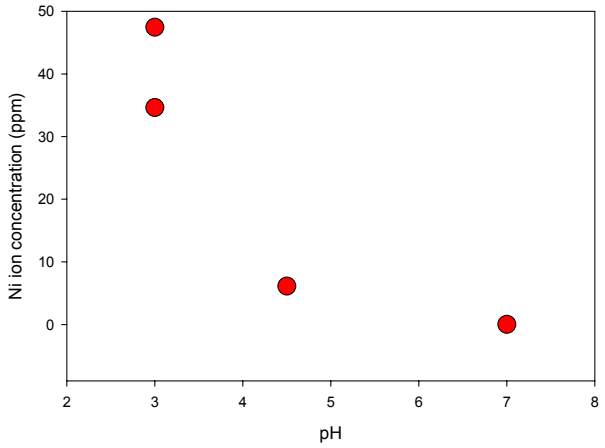
9.5931E-11 moles/kg H2O	4.9880E-06 ppm	Cr^{3+}
8.0831E-04 moles/kg H2O	4.7448E+01 ppm	Ni^{2+}
3.2677E-11 moles/kg H2O	1.8249E-06 ppm	Fe^{3+}

The calculated dissolved concentrations of chromium, nickel, and iron at 280 °C versus the pH measured at 25 °C are shown in the following page.

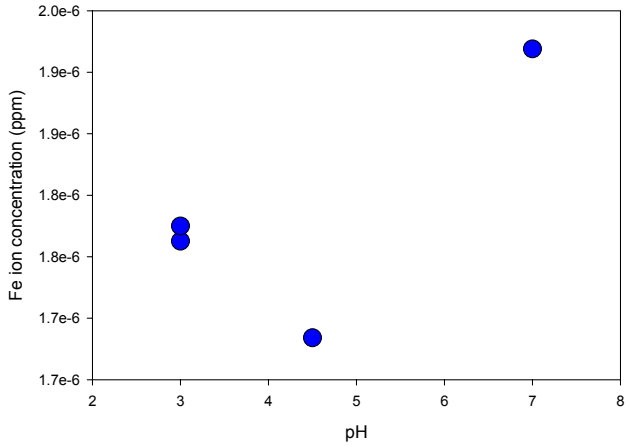
Dissolved Chromium Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



Dissolved Nickel Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



Dissolved Iron Concentration in $PbCl_2$ Solutions
in Contact with CrO(OH) and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



August 21, 2008

Below is an email from Andre Anderko (OLI Systems) advising of new model parameters for FeCr2O4 and NiCr2O4:

From: Andre Anderko [aanderko@olisystems.com]
Sent: Thursday, August 21, 2008 12:03 PM
To: rpabalan@cnwra.swri.edu
Cc: 'Berthold'
Subject: RE: Corrosion Analyzer MSE vs H+

Bobby:

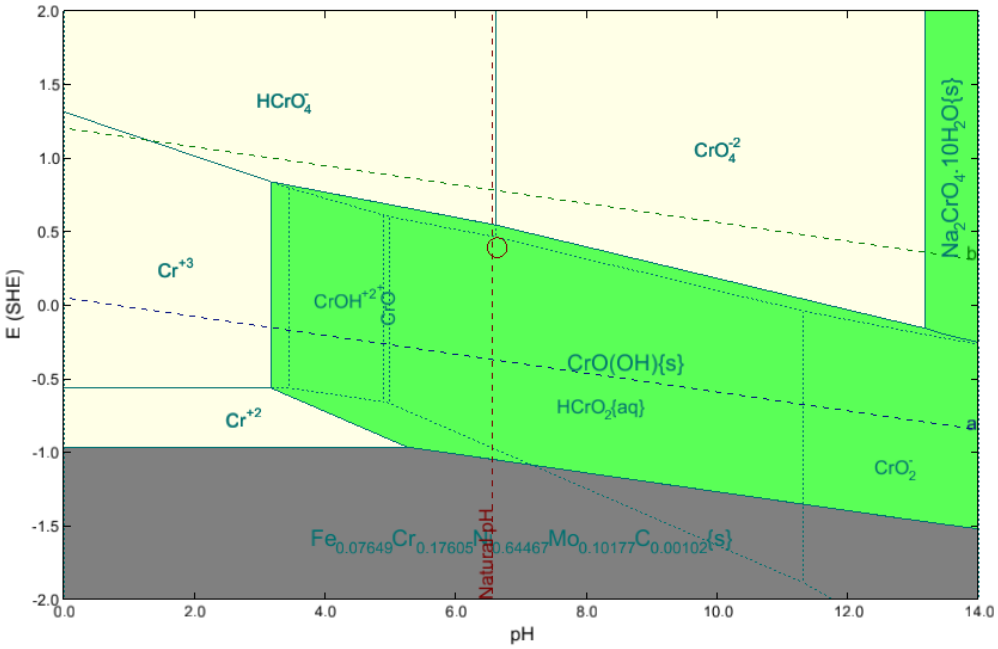
Some time ago, we discussed issues related to mixed oxides (Fe-Ni-Cr) in our software. I am writing to let you know that we have completed our analysis of FeCr2O4 and NiCr2O4 in addition to our previous work on NiFe2O4. The new parameters are in the latest build of the software (Analyzers 2.0.60 and ESP 8.0.60), which is available for downloading from our website. I am attaching a spreadsheet that compares our calculated results with experimental data.

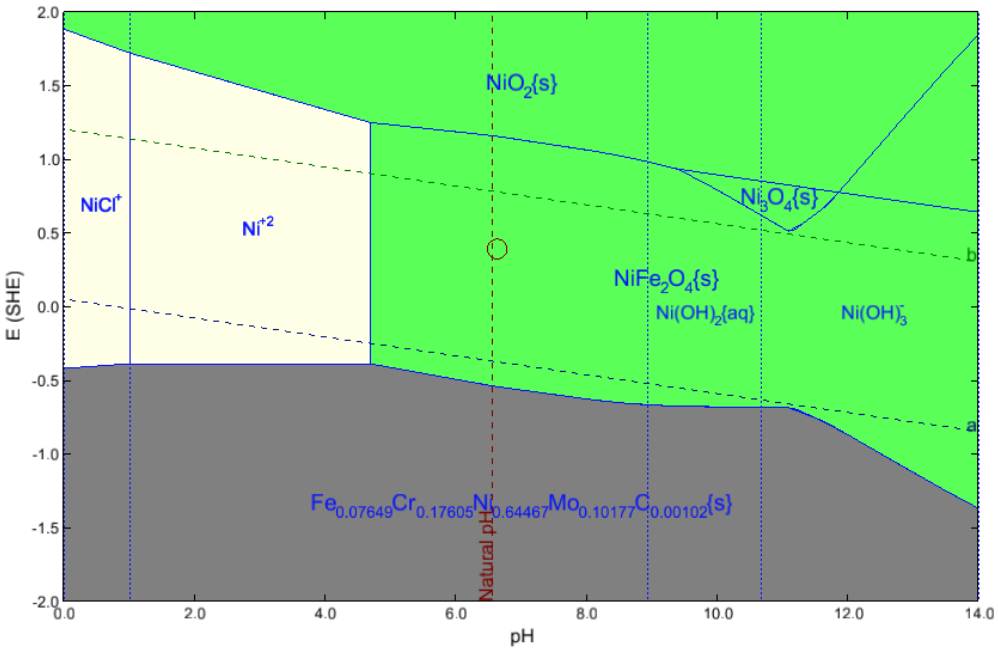
Best regards,
Andre

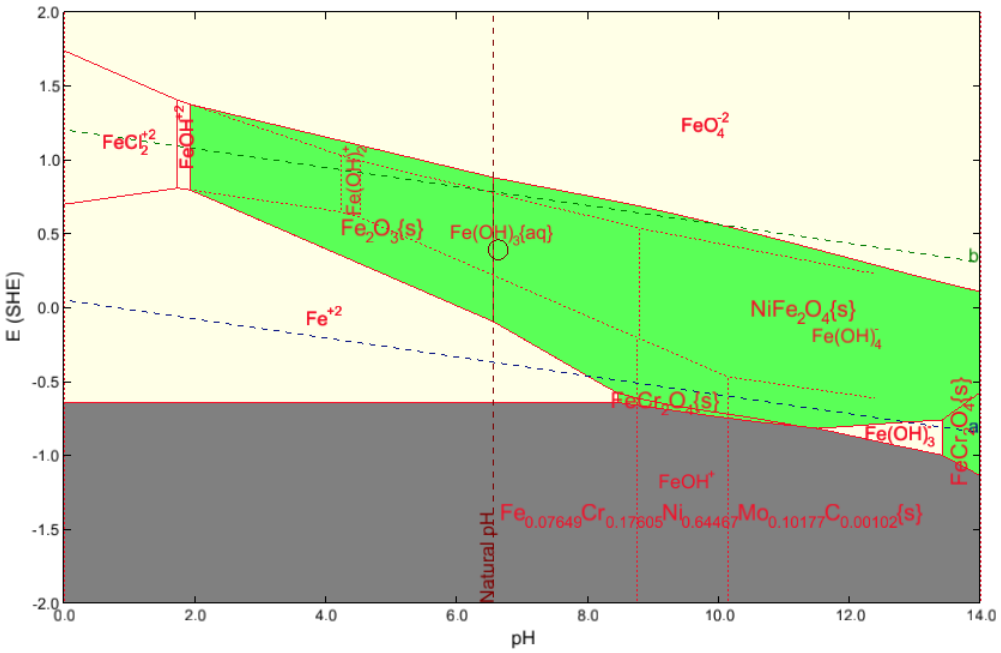
An updated version of the software will be downloaded from the OLI Systems website and installed for use in future calculations.

August 22, 2008

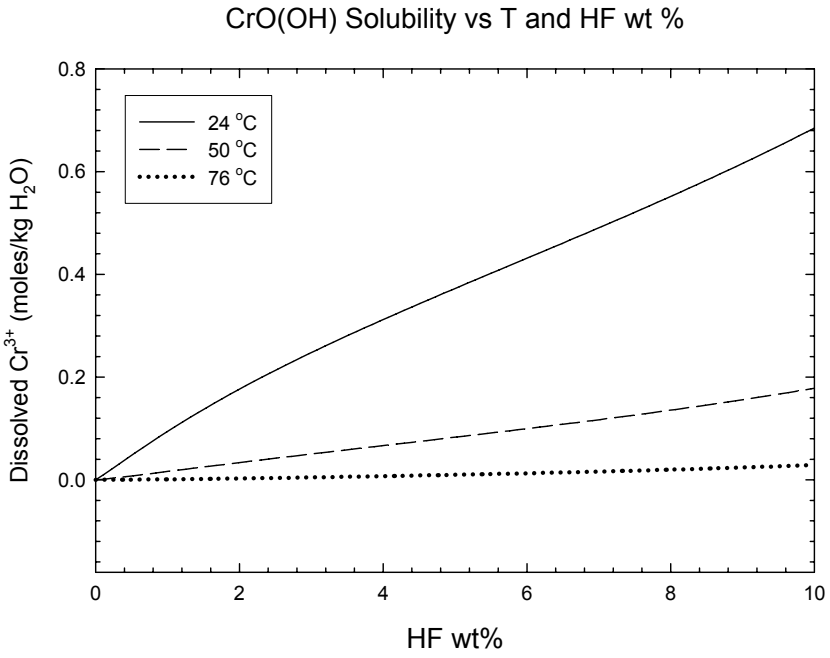
The following are the stability diagrams (chromium, nickel, and iron fields) of Alloy 276 at 50 °C and 1 bar in contact with pure water. The diagrams were calculated using CorrosionAnalyzer 2.0.

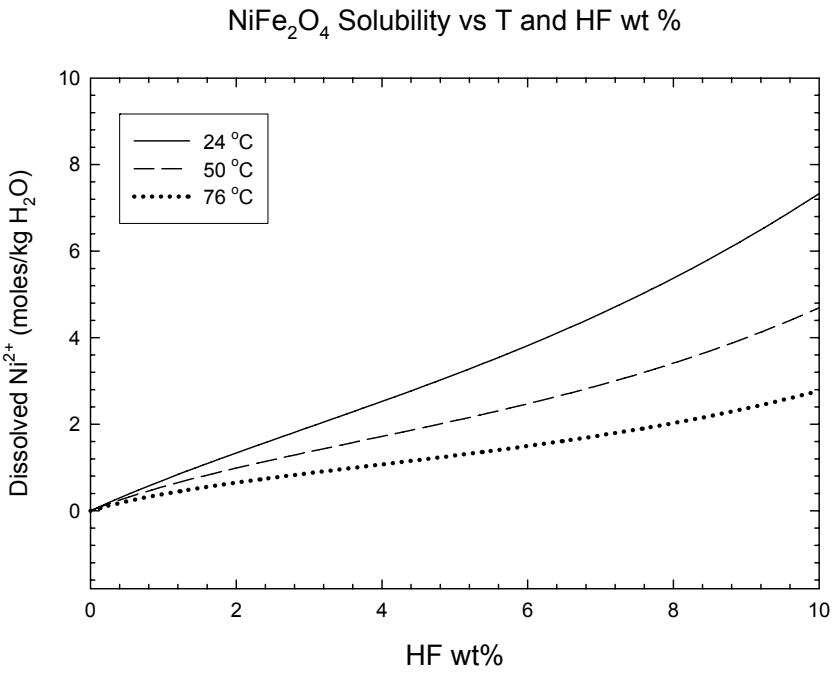




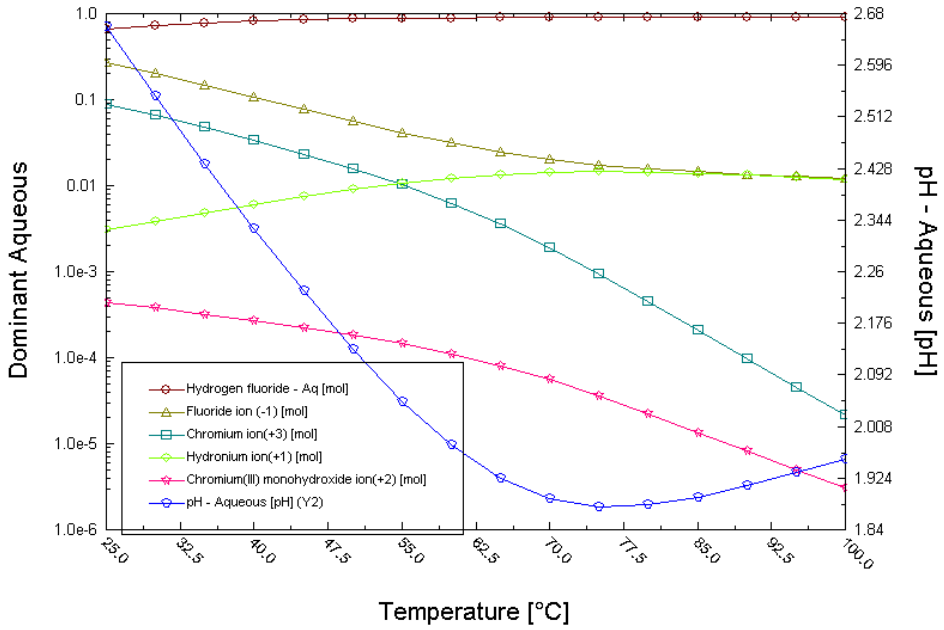


The following figures compare the solubility of CrO(OH) and NiFe2O4 versus HF concentration and temperature.



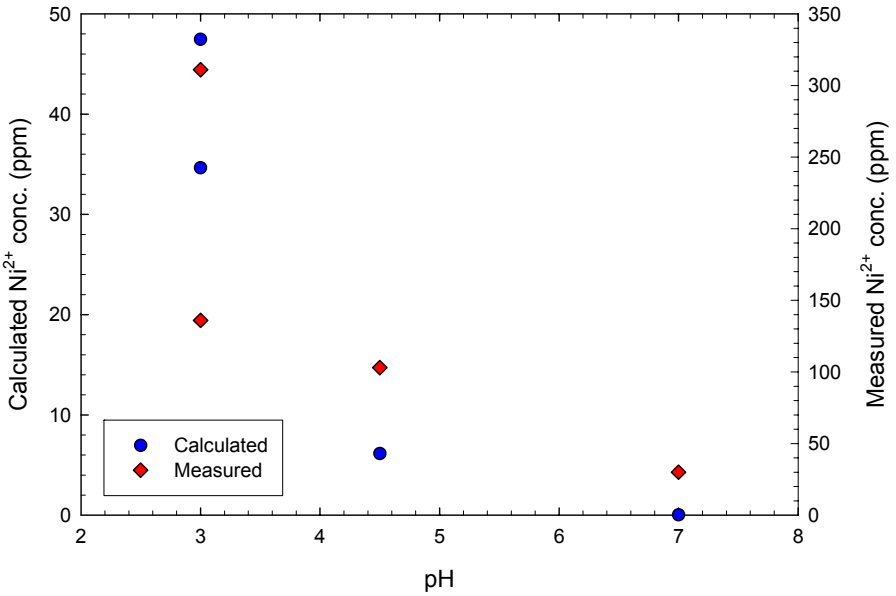


CorrosionAnalyzer Version 2.0 was used to calculate the solubility of CrO(OH) in HF solutions as a function of temperature. At a fixed HF concentration of 1 wt%, the pH and dominant aqueous species are plotted in the following figure.

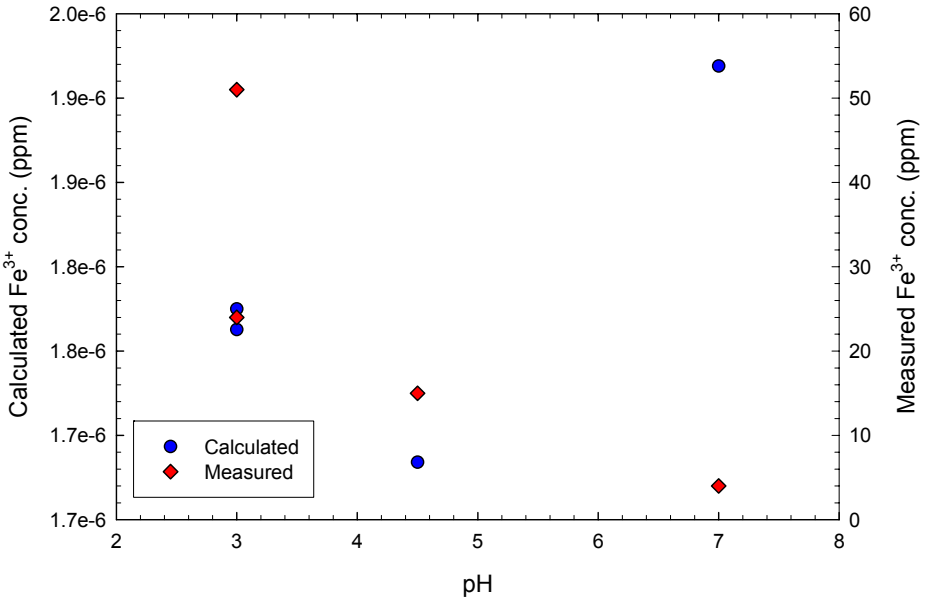


The following figures compare dissolved nickel and iron concentrations calculated using CorrosionAnalyzer 2.0 versus experimental data from Sakai et al. (1992):

Dissolved Nickel Concentration in $PbCl_2$ Solutions
in Contact with $CrO(OH)$ and $NiFe_2O_4$ (Alloy 600 Surface Oxides)



Dissolved Iron Concentration in $PbCl_2$ Solutions
in Contact with $CrO(OH)$ and $NiFe_2O_4$ (Alloy 600 Surface Oxides)

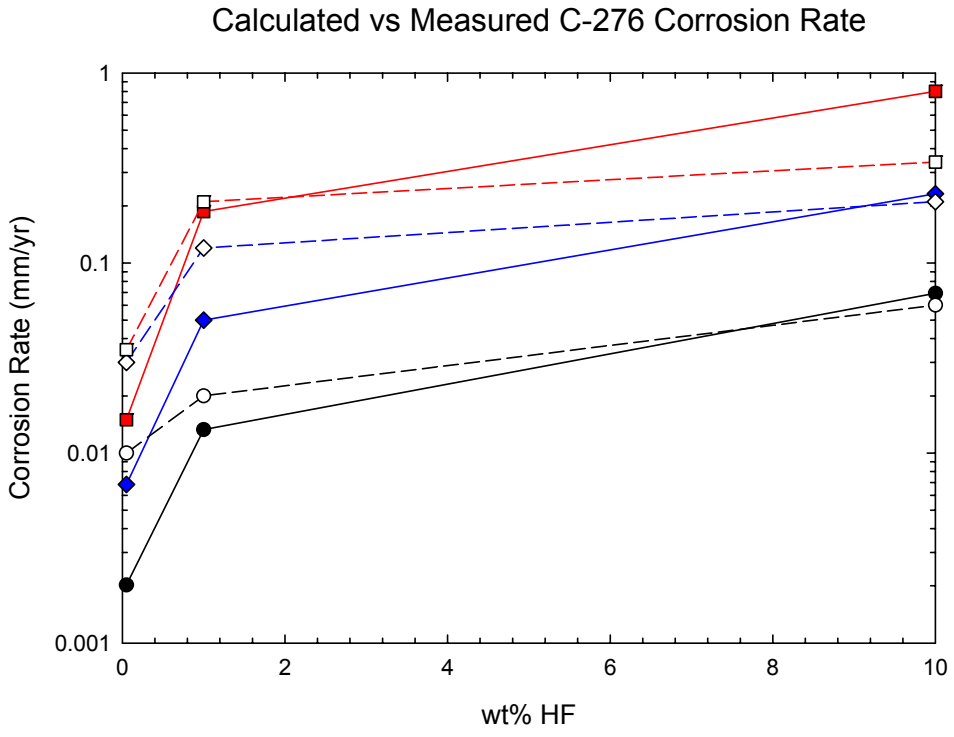


August 25, 2008

The following are the general corrosion rates of Alloy 276 calculated using CorrosionAnalyzer 2.0 (aqueous H+ model) at 24, 50, and 76 °C and various HF weight%. Values from Pawel (1994) also are listed.

wt% HF	pH, calc	24C Gen Cor Rate		Pawel 1994
0.05	2.43993	2.02E-03	mm/yr	0.01
1	1.73254	1.33E-02	mm/yr	0.02
10	0.975661	0.0693388	mm/yr	0.06
wt% HF	pH, calc	50C Gen Cor Rate		Pawel 1994
0.05	2.50572	6.84E-03	mm/yr	0.03
1	1.79986	0.0500626	mm/yr	0.12
10	1.02738	0.231235	mm/yr	0.21
wt% HF	pH, calc	76 C Gen Cor Rate		Pawel 1994
0.05	2.61739	0.0149851	mm/yr	0.03
1	1.91084	0.186628	mm/yr	0.21
10	1.12236	0.800537	mm/yr	0.34

The following figure compares the measured corrosion rate of C-276 reported by Pawel et al. (1994) at various HF wt% and temperatures with the general corrosion rate calculated using CorrosionAnalyzer 2.0 (aqueous H+ model).



Entries into Scientific Notebook No. 930E for the period March 1, 2008 through September 30, 2008, have been made by

4/22/10

Roberto T. Pabalan *I* Date

No original entry into this Scientific Notebook has been removed.

4/22/10

Roberto T. Pabalan *I* Date

ELECTRONIC NOTEBOOK #930E

October 1, 2008 through September 30, 2009

20.14002.01.353

Roberto T. Pabalan

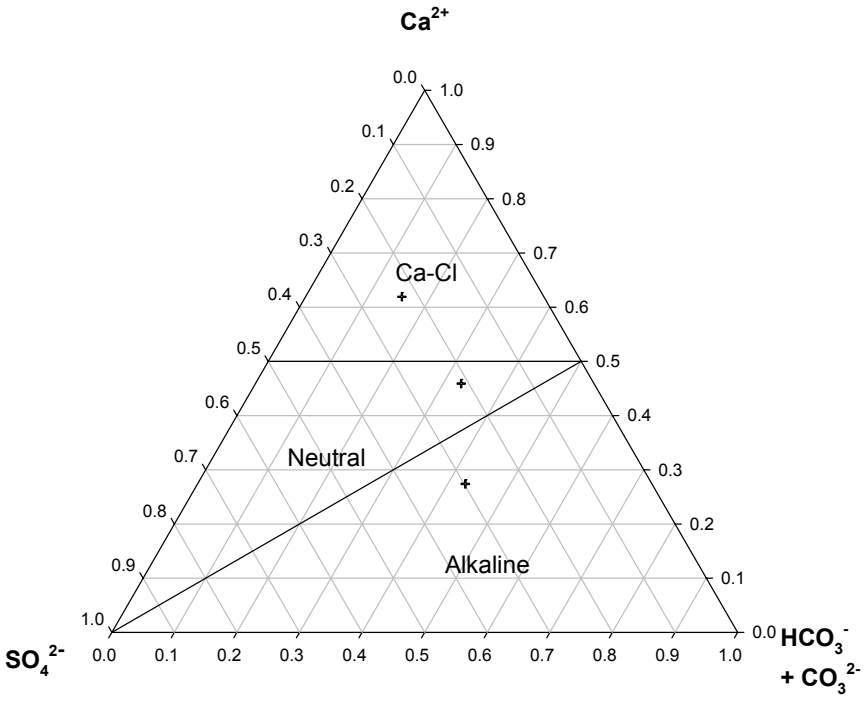
The entries in this electronic scientific notebook #930E document activities conducted during the period October 1, 2008, through September 30, 2009, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.14002.01.353).

January 6, 2009

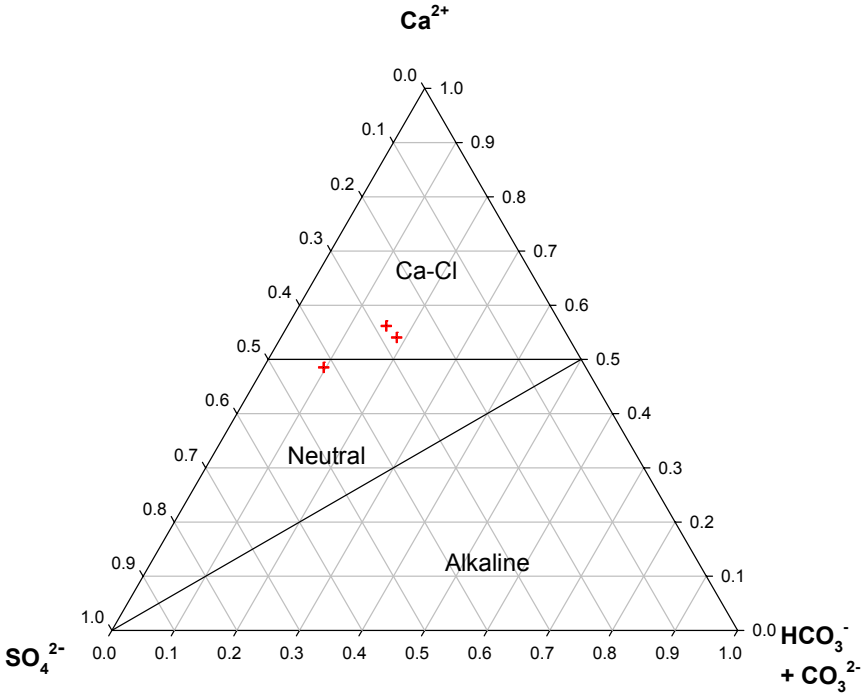
The following figures are ternary Ca^{2+}–SO_4^{2-}–(HCO_3^-+CO_3^{2-}) plots of Yucca Mountain water compositions listed in the document "COMPREHENSIVE COMPILATION OF AVAILABLE YUCCA MOUNTAIN POREWATER AND OTHER COMPOSITION DATA -- all_porewater_compositions_06_11_2007.pdf" that is available at www.lsnnet.gov. Page 1 of the file indicates the file was created by David Shields, with dates of 05/04/2006 to 06/11/2007. It is a comprehensive compilation of available Yucca Mountain porewater and other water composition data. It includes the USGS water composition data reported by Yang et al. (1996, 1998, 2003) and other DOE and Nye County results. The file indicates the sample collection method, lithology unit, hydrology unit, DTN number or source, and QA status, in addition to the chemical composition.

The data points plotted in the figure are only those that have a quality assurance status of "Q." The following table compares the number of data points plotted in the figures with those plotted previously in scientific notebook #679, page 157. In that figure, USGS data from samples taken mostly above the water table (i.e., unsaturated zone porewaters) were plotted. The figures below used all available "Q" data from the compilation by D. Shields.

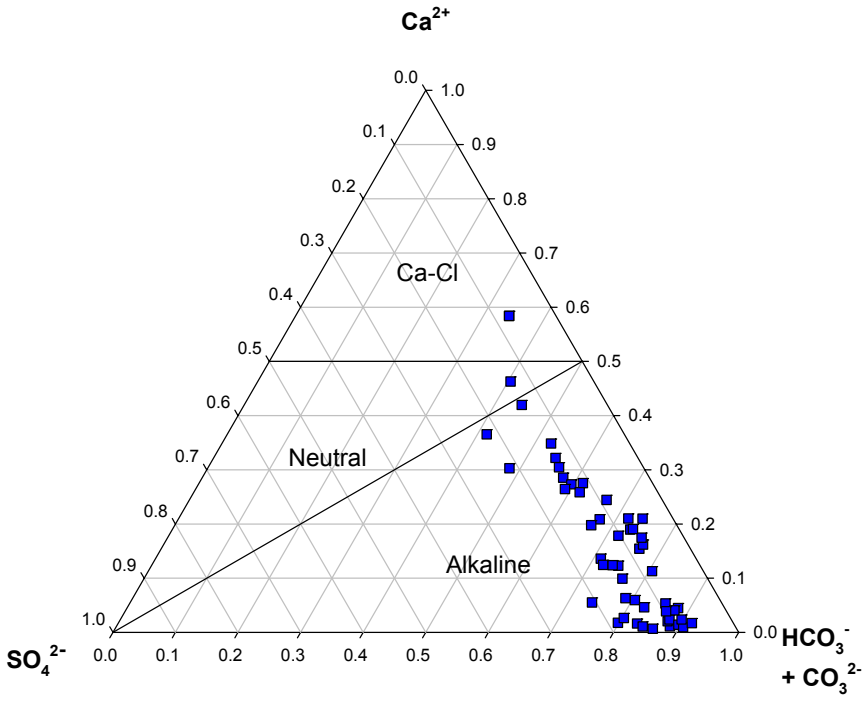
Sample Site	Number of data points plotted in the figures below	Number of USGS data points plotted in the figures below	Number of USGS data points plotted in previous work	Number of non-USGS data points plotted in the figures below
UZN55	3	3		
UZ-7A	3	3		
UZ-16	51	51	**26** (out of 30)	
UZ-14	61	61	**47**	
NRG-6	7	7	**7**	
NC-EWDP	**43**			**43**
SD-6	25 (out of 27)	25	**22**	
SD-12	14	14	**13**	
SD-7	19	19	**5** out of 14	
WT-24	36 (out of 38)	36	**18** out of 35	
ESF-HD-PERM	**7**			**7**
ESF-THERMALK	**7**			**7**
ESF-HD-ChemSamp	**17**			**17**
ESF-SR-MS	**6**			**6**
ESF-NR-MS	**5**			**5**
NRG-7A	7	7	**5**	
SD-9	37 (out of 49)	37	**13**	
ECRB-SYS-CS	**31**			**31**
TOTAL	**379**	**263**	**156**	**116**



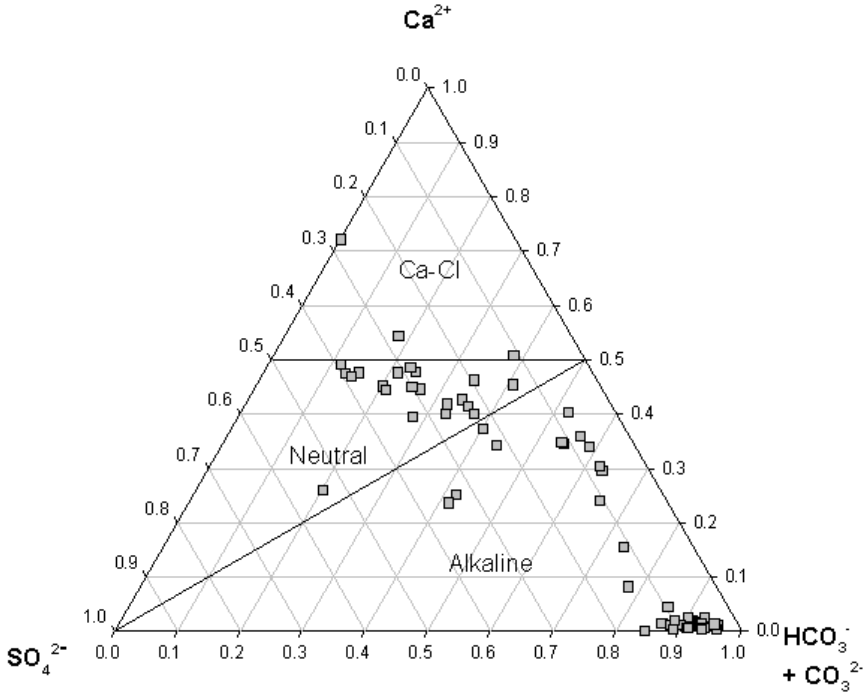
UZN55 Samples



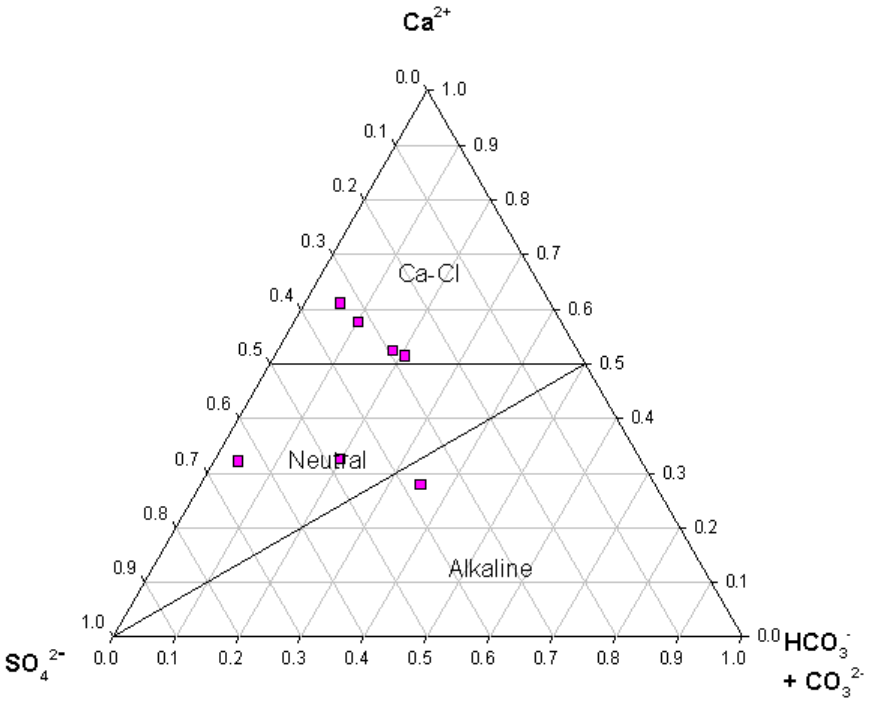
UZ-7A Samples



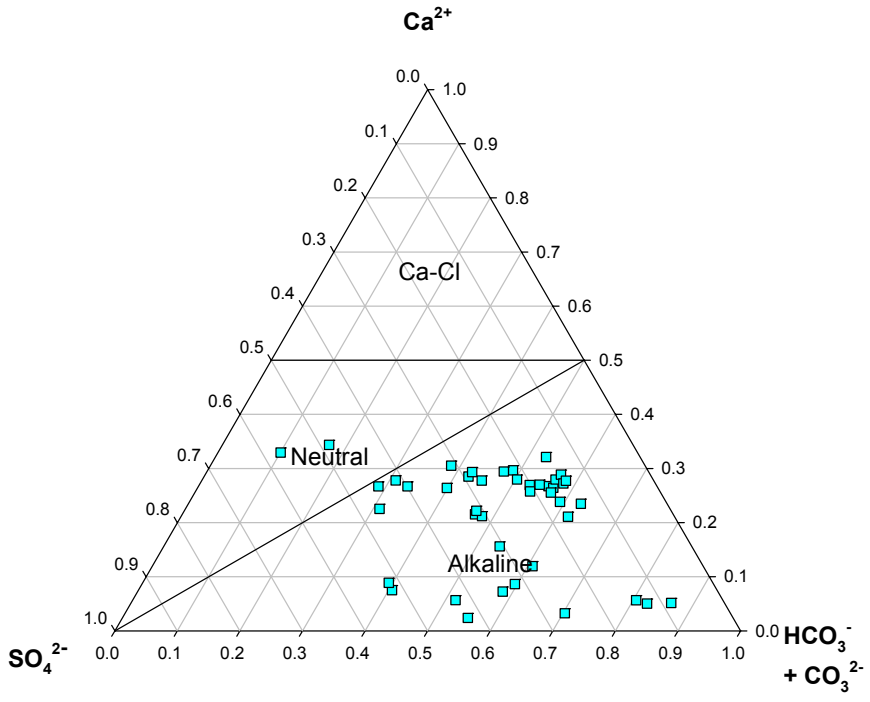
UZ-16 Samples



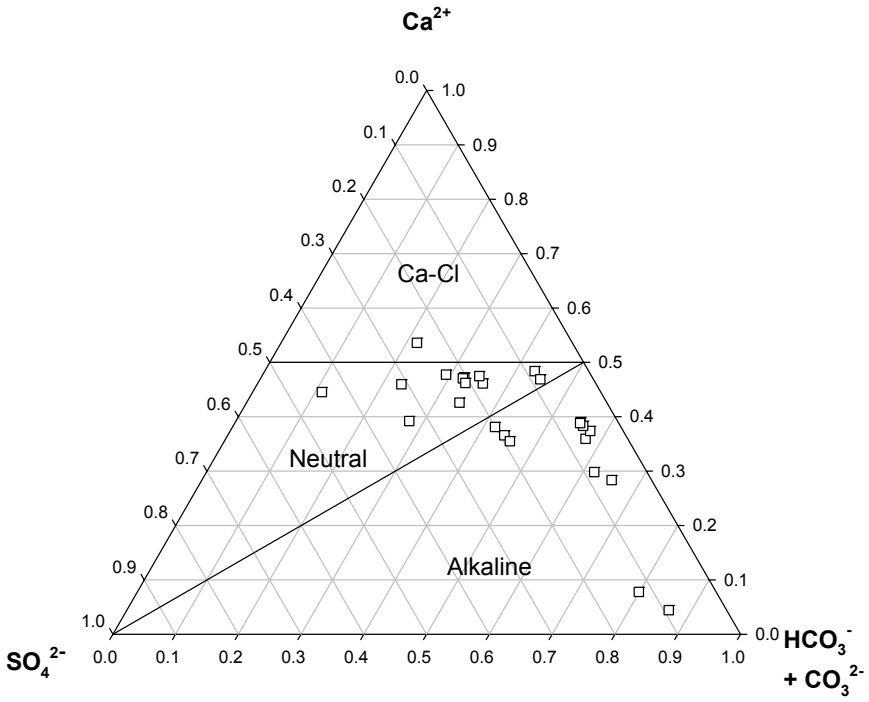
UZ-14 Samples



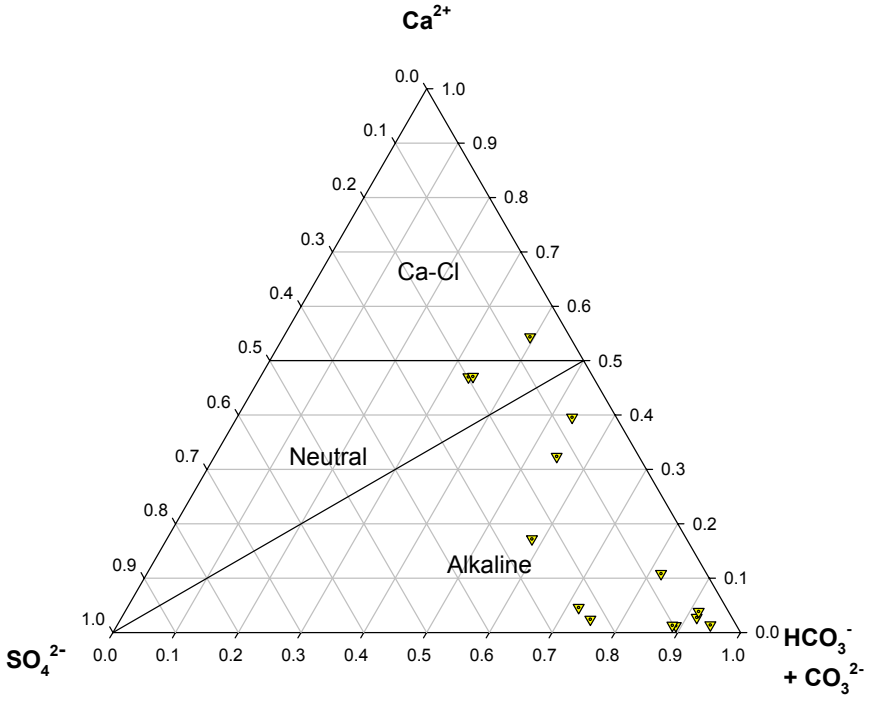
NRG-6 Samples



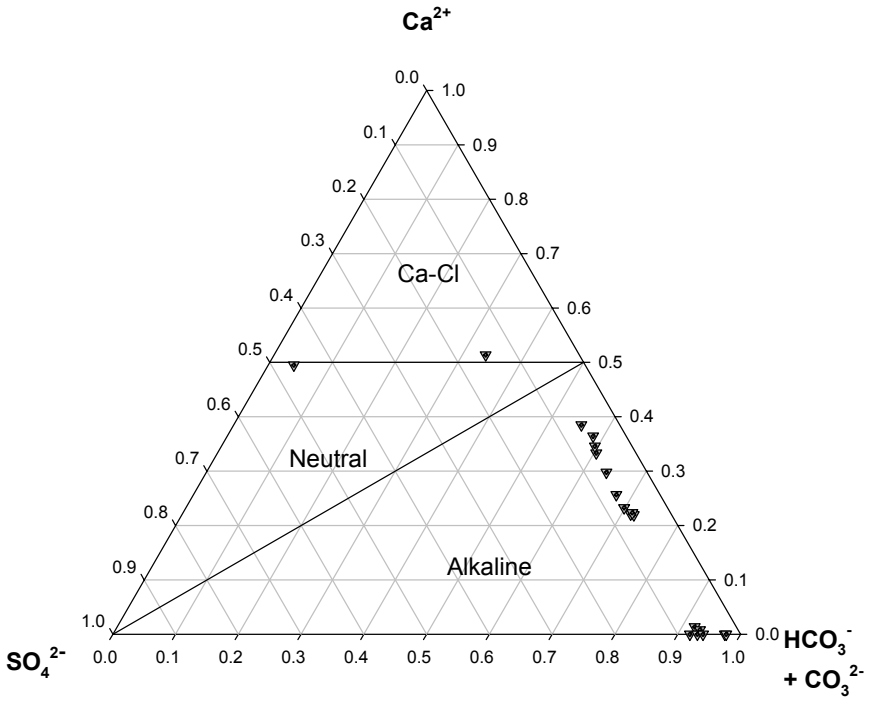
NC-EWDP Samples



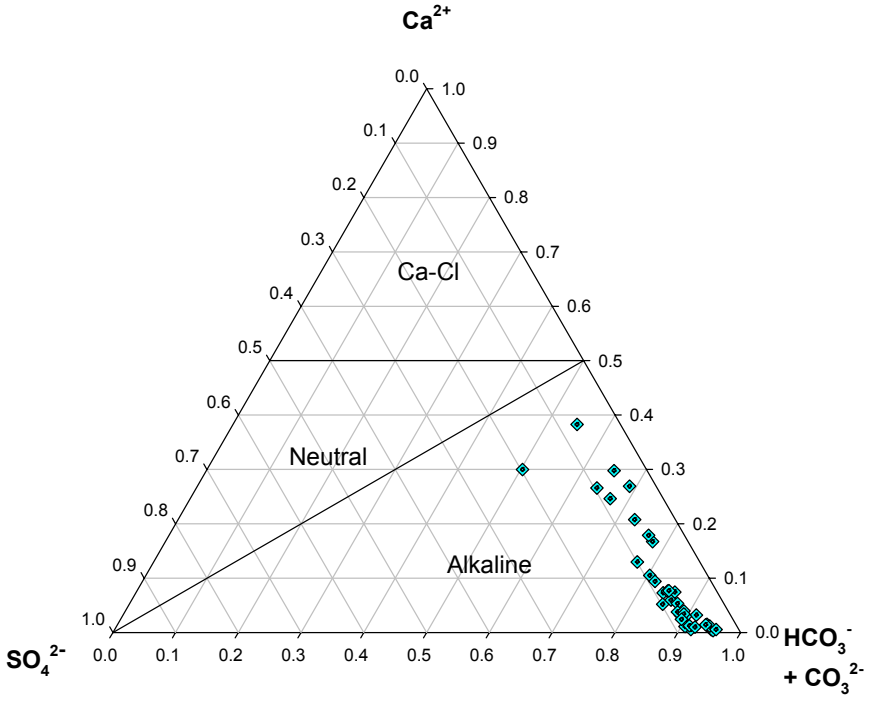
SD-6 Samples



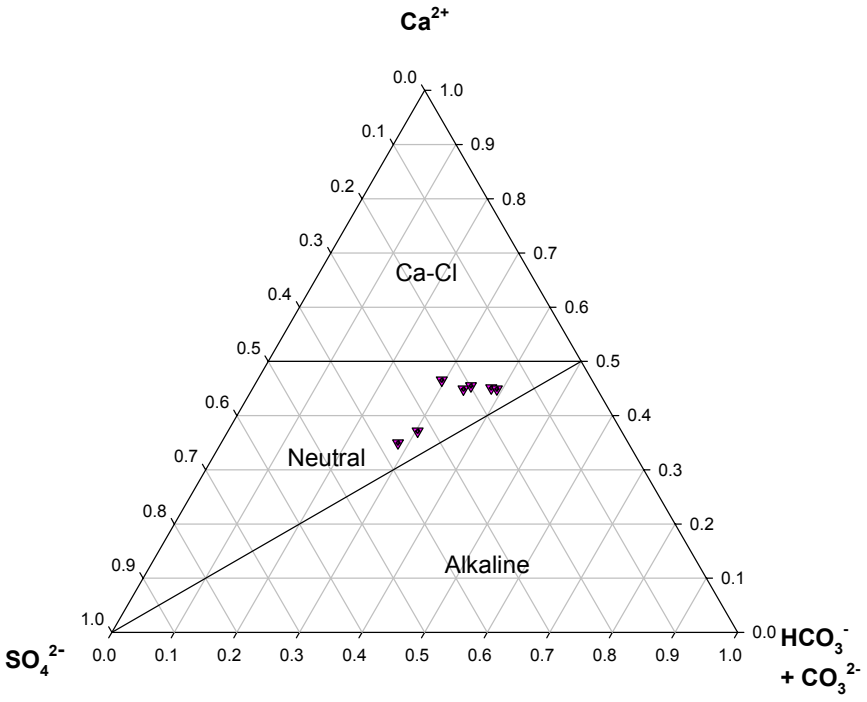
SD-12 Samples



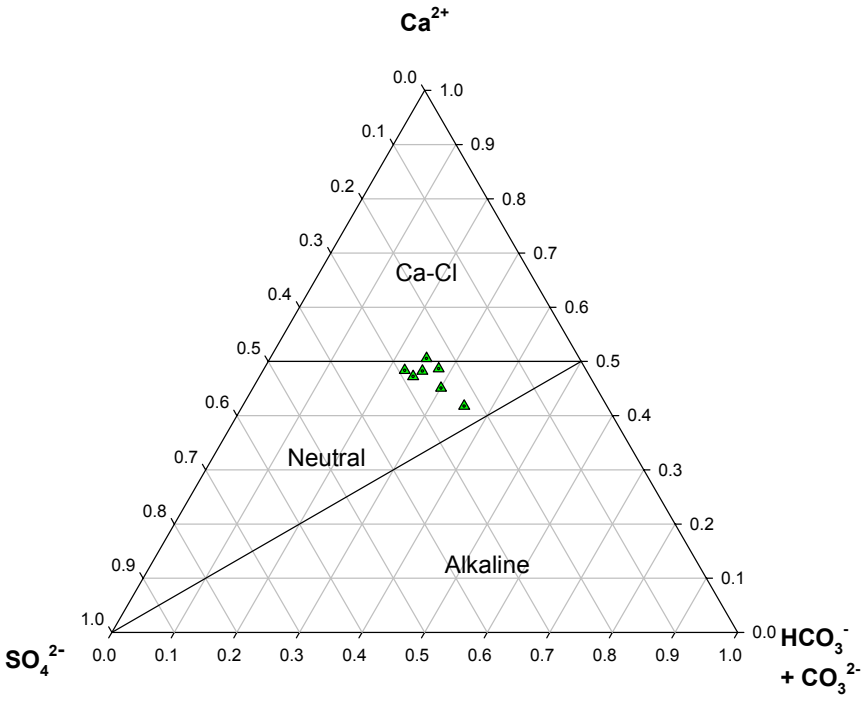
SD-7 Samples



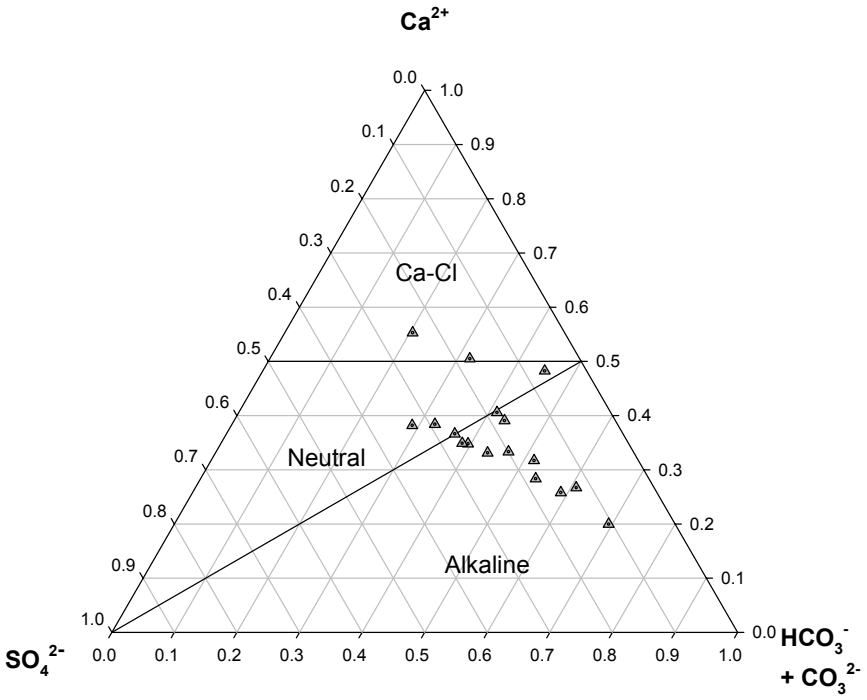
WT-24 Samples



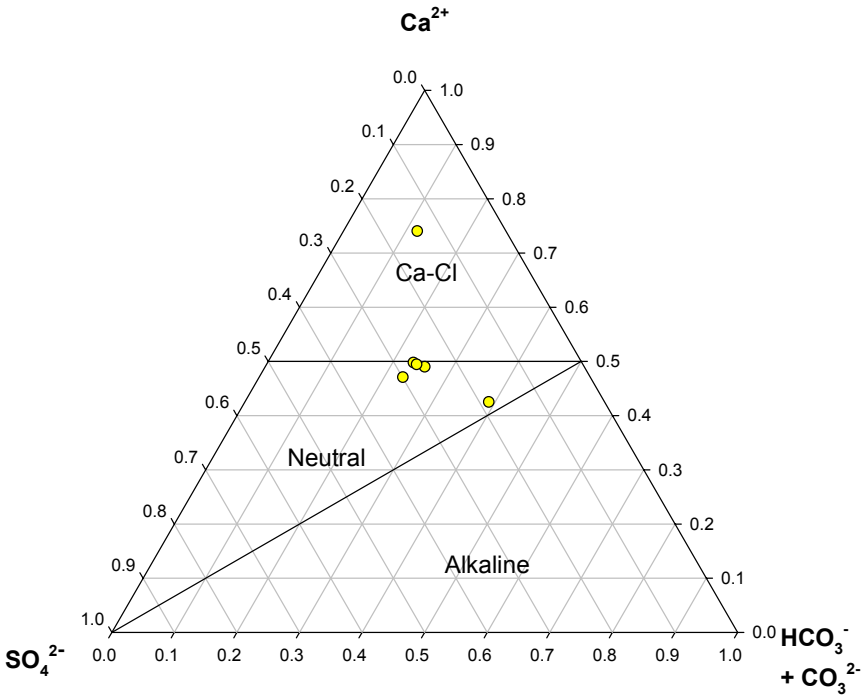
ESF-HD-PERM Samples



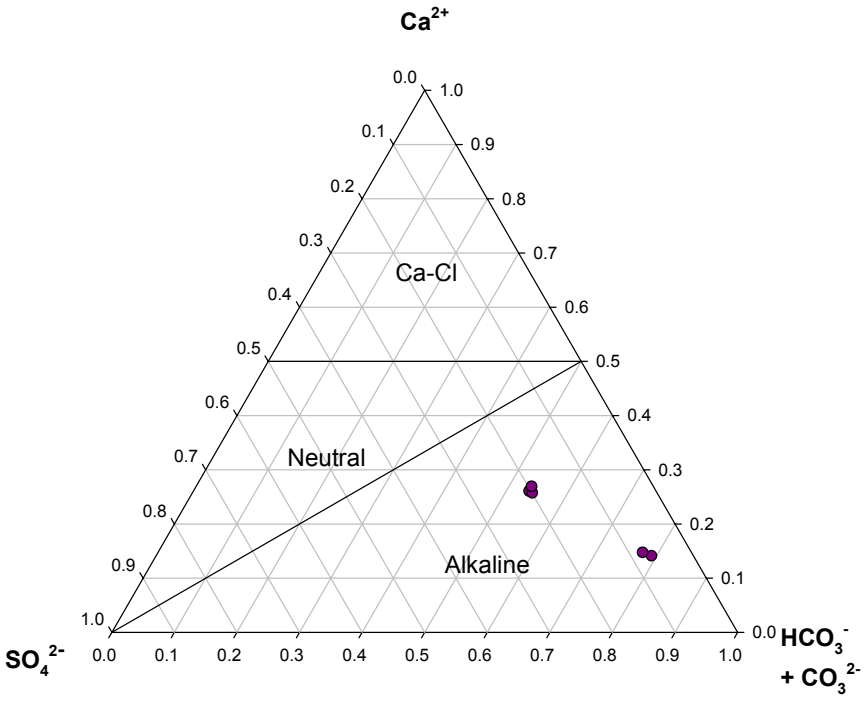
ESF-THERMALK Samples



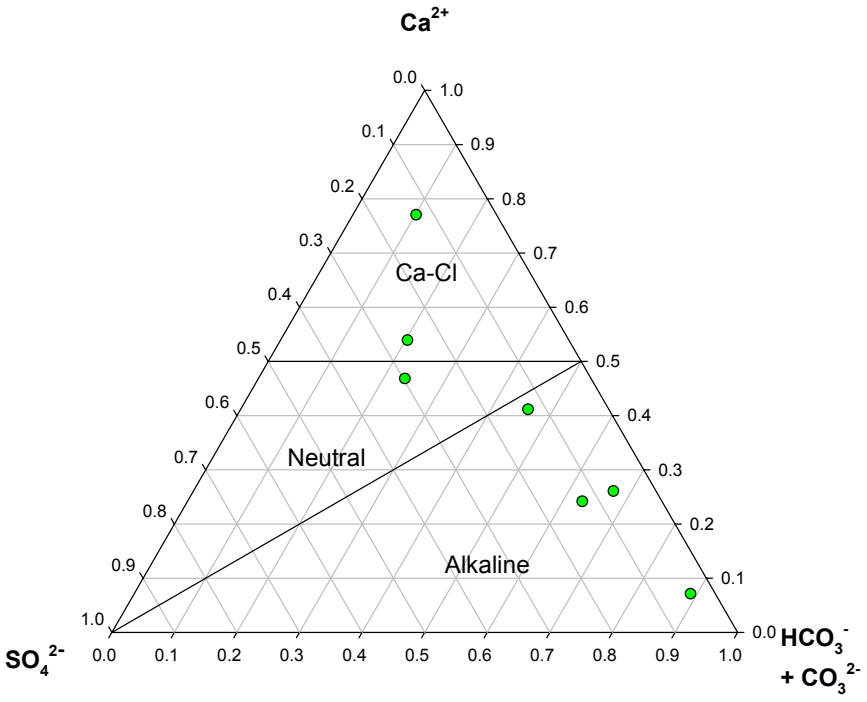
ESF-HD-ChemSamp Samples



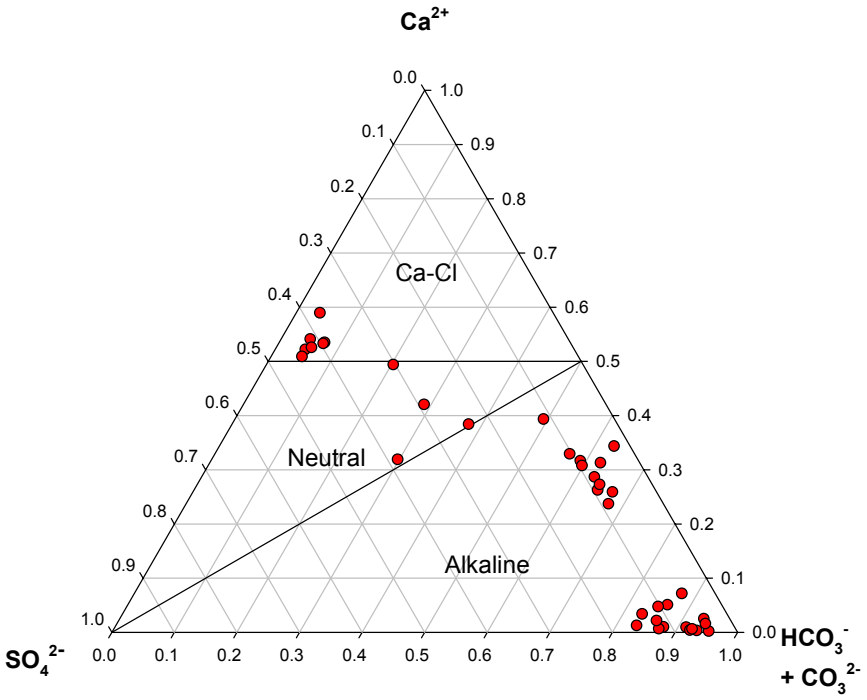
ESF-SR-MS Samples



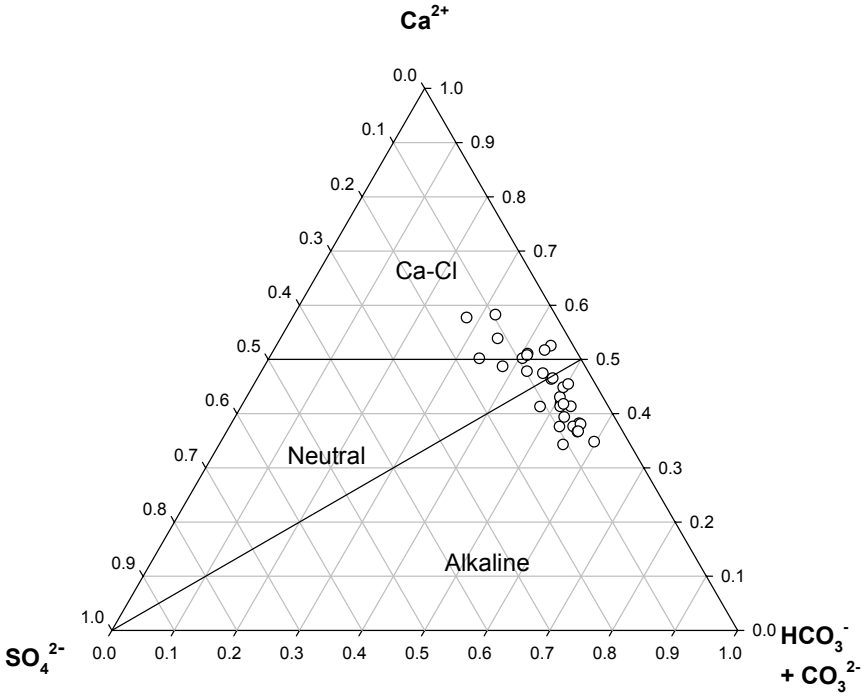
ESF-NR-MS Samples



NRG-7A Samples

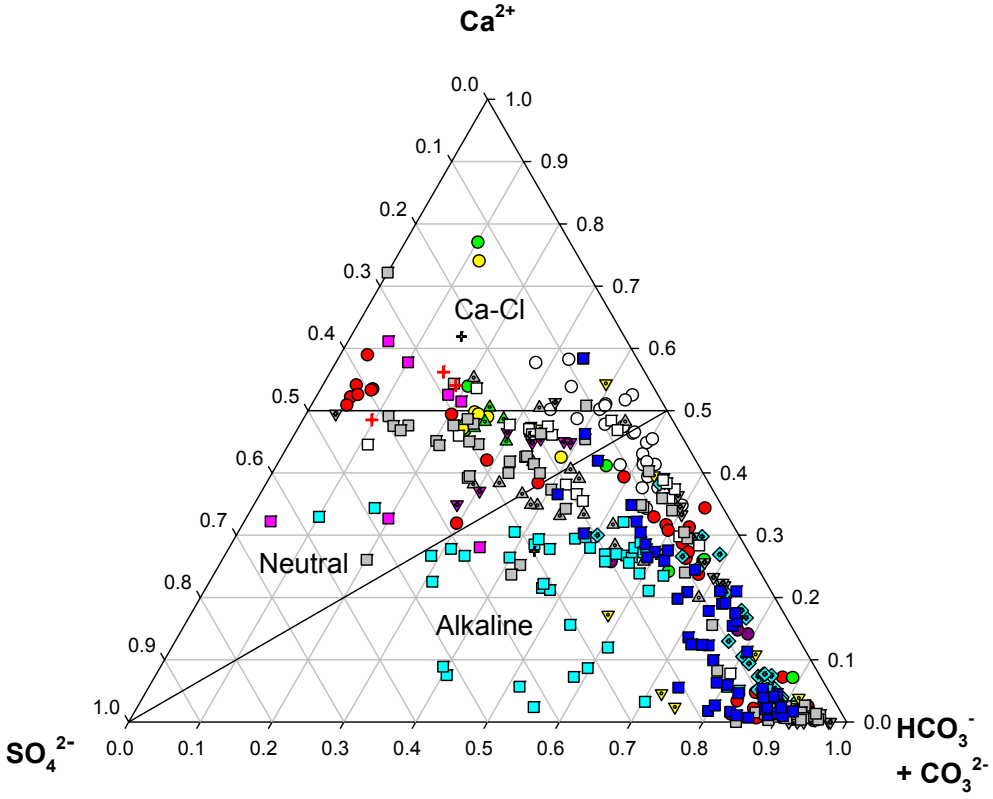


SD-9 Samples

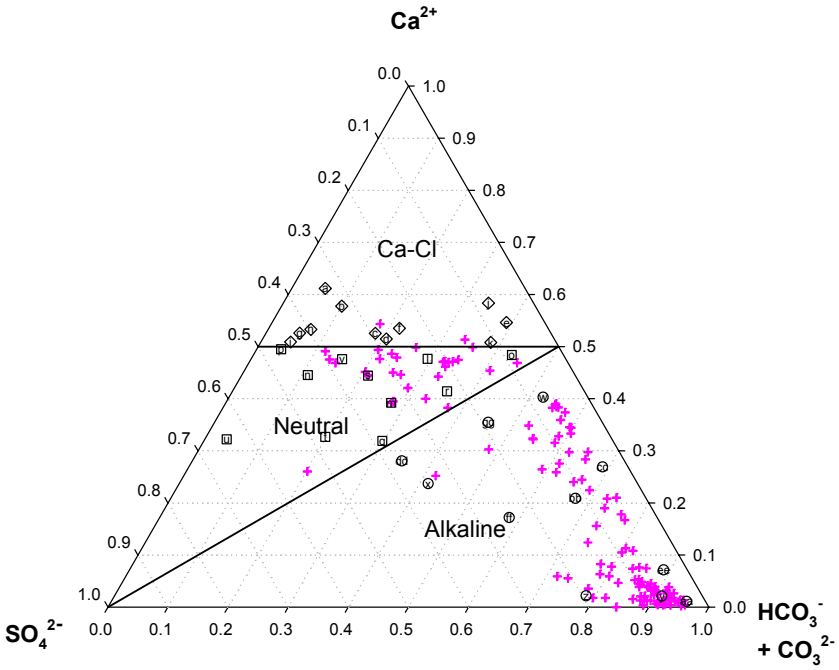


ECRB-SYS-CS Samples

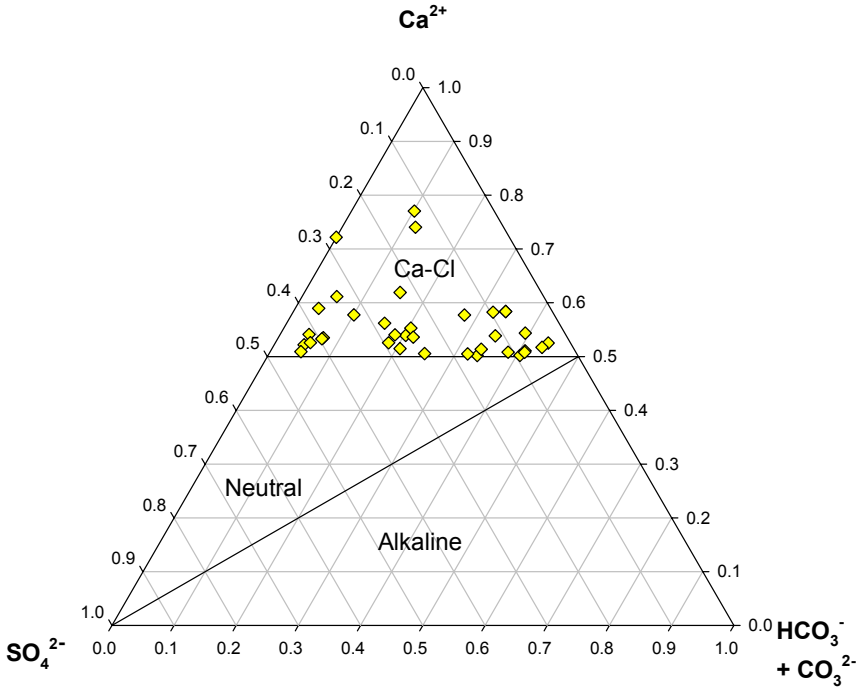
The following figure includes all 379 data points:



The following is from ESN#679 page 157 (156 points):



This figure includes only the Ca-Cl type waters (36 points; E-Ca>0.5):

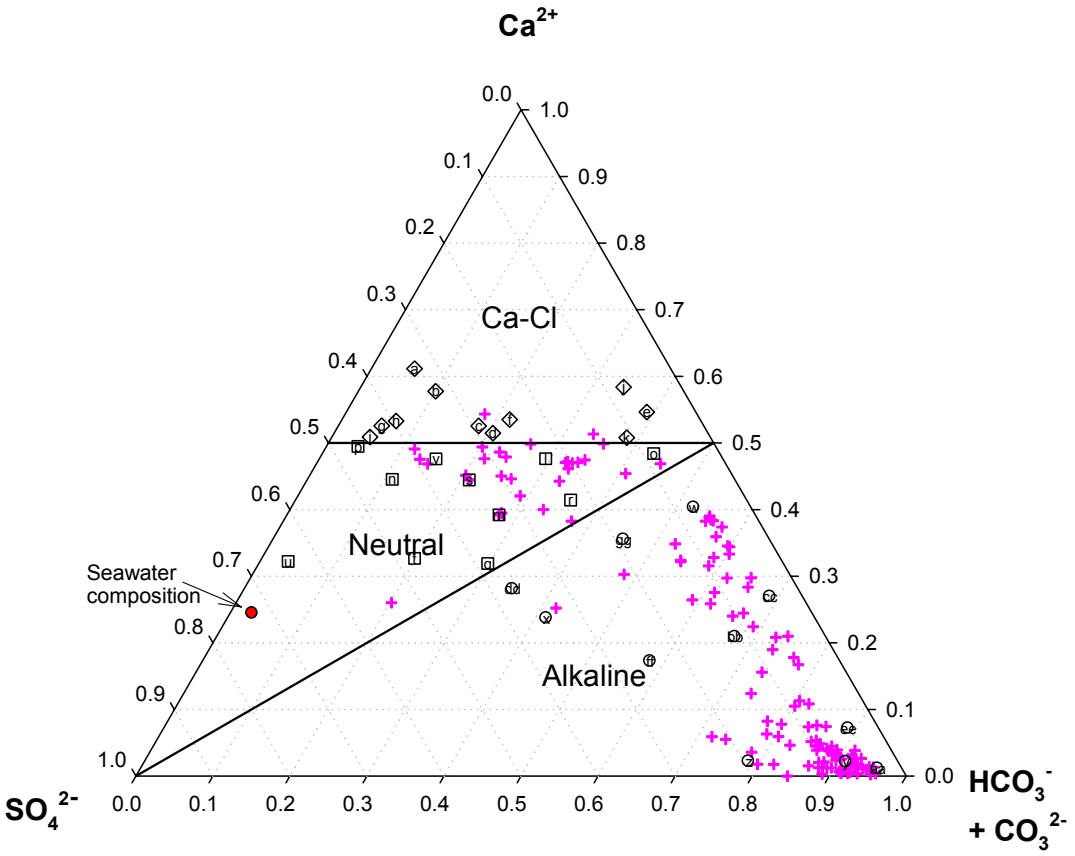


36 out of 379 water compositions are Ca-Cl type (9.5 %). This is close to the 8% value derived previously ESN#679, page 166) from Yucca Mountain unsaturated zone porewater compositions reported by Yang et al. (1996, 1998, 2003).

April 14, 2009

Nevada Contention #110 pertains to corrosion of rock bolts. Nevada claims that DOE ignored the potential corrosion of rock bolts in MgCl2-bearing solutions and cited a paper by Shoji and Ohnaka (1989) in which experimental data at 25 C showed that atmospheric stress corrosion cracking of stainless steel occurred in brines of MgCl2 and of seawater composition. The seawater test result was explained as being due to the MgCl2 present in the brine phase.

The following figure is a chemical divide diagram illustrating the compositions of Yucca Mountain porewaters including those used in evaporation simulations (see notebook #679E, page 157). Added to the figure is the composition of Inaqua seawater. As shown in the figure, seawater is a neutral type of brine.



The composition of Inaqua seawater (before and after charge balancing using StreamAnalyzer 2.0.30) is as follows:

	Input	Calculated		% Diff
Water	1.0000e6	9.8675e5	mg/L	-1.32538
Sodium ion(+1)	11300.0	11516.0	mg/L	1.91167
Potassium ion(+1)	414.000	414.000	mg/L	
Magnesium ion(+2)	1250.00	1250.00	mg/L	
Calcium ion(+2)	391.000	391.000	mg/L	
Chloride ion(-1)	20300.0	20300.0	mg/L	
Bicarbonate ion(-1)	142.000	142.000	mg/L	

Sulfate ion(-2)	2790.00	2790.00	mg/L
Bromide ion (-1)	69.7000	69.7000	mg/L

Evaporation at 110 C and 0.85 atm was simulated using StreamAnalyzer 2.0.30. The output is as follows:

Calculation Summary

Evap at 110 C, 0.85 atm Calculation for Work2

Unit Set: Default

Automatic Chemistry Model
Aqueous (H+ ion) Databanks:
Public

Isothermal Calculation

Temperature	110.000	°C
Pressure	0.850000	atm

Stream Inflows

Water	54.1698	mol
Calcium carbonate (calcite)	8.37311e-6	mol
Calcium hydroxide	9.74756e-3	mol
Carbon dioxide	2.31883e-3	mol
Hydrogen bromide	8.72293e-4	mol
Hydrogen chloride	0.572587	mol
Magnesium hydroxide	0.0514295	mol
Potassium hydroxide	0.0105886	mol
Sodium hydroxide	0.500913	mol
Sulfur trioxide	0.0290431	mol

Stream Parameters

Row Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amt - Total Inflow	55.347	mol
Temperature	110.000	°C
Pressure	0.850000	atm

Aqueous Properties

pH	*4.42699*	*pH*
Ionic Strength	0.168429	mol/mol
Osmotic Pressure	876.957	atm
Electrical Cond, specific	0.698990	1/(ohm-cm)
Electrical Cond, molar	7.63504	cm2/ohm-mol
Viscosity, absolute	1.10127	cP
Viscosity, relative	4.32584	cP/cP H2O

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd Liquid**
	--	g/ml	g/ml	g/ml	g/ml
Density	--	1.26429	4.90318e-4	2.24289	0.0

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd Liquid**
	cal	cal	cal	cal	cal
Enthalpy	-3.20016e6	-50347.9	-3.09603e6	-53786.6	0.0

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd Liquid**
	cal/g K	cal/g K	cal/g K	cal/g K	cal/g K

Heat Capacity	0.0	0.0	0.0	0.0	0.0

Scaling Tendencies

Row Filter Applied: Only Non Zero Values

solids within temperature range		**Temperature Range**		
Sodium chloride	1.00000	0.0	350.000 °C	inside range
Magnesium sulfate monohydrate	1.00000	69.0000	240.000 °C	inside range
Calcium sulfate	1.00000	0.0	455.000 °C	inside range
Magnesium sulfate-0.25-(magnesium hydroxide)-hemihydrate	1.00000	data valid through range		inside range
Potassium chloride	0.709804	0.0	200.000 °C	inside range
Magnesium sulfate-0.5-(magnesium hydroxide)	0.440011	data valid through range		inside range
Calcium sulfate dihydrate	0.108867	0.0	126.000 °C	inside range
Sodium sulfate	0.0393408	19.0000	241.000 °C	inside range
Magnesium chloride hexahydrate	0.0205046	0.0	116.700 °C	inside range
Potassium sulfate(VI)	0.0195819	9.70000	292.000 °C	inside range
Glaserite	0.0165058	35.0000	150.000 °C	inside range
Sodium bromide	5.15127e-3	51.0000	350.000 °C	inside range
Potassium bromide	4.45057e-3	0.0	421.000 °C	inside range
Magnesium hydroxide	1.99441e-3	data valid through range		inside range
Magnesium chloride hydroxide	6.39862e-5	data valid through range		inside range
Potassium bisulfate(VI)	4.19696e-6	data valid through range		inside range
Magnesium carbonate	2.78618e-6	data valid through range		inside range
Potassium magnesium chloride dihydrate	2.75903e-6	data valid through range		inside range
Calcium chloride dihydrate	1.86932e-6	45.0900	175.510 °C	inside range
Sodium bisulfate	5.58078e-7	data valid through range		inside range
Magnesium carbonate trihydrate	6.21435e-8	data valid through range		inside range
Calcium carbonate (calcite)	1.93669e-8	data valid through range		inside range
Sodium bicarbonate	2.23552e-9	0.0	200.000 °C	inside range
Potassium bicarbonate	1.47728e-10	data valid through range		inside range
Potassium magnesium chloride	7.67444e-11	data valid through range		inside range
Calcium hydroxide	6.81070e-13	data valid through range		inside range
Potassium hydroxide monohydrate	1.23955e-13	33.0000	143.000 °C	inside range

Sodium carbonate	1.74245e-14	109.000	300.000 °C	inside range
Sodium carbonate monohydrate	1.05169e-14	34.7600	112.500 °C	inside range
Hexasodium carbonate bissulfate	5.50073e-16	30.0000	150.000 °C	inside range
Calcium bromide	1.40394e-16	data valid through range		inside range
Potassium hydroxide	3.17884e-17	data valid through range		inside range
Potassium carbonate 1.5 hydrate	1.79047e-18	data valid through range		inside range
Magnesium bromide	5.20611e-20	data valid through range		inside range
Potassium carbonate	2.26758e-20	data valid through range		inside range
Sodium bicarbonate carbonate dihydrate	3.12639e-23	21.2600	150.000 °C	inside range
Pentasodium bicarbonate carbonate	1.00000e-35	100.000	200.000 °C	inside range
Potassium sesquicarbonate sesquihydrate	1.00000e-35	data valid through range		inside range

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

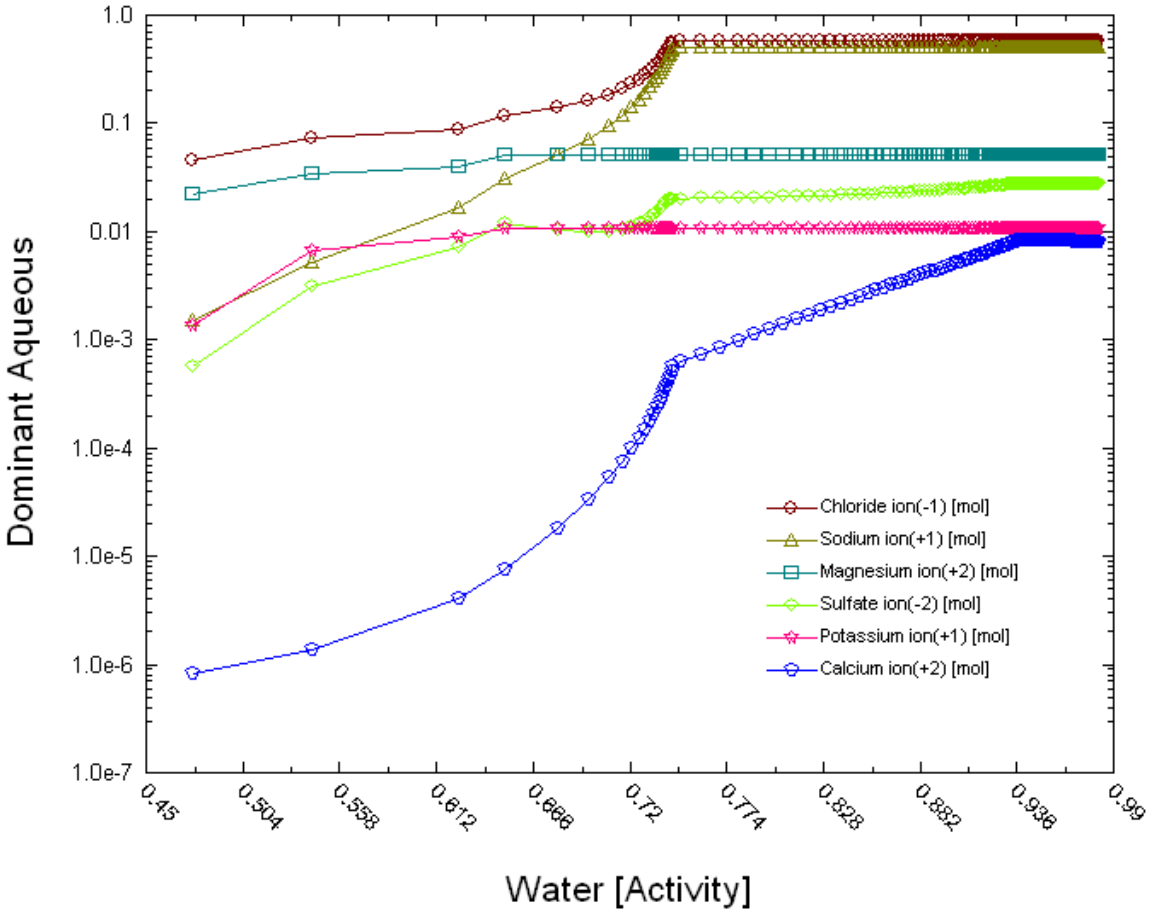
	Total	Aqueous	Aqueous moles/kg H2O	Vapor	Solid
	mol	mol		mol	mol
Water	54.7668	0.572145	55.5093	54.1947	0
Calcium carbonate (calcite)	1.03E-16	1.03E-16	9.99E-15	0	0
Carbon dioxide	2.33E-03	7.78E-10	7.55E-08	2.33E-03	0
Hydrogen bromide	4.80E-09	5.67E-17	5.5E-15	4.80E-09	0
Hydrogen chloride	5.22E-05	8.35E-11	8.1E-09	5.22E-05	0
Sulfur trioxide	1.70E-24	3.40E-25	3.3E-23	1.36E-24	0
Calcium chloride	4.94E-12	4.94E-12	4.79E-10	0	0
Calcium sulfate	9.73E-03	1.14E-06	0.000111	0	9.73E-03
Magnesium carbonate	4.72E-13	4.72E-13	4.58E-11	0	0
Magnesium sulfate	9.68E-03	9.68E-03	0.93915	0	0
Magnesium sulfate monohydrate	3.04E-03	0	0	0	3.04E-03
Magnesium sulfate-0.25-(magnesium hydroxide)-hemihydrate	4.76E-03	0	0	0	4.76E-03
Potassium bisulfate(VI)	7.26E-09	7.26E-09	7.04E-07	0	0
Potassium chloride	7.65E-04	7.65E-04	0.07422	0	0
Sodium bicarbonate	4.90E-13	4.90E-13	4.75E-11	0	0
Sodium bromide	8.34E-05	8.34E-05	0.008091	0	0
Sodium chloride	0.487368	0	0	0	0.487368
Sulfuric(VI) acid	2.54E-19	2.63E-22	2.55E-20	2.54E-19	0
Bicarbonate ion(-1)	*4.37E-12*	*4.37E-12*	*4.24E-10*	*0*	*0*
Bisulfate(VI) ion (-1)	*6.36E-07*	*6.36E-07*	*6.17E-05*	*0*	*0*
Bromide ion (-1)	*7.89E-04*	*7.89E-04*	*0.076548*	*0*	*0*
Calcium bicarbonate ion(+1)	7.40E-13	7.40E-13	7.18E-11	0	0
Calcium hydroxide ion(+1)	1.57E-11	1.57E-11	1.52E-09	0	0

Calcium ion(+2)	*2.25E-05*	*2.25E-05*	*0.002183*	*0*	*0*
Calcium monochloride ion(+1)	2.65E-06	2.65E-06	0.000257	0	0
Carbonate ion(-2)	*1.45E-15*	*1.45E-15*	*1.41E-13*	*0*	*0*
Chloride ion(-1)	*0.084399*	*0.084399*	*8.18836*	*0*	*0*
Hydrogen ion(+1)	1.94E-07	1.94E-07	1.88E-05	0	0
Hydroxide ion(-1)	2.91E-10	2.91E-10	2.82E-08	0	0
Magnesium bicarbonate ion(+1)	1.13E-08	1.13E-08	1.1E-06	0	0
Magnesium hydroxide ion(+1)	1.21E-06	1.21E-06	0.000117	0	0
Magnesium ion(+2)	*0.032762*	*0.032762*	*3.178557*	*0*	*0*
Potassium ion(+1)	*9.15E-03*	*9.15E-03*	*0.88773*	*0*	*0*
Potassium sulfate(VI) ion(-1)	6.74E-04	6.74E-04	0.065391	0	0
Sodium carbonate ion(-1)	1.93E-16	1.93E-16	1.87E-14	0	0
Sodium ion(+1)	*0.013461*	*0.013461*	*1.305981*	*0*	*0*
Sodium sulfate ion(-1)	4.58E-37	4.58E-37	4.44E-35	0	0
Sulfate ion(-2)	*1.16E-03*	*1.16E-03*	*0.112543*	*0*	*0*
Total (by phase)	55.4271	0.725099	70.34884	54.1971	0.504893

April 14, 2009

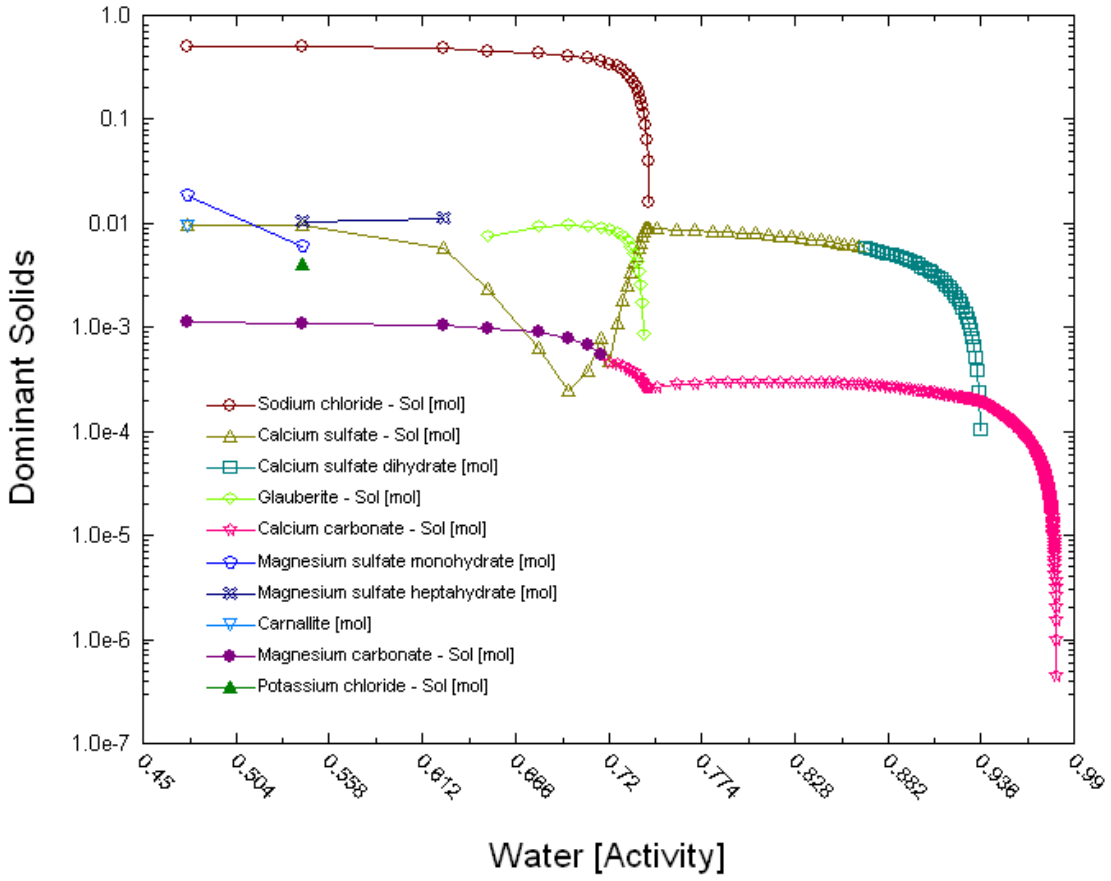
Evaporations simulation of Inaqua seawater was conducted using StreamAnalyzer 2.0.30 (MSE model) The Inaqua seawater composition was used as input, and the calculation type was specified as isothermal and as a composition survey (with water ranging from 55.4801 to 5E-7 moles; 251 points were calculated).

The resulting (six) dominant aqueous species are plotted as follows:



As indicated in the above figure, with increasing evaporation (decreasing water activity or relative humidity – going from right to left of the diagram), the brine that forms eventually becomes dominated by MgCl2 – consistent with the interpretation of Shoji and Ohnaka that Mg and Cl are the species that cause atmospheric stress corrosion cracking of stainless steel.

The 10 dominant solids are shown in the following figure:

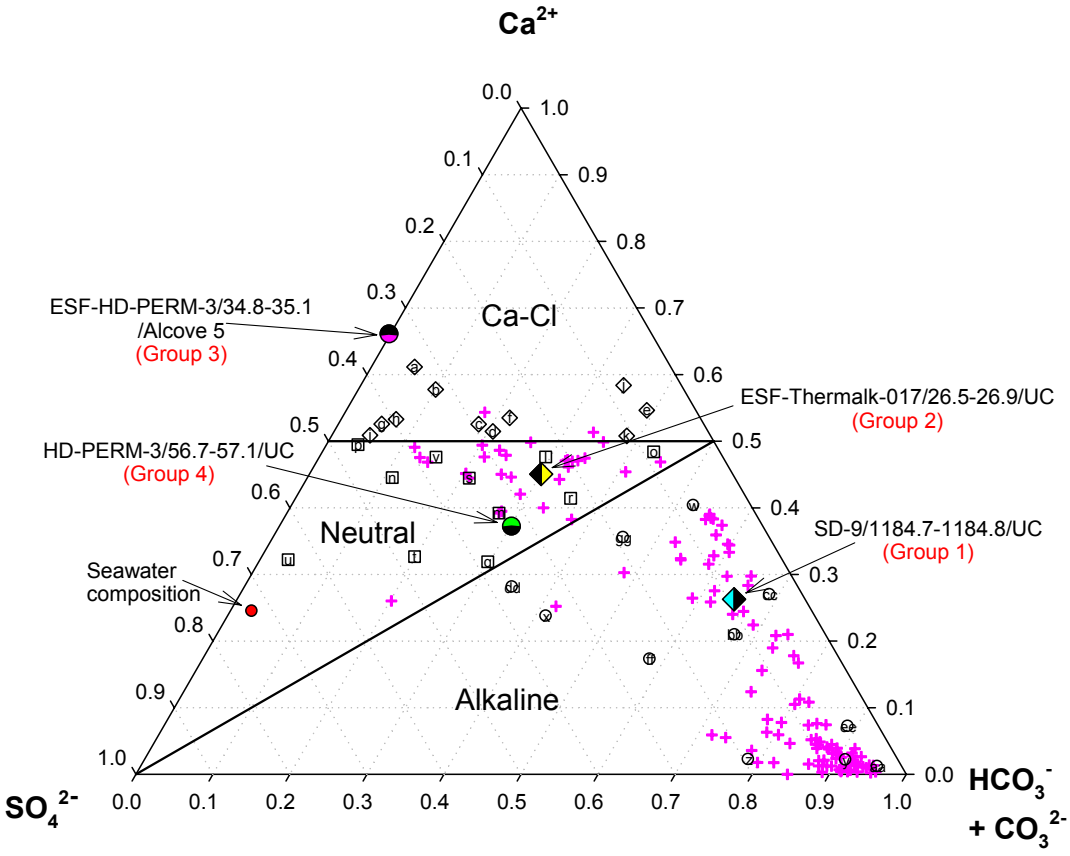


The following compositions were taken from ESF #930E, page 52. These are DOE representations of Yucca Mountain porewaters used in the Safety Analysis Report.

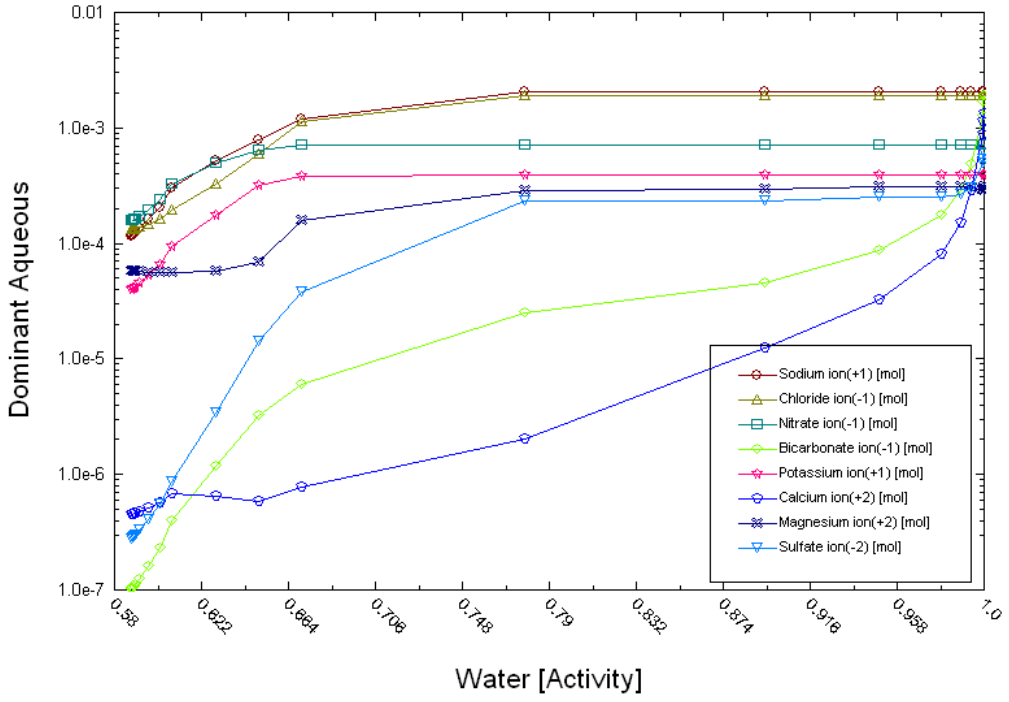
Table 1. Chemical Compositions (mg/L) of Four Pore Waters Used to Represent Near-Field Water Chemistry. Values Taken From Helean (2007). Values are the Same as in Table 2.3.5-5 of the DOE SAR.

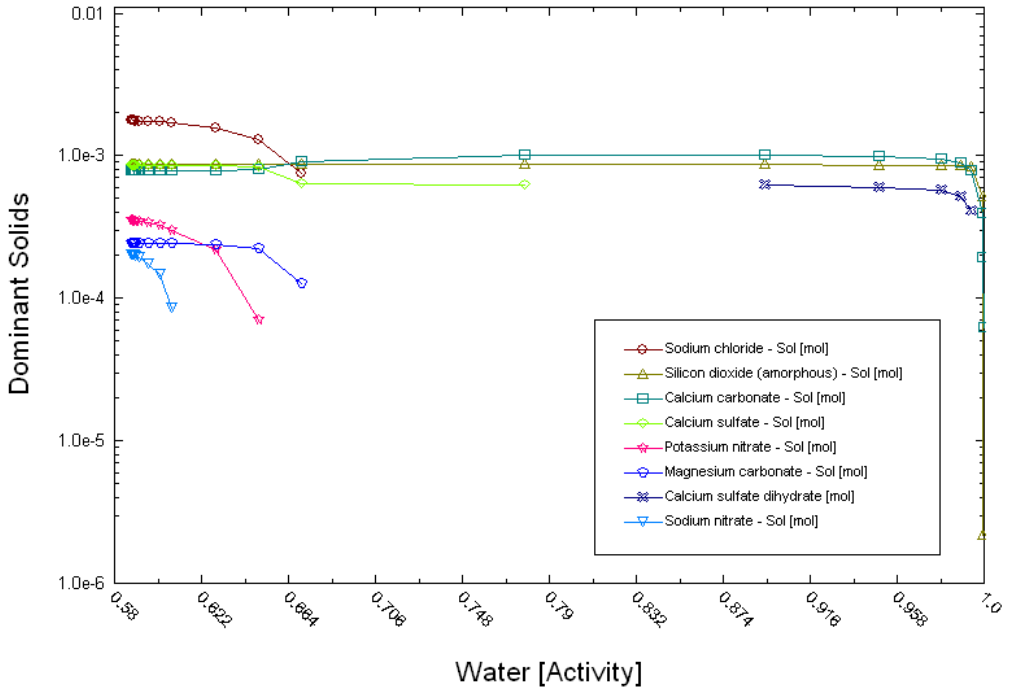
	Pore Water Identification			
	ESF-Thermalk-017/26.5-26.9/UC (Group 2)	SD-9/1184.7-1184.8/UC (Group 1)	HD-PERM-3/56.7-57.1/UC (Group 4)	ESF-HD-PERM-3/34.8-35.1/Alcove 5 (Group 3)
Na^+	45	59	123	62
K^+	14.4	4.8	13.8	9
Mg^{2+}	7.9	0.7	16.7	17.4
Ca^{2+}	62	19	59.9	97
Cl^-	67	23	146	123
SO_4^{2-}	82	16	126	120
HCO_3^-	126	142	149	—
NO_3^-	44	16	57.4	10
F^-	1.4	2.2	1.3	0.76
SiO_2	52	42	—	75

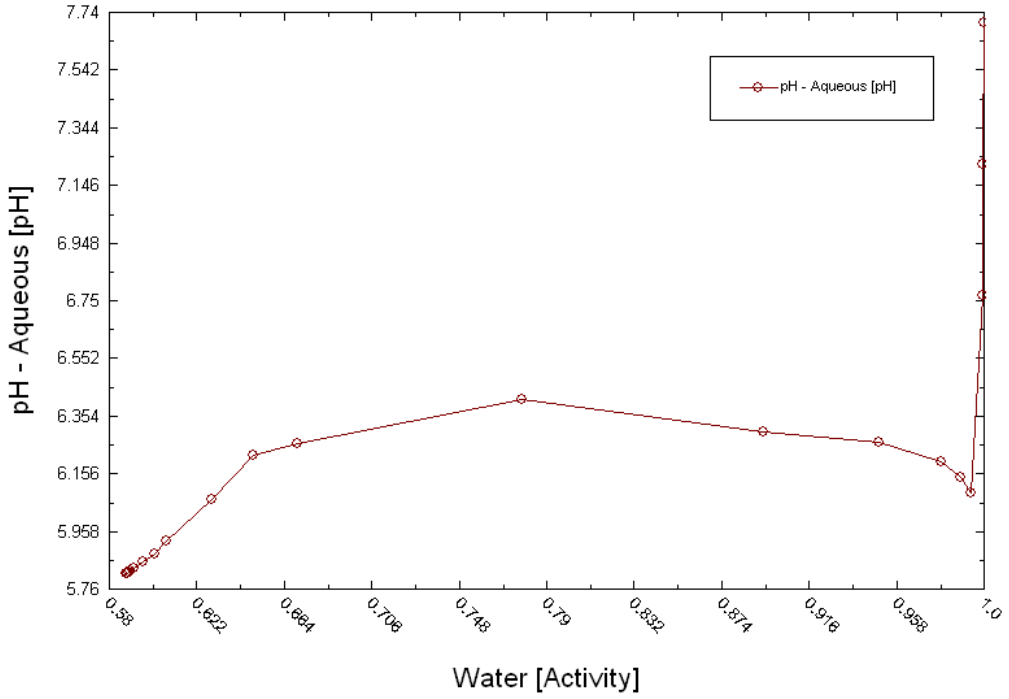
The following is a chemical divide plot showing the compositions of Yucca Mountain pore waters used by DOE in its SAR near-field chemistry model, along with the compositions of pore waters sampled by the USGS from the YM unsaturated zone.



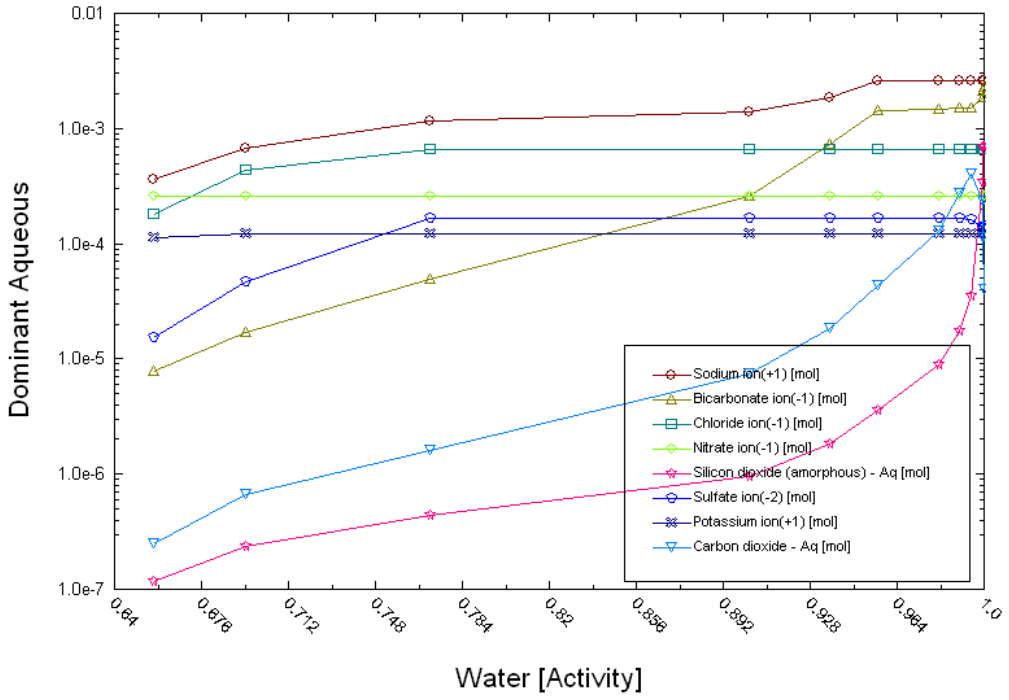
Evaporation simulations were done using StreamAnalyzer 2.0.30. The results for ESF-Thermal-017/26.5-26.9/UC are as follows:

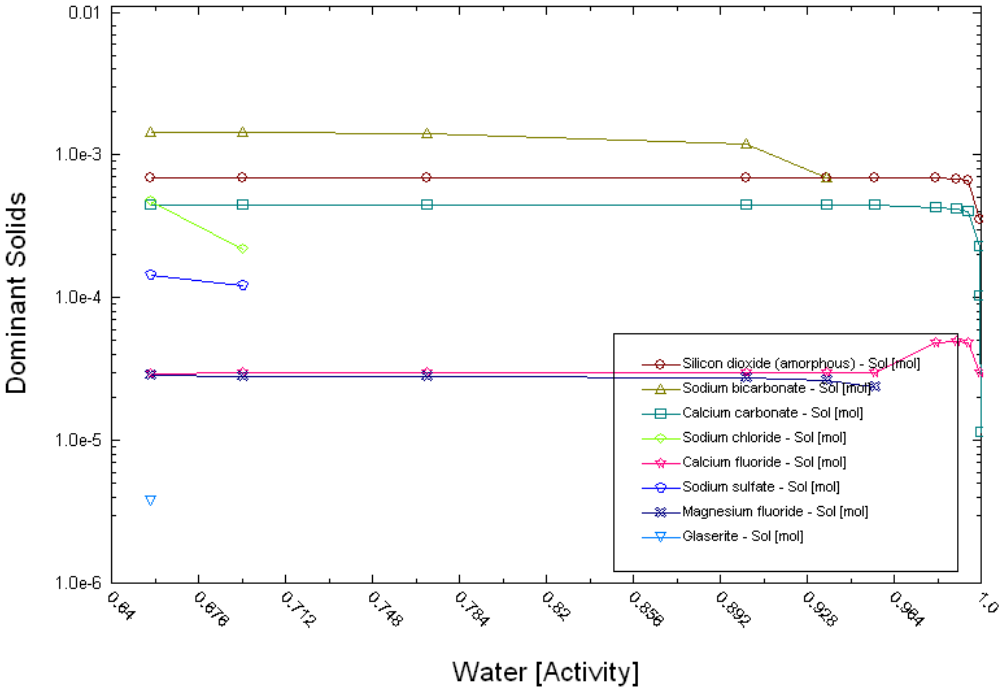


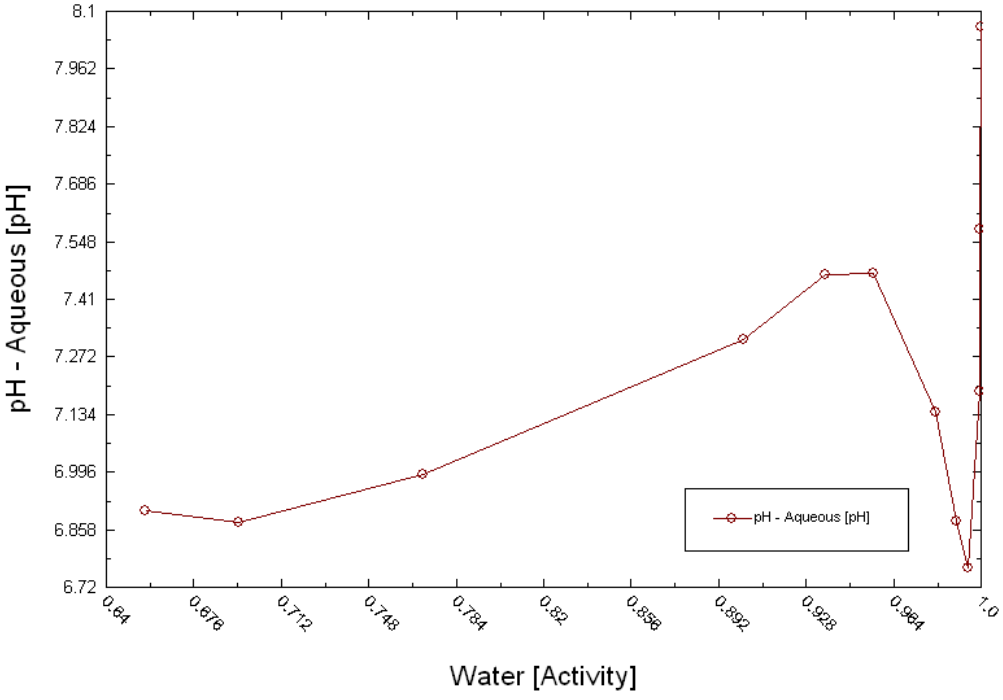




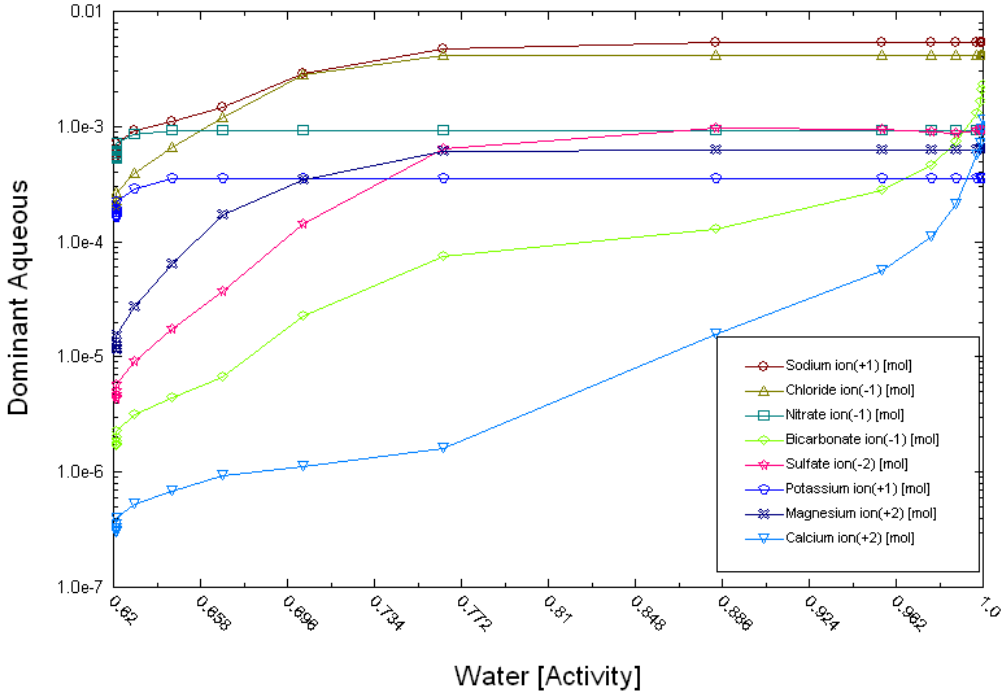
The results for SD-9/1184.7-1184.8/UC are as follows:

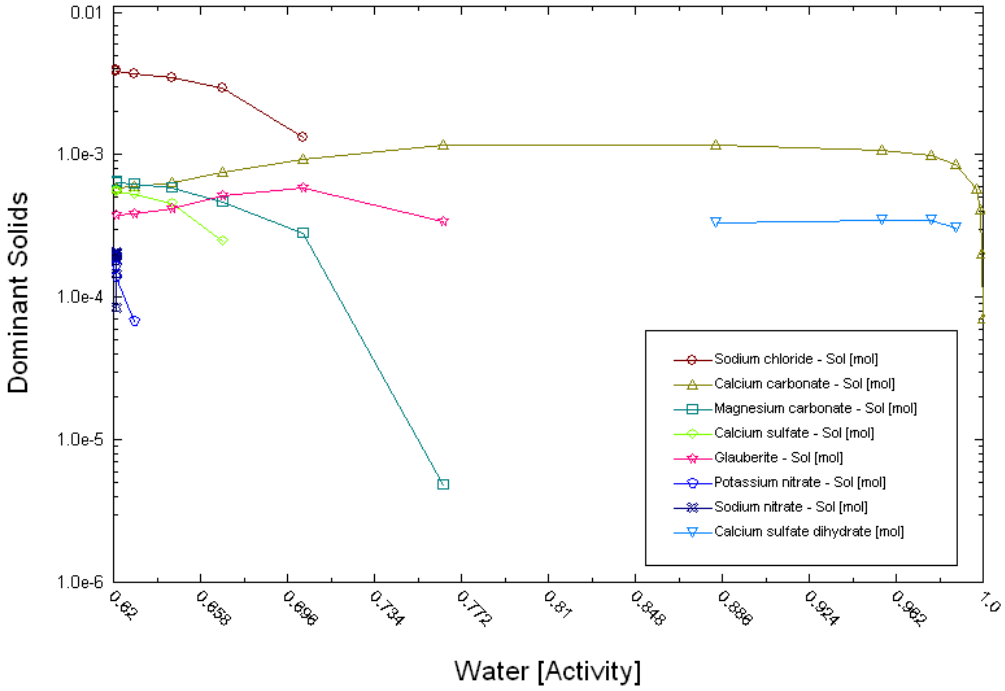


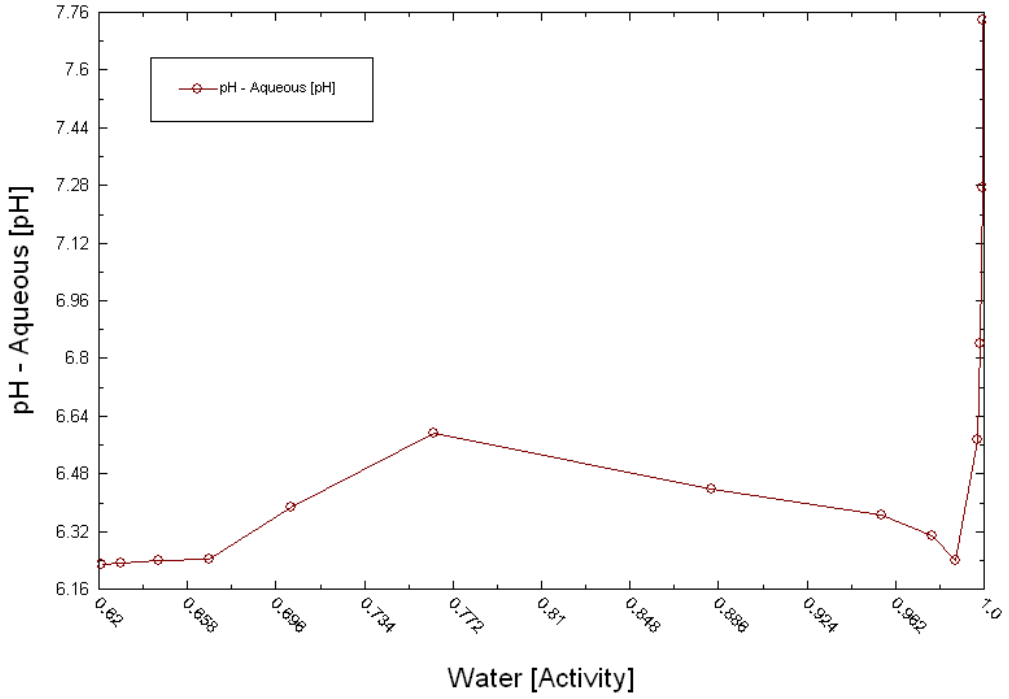

Dominant Solids
0.01
1.0e-3
1.0e-4
1.0e-5
1.0e-6
0.64
0.676
0.712
0.748
0.784
0.82
0.856
0.892
0.928
0.964
1.0
Water [Activity]
Silicon dioxide (amorphous) - Sol [mol]
Sodium bicarbonate - Sol [mol]
Calcium carbonate - Sol [mol]
Sodium chloride - Sol [mol]
Calcium fluoride - Sol [mol]
Sodium sulfate - Sol [mol]
Magnesium fluoride - Sol [mol]
Glaserite - Sol [mol]


pH - Aqueous [pH]
8.1
7.962
7.824
7.686
7.548
7.41
7.272
7.134
6.996
6.858
6.72
0.64
0.676
0.712
0.748
0.784
0.82
0.856
0.892
0.928
0.964
1.0
Water [Activity]
pH - Aqueous [pH]

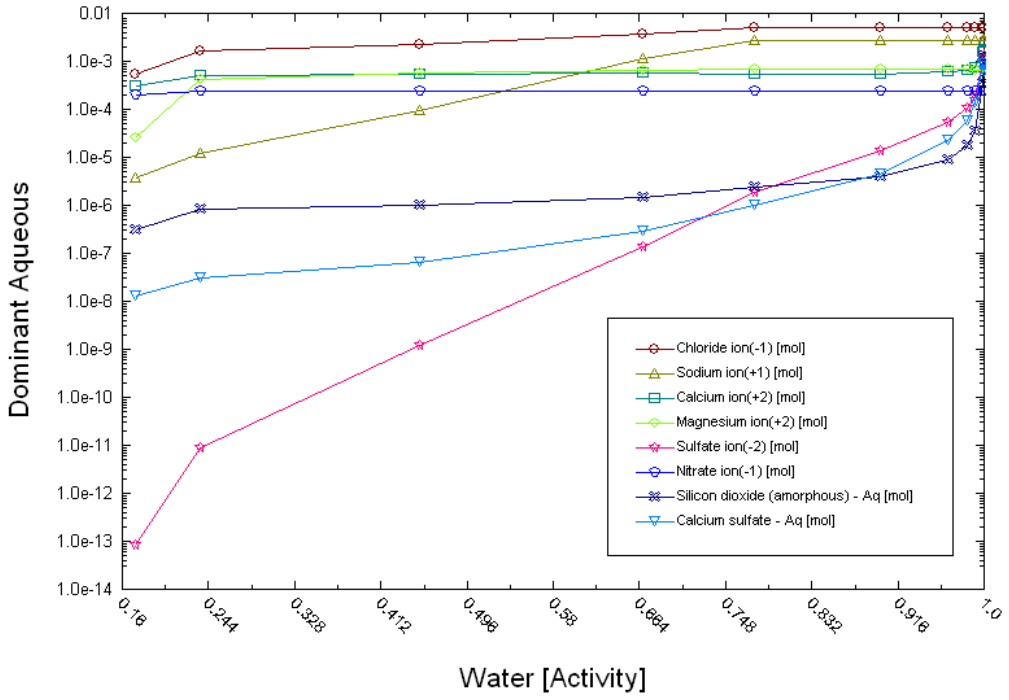
The results for HD-PERM-3/56.7-57.1/UC are as follows:

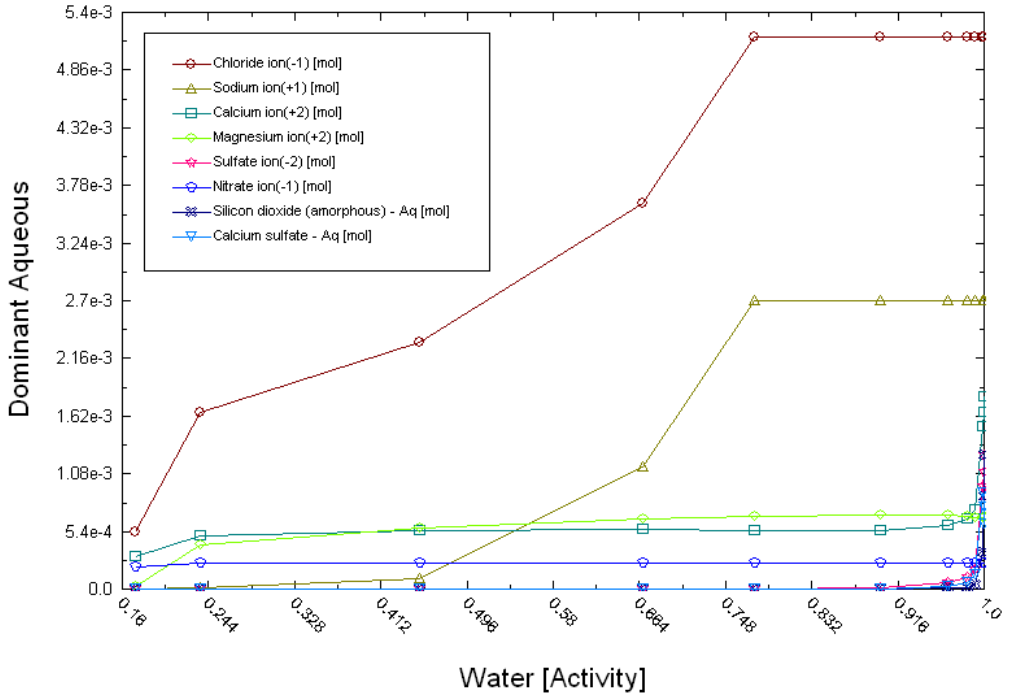


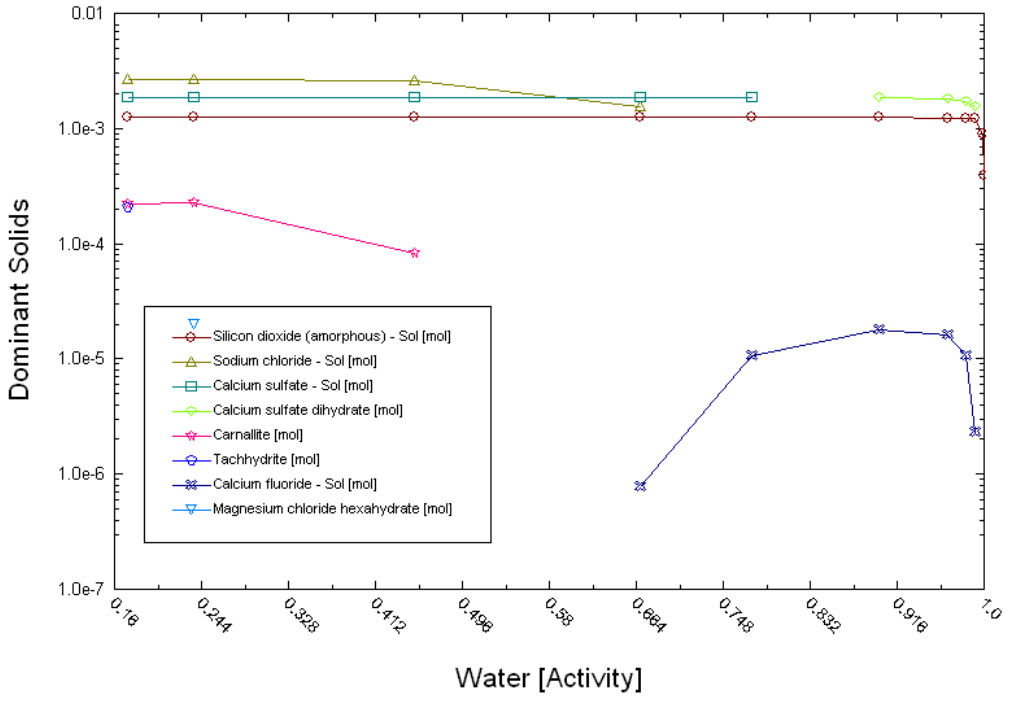


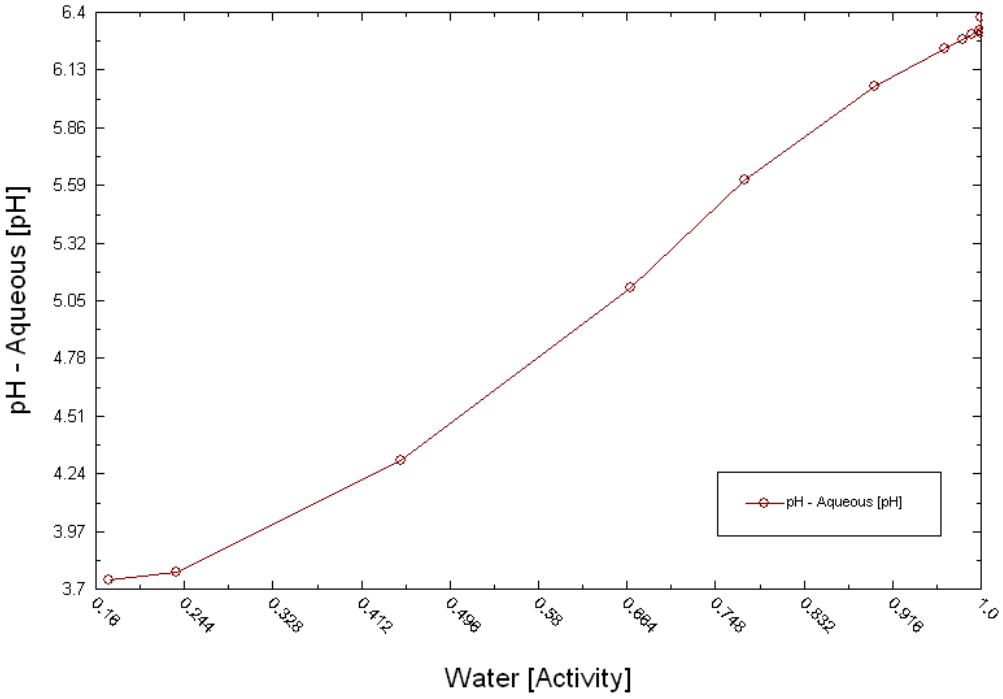


The results for ESF-HD-PERM-3/34.8-35.1/Alcove 5 are as follows:




Dominant Aqueous
Water [Activity]
Chloride ion(-1) [mol]
Sodium ion(+1) [mol]
Calcium ion(+2) [mol]
Magnesium ion(+2) [mol]
Sulfate ion(-2) [mol]
Nitrate ion(-1) [mol]
Silicon dioxide (amorphous) - Aq [mol]
Calcium sulfate - Aq [mol]
5.4e-3
4.86e-3
4.32e-3
3.78e-3
3.24e-3
2.7e-3
2.16e-3
1.62e-3
1.08e-3
5.4e-4
0.0
0.16
0.244
0.328
0.412
0.496
0.58
0.664
0.748
0.832
0.916
1.0


Dominant Solids
Water [Activity]
Silicon dioxide (amorphous) - Sol [mol]
Sodium chloride - Sol [mol]
Calcium sulfate - Sol [mol]
Calcium sulfate dihydrate [mol]
Carnallite [mol]
Tachhydrite [mol]
Calcium fluoride - Sol [mol]
Magnesium chloride hexahydrate [mol]
0.01
1.0e-3
1.0e-4
1.0e-5
1.0e-6
1.0e-7
0.16
0.244
0.328
0.412
0.496
0.58
0.664
0.748
0.832
0.916
1.0


6.4
6.13
5.86
5.59
5.32
5.05
4.78
4.51
4.24
3.97
3.7
pH - Aqueous [pH]
0.16
0.244
0.328
0.412
0.496
0.58
0.664
0.748
0.832
0.916
1.0
Water [Activity]
pH - Aqueous [pH]

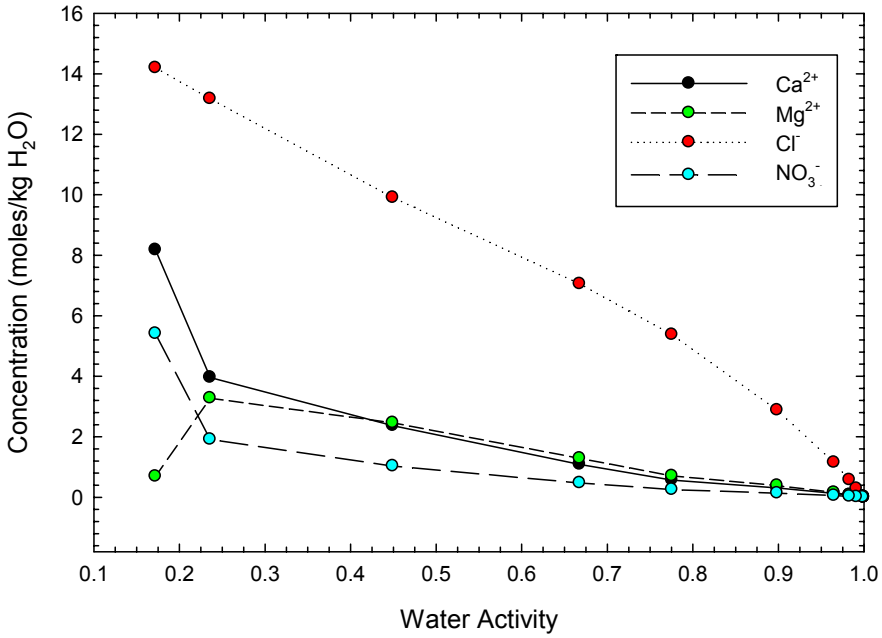
April 21, 2009 — The calculated speciation for ESF-HD-PERM-3/34.8-35.1/Alcove 5 is indicated in the following table:

H2O	CaCl2 - Aq	Ca+2	CaF+1	Cl-1	Mg+2	MgF+1	NO3-1	K+1	Na+1	SO4-2
mol	mol	mol	mol	mol	mol	mol	mol	mol	mol	mol
55.341	4.53E-12	1.81E-03	1.84E-06	5.17E-03	6.76E-04	4.03E-05	2.41E-04	2.30E-04	2.70E-03	1.25E-03
25.0034	1.57E-11	1.65E-03	1.96E-06	5.17E-03	6.69E-04	4.67E-05	2.41E-04	2.30E-04	2.70E-03	1.09E-03
10.0034	6.04E-11	1.52E-03	1.97E-06	5.17E-03	6.64E-04	5.14E-05	2.41E-04	2.30E-04	2.70E-03	9.61E-04
1.00036	7.95E-10	7.42E-04	8.41E-07	5.17E-03	6.63E-04	5.29E-05	2.41E-04	2.30E-04	2.70E-03	1.88E-04
0.500049	1.68E-09	6.52E-04	4.24E-07	5.17E-03	6.79E-04	3.74E-05	2.41E-04	2.30E-04	2.70E-03	1.06E-04
0.249876	3.94E-09	5.96E-04	1.90E-07	5.17E-03	6.89E-04	2.69E-05	2.41E-04	2.30E-04	2.70E-03	5.49E-05
0.099759	2.17E-08	5.53E-04	5.06E-08	5.17E-03	6.92E-04	2.34E-05	2.41E-04	2.30E-04	2.70E-03	1.39E-05
0.053448	1.94E-07	5.48E-04	1.86E-08	5.17E-03	6.78E-04	3.83E-05	2.41E-04	2.30E-04	2.70E-03	1.85E-06
0.028448	6.26E-07	5.56E-04	1.15E-08	3.61E-03	6.58E-04	5.81E-05	2.41E-04	2.30E-04	1.14E-03	1.40E-07
0.012949	5.15E-06	5.52E-04	2.87E-09	2.31E-03	5.73E-04	5.97E-05	2.41E-04	1.47E-04	9.31E-05	1.23E-09
6.98E-03	5.98E-05	4.98E-04	6.93E-10	1.66E-03	4.12E-04	5.97E-05	2.41E-04	5.90E-06	1.23E-05	8.82E-12
2.09E-03	2.73E-05	3.08E-04	2.35E-09	5.35E-04	2.59E-05	5.97E-05	2.04E-04	7.43E-06	3.71E-06	8.45E-14

In terms of moles/kgH2O, the speciation is as follows. The first column is the calculated water activity.

H2O	CaCl2 - Aq	**Ca+2**	CaF+1	**Cl-1**	**Mg+2**	MgF+1	**NO3-1**	K+1	**Na+1**	SO4-2
Activity	molal	molal	molal	molal	molal	molal	molal	molal	molal	molal
0.999762	4.55E-12	0.001811	1.85E-06	0.005189	0.000678	4.04E-05	0.000241	0.000231	0.002705	0.001254
0.999504	3.48E-11	0.003663	4.36E-06	0.011486	0.001486	0.000104	0.000534	0.000511	0.005987	0.00243
0.998855	3.35E-10	0.008416	1.09E-05	0.028709	0.003687	0.000285	0.001335	0.001277	0.014965	0.005334
0.991302	4.41E-08	0.041167	4.67E-05	0.287083	0.036787	0.002938	0.013345	0.012773	0.149646	0.010406
0.982953	1.87E-07	0.072391	4.71E-05	0.574317	0.075324	0.004147	0.026698	0.025553	0.299371	0.011739
0.964989	8.75E-07	0.132395	4.21E-05	1.149315	0.153064	0.005973	0.053427	0.051136	0.599098	0.012193
0.898563	1.2E-05	0.307843	2.82E-05	2.878786	0.385316	0.013039	0.133824	0.128086	1.50062	0.007732
0.775577	0.000202	0.569596	1.93E-05	5.372825	0.703788	0.039733	0.24978	0.23907	2.800874	0.001924
0.667729	0.001222	1.085327	2.25E-05	7.051129	1.283582	0.11335	0.469288	0.449166	2.22061	0.000273
0.449553	0.022085	2.367648	1.23E-05	9.904432	2.457174	0.255704	1.030948	0.630795	0.39923	5.27E-06
0.23597	0.475362	3.957232	5.51E-06	13.17097	3.27481	0.47431	1.912225	0.04689	0.097914	7.02E-08
0.17207	7.24E-01	8.173334	6.24E-05	14.19201	0.688105	1.58239	5.408745	0.197041	0.098356	2.24E-09

The concentration (moles/kg H2O) of Mg^{2+}, Ca^{2+}, and Cl^{-} are plotted in the following figure:



The following is a summary discussion of the preceding calculations relevant to the Nevada contention on rock bolt corrosion.

Technical Issue: Rock Bolt Corrosion — Nevada Contention #Nev-Safety-110

Nevada contended that DOE neglected to consider the degradation of the emplacement drift ground support during the preclosure period because the DOE analysis ignored the potential stress corrosion cracking (SCC) of the rock bolts, which could occur at temperatures below 100 °C based on experimental data reported by Shoji and Ohnaka (1989). Shoji and Ohnaka (1989) reported that SCC of stainless steel can occur at temperatures as low as 25 °C in the presence of salt deposits containing $MgCl_2$. Shoji and Ohnaka (1989) observed SCC of stainless steel in pure $MgCl_2$ solutions and also in brines formed by evaporation of synthetic seawater. The authors explained the seawater results as being due to the dominance of dissolved $MgCl_2$ in concentrated seawater brines. [The data of Shoji and Ohnaka (1989) also show SCC occurred in $CaCl_2$ solutions, although Nevada did not mention this result in its contention].

The analyses presented in this writeup were done to determine if the Nevada contention has technical merit and to test the hypotheses that brines rich in dissolved $MgCl_2$ and $CaCl_2$ could form by evaporation of initially dilute Yucca Mountain pore waters that could be present above the repository drift. The analyses were done by simulating the evaporation of waters of different compositions using the chemical modeling software StreamAnalyzer Version 2.0.30. The evaporation simulations were conducted for a constant temperature of 25 °C.

Analysis 1:

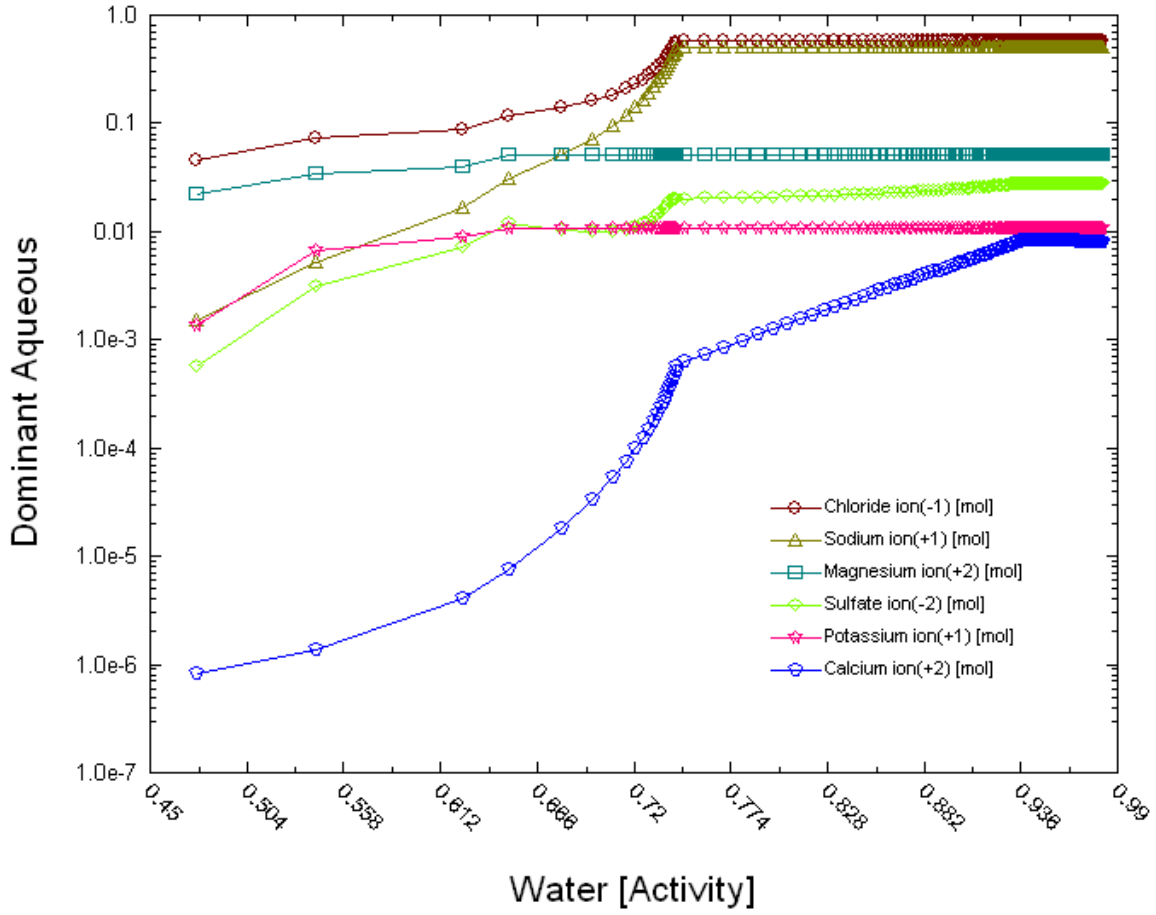
Analysis 1 used the composition of seawater as input to the evaporation simulation. Seawater has a multi-ionic composition, although the dominant cation is Na^+ and the dominant anion is Cl^-Shoji and Ohnaka (1989) speculated that SCC of stainless steel occurred in their tests because $MgCl_2$ is the dominant dissolved component in the evaporated synthetic seawater. Analysis 1 was done to confirm that evaporation of seawater results in a brine composition dominated by Mg^{2+} and Cl^- ions.

The following composition of seawater, taken from McCaffrey et al. (1987; "The evaporation path of seawater and the coprecipitation of Br- and K+ with halite." Journal of Sedimentary Petrology 57: 928-937), was used as input to the seawater evaporation simulation.

Table 1. Seawater Composition (McCaffrey et al., 1987)

	concentration (mg/L)
Na+	11,300
K+	414
Mg2+	1,250
Ca2+	391
Cl-	20,300
HCO3-	142
SO42-	2,790
Br-	69.7

The resulting most dominant aqueous species are plotted in the following figure as a function of water activity (equivalent to relative humidity). In the diagram, the degree of evaporation increases going from right to left.



As indicated in the above figure, with increasing degree of evaporation, the brine eventually becomes dominated by Mg^{2+} and Cl^{-}—consistent with the interpretation of Shoji and Ohnaka (1989).

Analysis 2:

With respect to the proposed Yucca Mountain repository, the concern is that pore waters in contact with the rock bolts above the emplacement drift will evaporate and become corrosive. Evaporation could result from the elevated temperature imposed by the high level wastes or by the drying effect of the ventilation system. To provide preliminary information regarding this issue, evaporation simulations were conducted using StreamAnalyzer Version 2.0.30 and compositions representative of Yucca Mountain pore waters.

In the near-field chemistry model discussed in the Safety Analysis Report, the DOE selected the four compositions listed in the following table (Table 2) to represent the chemistry of Yucca Mountain pore waters.

Table 2. Chemical Compositions (mg/L) of Four Pore Waters Used to Represent the Water Chemistry in the Near-Field Chemistry Model. Values are from Table 2.3.5-5 of the DOE Safety Analysis Report.				
	Pore Water Identification			
	ESF-Thermalk-017/26.5-26.9/UC	SD-9/1184.7-1184.8/UC	HD-PERM-3/56.7-57.1/UC	ESF-HD-PERM-3/34.8-35.1/Alcove 5
Na^+	45	59	123	62
K^+	14.4	4.8	13.8	9
Mg^{2+}	7.9	0.7	16.7	17.4
Ca^{2+}	62	19	59.9	97
Cl^-	67	23	146	123
SO_4^{2-}	82	16	126	120
HCO_3^-	126	142	149	—
NO_3^-	44	16	57.4	10
F^-	1.4	2.2	1.3	0.76
SiO_2	52	42	—	75

The above compositions can be compared to other Yucca Mountain pore water compositions by means of a Ca^{2+}–SO_4^{2-}–ΣCO_3^{2-} ternary diagram, as shown in the following figure.

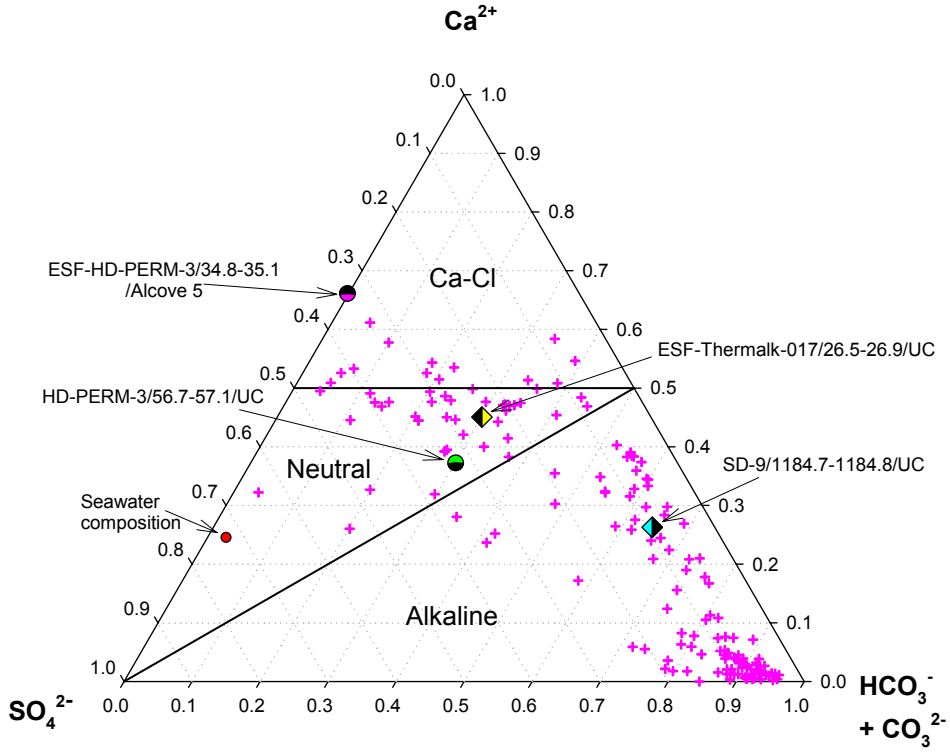


Figure 1. Ternary (Ca-SO_4-HCO_3) Phase Diagram Plotting Yucca Mountain Unsaturated Zone Pore Water Compositions (+) Reported by Yang, et al. (2003, 1998, 1996) and the Four Pore Water Compositions DOE Used in Its Near-Field Chemistry Model. Also Shown is the Seawater Composition. Chemical Divide Lines Separate the Compositions Into Three Brine Types: (i) Calcium-Chloride, (ii) Neutral, and (iii) Alkaline.

The above figure divides the composition space into three fields. Compositions located in the same field tend to evolve by evaporation into a similar brine type—Ca-Cl, neutral, or alkaline—based on the chemical divide concept discussed by Hardie and Eugster (1970). The compositions in Table 2 were used as input to evaporation simulations conducted at 25 °C. The results are shown in Figure 2.

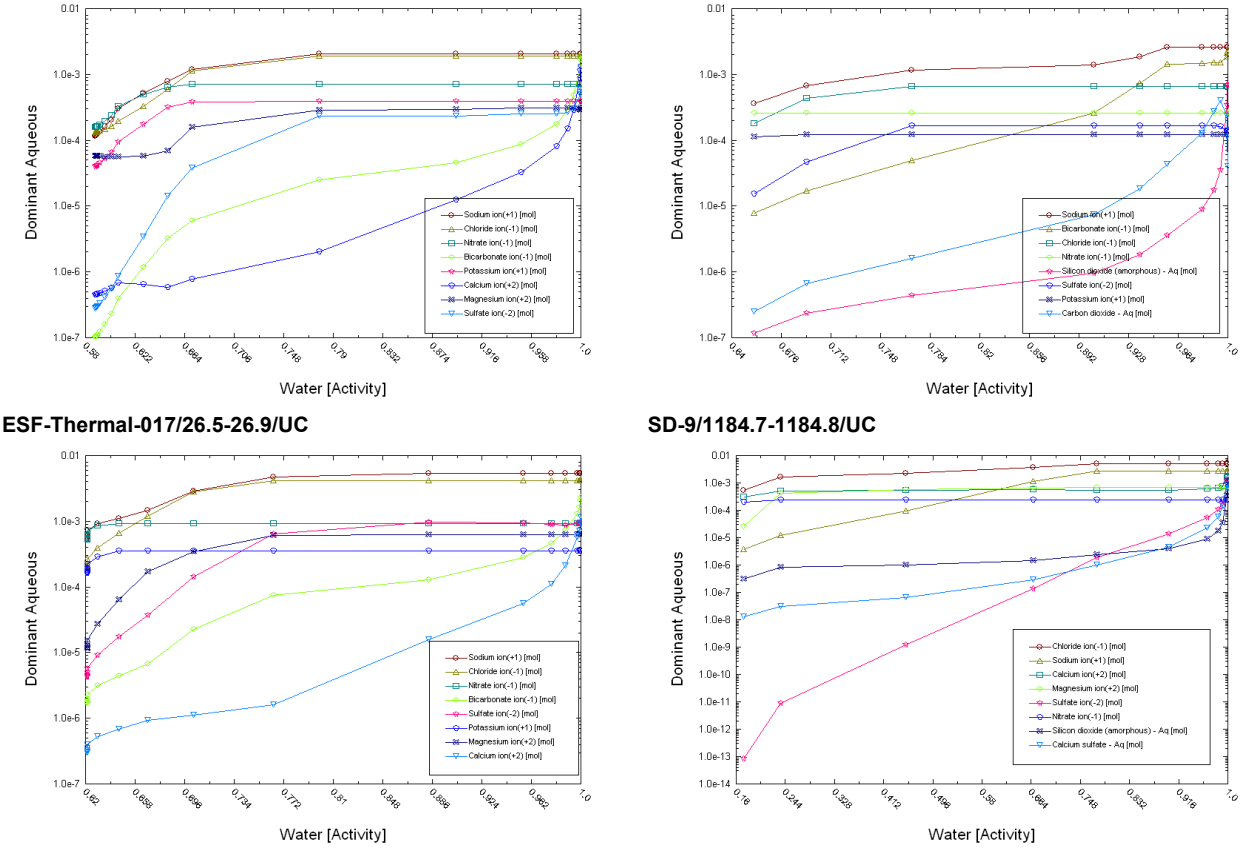
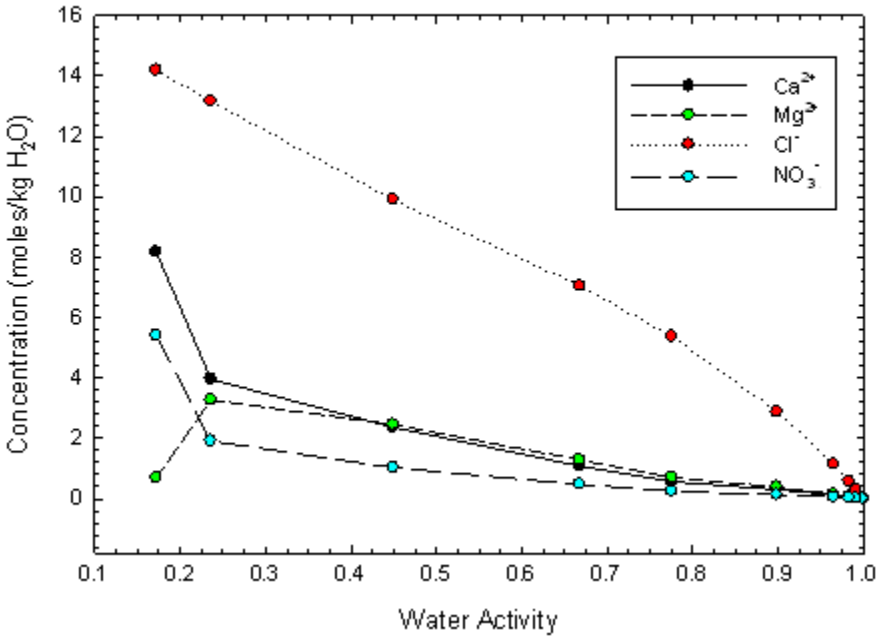


Figure 2. Dominant Aqueous Species in Evaporating Yucca Mountain Pore Waters Calculated at 25 °C Using StreamAnalyzer Version 2.0.30. Degree of Evaporation Increases from Right to Left of the Diagrams. The Pore Water Compositions Used as Input to the Evaporation Simulations Were Taken from the DOE Safety Analysis Report Table 2.3.5-5.

Of the four pore water compositions used as input in the calculations, ESF-HD-PERM-3/34.8-35.1/Alcove 5 resulted in brines that are dominated by Ca^{2+}, Mg^{2+}, and Cl^- ions. The other three pore water compositions resulted in brines dominated by Na^+ and Cl^- ions.

Thus, a preliminary conclusion can be made that there is a potential for rock bolts used in the Yucca Mountain ground support system to corrode by SCC if evaporation of initially dilute pore waters occurs due to thermal effects or due to ventilation during the preclosure period.

The calculated concentrations of Mg^{2+}, Ca^{2+}, Cl^{-}, and NO_3^{-} (moles/kg H_2O) for pore water composition ESF-HD-PERM-3/34.8-35.1/Alcove 5 as a function of degree of evaporation is shown in the following figure. Evaporation of the initially dilute pore water results in high concentrations of Mg^{2+}, Ca^{2+}, Cl^{-}, and NO_3^{-}. The decrease in Mg^{2+} concentration below a water activity of ~0.25 is due to the formation of an MgF^{+} aqueous complex.



End of Summary Discussion

April 30, 2009

In the DOE response to RAI 3.2.2.1.3.3-003, the composition of 125 TSw pore waters were tabulated. J. Myers requested that a Piper plot be generated to show the composition of the 90 compositions that were not excluded from the DOE screening process. Because some of the 90 compositions do not have HCO3– data, GWB React was used to derive HCO3– values. The React calculation specified a log fCO2 of -3.0, and charge balance on H+.

For pore water sample SD-9/991.7-992.1/UC, the React script is as follows:

```
Temperature is 25 C
      Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
      Working directory:  d:\gwb\test runs
      Options: Debye-Huckel

      Basis is:
       H2O                          1 free kg
       Na+                         61 mg/l
       K+                         5.4 mg/l
       Mg++                        .6 mg/l
       Calcite  (swapped for Ca++)     1 gram
       Cl-                        26 mg/l
       SO4--                       13 mg/l
       NO3-  (swapped for NH3(aq))     20 mg/l
       F-                         3.3 mg/l
       Br-                        .1 mg/l
       Quartz  (swapped for SiO2(aq))  1 gram
       CO2(g)  (swapped for HCO3-)     -3 log fugacity
       H+                          charge balance
       O2(g)  (swapped for O2(aq))     .21 fugacity
      Reactants:
       Fix fugacity of CO2(g)
```

The output is as follows:

```
        Step #     0            Xi = 0.0000
        Temperature =  25.0 C    Pressure =  1.013 bars
        pH =  8.098              log fO2 =   -0.678
        Eh =   0.7400 volts      pe =  12.5090
        Ionic strength      =    0.004116
        Activity of water   =    0.999974
        Solvent mass        =    1.000000 kg
        Solution mass       =    1.000294 kg
        Solution density    =    1.013    g/cm3
        Chlorinity          =    0.000724 molal
        Dissolved solids    =        294 mg/kg sol'n
        Rock mass           =    0.001954 kg
        Carbonate alkalinity=      105.74 mg/kg as CaCO3

                     moles       moles        grams         cm3
 Reactants           remaining   reacted      reacted       reacted
--------------------------------------------------------------------------------
 CO2(g)            -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
--------------------------------------------------------------------------------
 Calcite              0.009591     -2.018        0.9599         0.3542
 Quartz                0.01654     -1.781        0.9939         0.3753
                                                 _____          _____
       (total)                                    1.954          0.7295

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
--------------------------------------------------------------------------------
 Na+                  0.002612        60.02      0.9331        -2.6132
 HCO3-                 0.002063        125.8      0.9331        -2.7156
```

Cl-	0.0007240	25.66	0.9318	-3.1710
Ca++	0.0003825	15.33	0.7650	-3.5337
NO3-	0.0003181	19.72	0.9318	-3.5281
O2(aq)	0.0002654	8.490	1.0000	-3.5761
F-	0.0001712	3.252	0.9324	-3.7969
K+	0.0001363	5.328	0.9318	-3.8962
SO4--	0.0001278	12.27	0.7571	-4.0144
SiO2(aq)	0.0001002	6.016	1.0000	-3.9993
CO2(aq)	3.397e-005	1.495	1.0000	-4.4689
Mg++	2.326e-005	0.5651	0.7725	-4.7456
CO3--	1.490e-005	0.8940	0.7591	-4.9464
CaCO3(aq)	7.031e-006	0.7035	1.0000	-5.1530
CaHCO3+	6.722e-006	0.6794	0.9331	-5.2026
NaHCO3(aq)	6.688e-006	0.5617	1.0000	-5.1747
CaSO4(aq)	3.656e-006	0.4976	1.0000	-5.4370
NaSO4-	1.669e-006	0.1987	0.9331	-5.8076
HSiO3-	1.501e-006	0.1156	0.9331	-5.8538
OH-	1.359e-006	0.02311	0.9324	-5.8971
Br-	1.236e-006	0.09872	0.9318	-5.9387
CaNO3+	4.659e-007	0.04755	0.9331	-6.3618
MgSO4(aq)	4.485e-007	0.05397	1.0000	-6.3483
MgHCO3+	4.024e-007	0.03432	0.9331	-6.4255
NaCl(aq)	2.747e-007	0.01605	1.0000	-6.5612
CaF+	2.406e-007	0.01421	0.9331	-6.6489
MgCO3(aq)	1.936e-007	0.01632	1.0000	-6.7131
NaHSiO3(aq)	1.519e-007	0.01520	1.0000	-6.8185
KSO4-	9.979e-008	0.01348	0.9331	-7.0310
NaCO3-	9.658e-008	0.008013	0.9331	-7.0452
MgF+	6.919e-008	0.002995	0.9331	-7.1900
CaCl+	4.264e-008	0.003220	0.9331	-7.4002
NaF(aq)	3.911e-008	0.001642	1.0000	-7.4077

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Calcite	0.0000 sat	Coesite	-0.8100
Quartz	0.0000 sat	Monohydrocalcite	-0.8337
Dolomite-ord	-0.0280	Cristobalite(bet	-0.9940
Dolomite	-0.0280	Fluorite	-1.0904
Ice	-0.1387	SiO2(am)	-1.2857
Aragonite	-0.1444	Dolomite-dis	-1.5724
Tridymite	-0.1715	Magnesite	-1.6568
Chalcedony	-0.2712	Talc	-2.7843
Cristobalite(alp	-0.5505	Sellaite	-2.9550

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

Gases	fugacity	log fug.
O2(g)	0.2100	-0.678
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	9.829e-014	-13.007
HCl(g)	2.664e-018	-17.574
N2(g)	1.365e-019	-18.865
NO2(g)	7.954e-020	-19.099
HBr(g)	1.207e-023	-22.918
Br2(g)	1.369e-024	-23.864
NO(g)	1.163e-025	-24.934
Cl2(g)	4.717e-028	-27.326
SiF4(g)	4.115e-037	-36.386
H2(g)	6.115e-042	-41.214
CO(g)	1.910e-048	-47.719
SO2(g)	7.061e-057	-56.151
NH3(g)	4.259e-069	-68.371
Na(g)	3.272e-075	-74.485
K(g)	3.268e-077	-76.486
F2(g)	5.041e-082	-81.297
Mg(g)	9.751e-130	-129.011
H2S(g)	3.988e-144	-143.399

CH4(g)	1.116e-145	-144.952
Ca(g)	2.358e-151	-150.627
C(g)	9.776e-190	-189.010
Si(g)	4.226e-221	-220.374
S2(g)	9.486e-231	-230.023
C2H4(g)	6.568e-238	-237.183

		In fluid		Sorbed	Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Br-	1.24e-006	1.24e-006	0.0987			
Ca++	0.00999	0.000401	16.1			
Cl-	0.000724	0.000724	25.7			
F-	0.000172	0.000172	3.26			
H+	-0.00990	-0.000310	-0.312			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.0117	0.00213	130.			
K+	0.000136	0.000136	5.33			
Mg++	2.44e-005	2.44e-005	0.592			
NH3(aq)	0.000319	0.000319	5.42			
Na+	0.00262	0.00262	60.2			
O2(aq)	0.000903	0.000903	28.9			
SO4--	0.000134	0.000134	12.8			
SiO2(aq)	0.0166	0.000102	6.12			

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Bromine	1.236e-006	1.236e-006	0.09873		
Calcium	0.009991	0.0004007	16.05		
Carbon	0.01172	0.002133	25.61		
Chlorine	0.0007243	0.0007243	25.67		
Fluorine	0.0001715	0.0001715	3.258		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	2.438e-005	2.438e-005	0.5924		
Nitrogen	0.0003186	0.0003186	4.461		
Oxygen	55.58	55.52	8.880e+005		
Potassium	0.0001364	0.0001364	5.332		
Silicon	0.01664	0.0001018	2.859		
Sodium	0.002620	0.002620	60.23		
Sulfur	0.0001337	0.0001337	4.284		

For pore water sample ECRB-SYS-CS2350.5,0-5.7/UC, the script is

```
Temperature is 25 C
    Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
    Working directory:  d:\gwb\test runs
    Options: Debye-Huckel

    Basis is:
     H2O                          1 free kg
     Na+                        110 mg/l
     K+                        11.2 mg/l
     Mg++                       10.8 mg/l
     Calcite  (swapped for Ca++)     1 gram
     Cl-                        45 mg/l
     SO4--                        22 mg/l
     NO3-  (swapped for NH3(aq))     6.3 mg/l
     F-                         5.9 mg/l
     Br-                        .1 mg/l
     Quartz  (swapped for SiO2(aq))  1 gram
     CO2(g)  (swapped for HCO3-)     -3 log fugacity
     H+                           charge balance
     O2(g)  (swapped for O2(aq))     .21 fugacity
    Reactants:
     Fix fugacity of CO2(g)
```

The result is as follows:

```
Step #     0            Xi = 0.0000
Temperature =  25.0 C    Pressure =  1.013 bars
pH =  8.362              log fO2 =   -0.678
Eh =   0.7244 volts      pe =  12.2454
Ionic strength      =    0.006834
Activity of water   =    0.999955
Solvent mass        =    1.000000 kg
Solution mass       =    1.000478 kg
Solution density    =    1.013    g/cm3
Chlorinity          =    0.001254 molal
Dissolved solids    =         477 mg/kg sol'n
Rock mass           =    0.001980 kg
Carbonate alkalinity=      200.92 mg/kg as CaCO3

                    moles       moles        grams         cm3
Reactants           remaining   reacted      reacted       reacted
-------------------------------------------------------------------------------
CO2(g)            -- fixed fugacity buffer --

Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
Calcite              0.009857     -2.006         0.9866          0.3641
Quartz               0.01654      -1.781         0.9938          0.3753
                                  ___________    ___________
     (total)                        1.980          0.7393

Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------------
Na+                 0.004698        108.0       0.9165        -2.3659
HCO3-               0.003853        235.0       0.9165        -2.4521
Cl-                 0.001253        44.39       0.9145        -2.9410
Mg++                0.0004027       9.783       0.7267        -3.5336
F-                  0.0003045       5.782       0.9155        -3.5547
K+                  0.0002826       11.05       0.9145        -3.5876
O2(aq)              0.0002654       8.489       1.0000        -3.5761
SO4--               0.0002086       20.03       0.7043        -3.8329
Ca++                0.0001214       4.864       0.7160        -4.0608
NO3-                0.0001003       6.217       0.9145        -4.0374
SiO2(aq)            0.0001002       6.015       1.0000        -3.9993
CO3--               5.384e-005      3.229       0.7073        -4.4193
CO2(aq)             3.397e-005      1.494       1.0000        -4.4689
NaHCO3(aq)          2.168e-005      1.821       1.0000        -4.6639
MgHCO3+             1.224e-005      1.044       0.9165        -4.9500
MgSO4(aq)           1.110e-005      1.335       1.0000        -4.9549
MgCO3(aq)           1.062e-005      0.8947      1.0000        -4.9740
CaCO3(aq)           7.031e-006      0.7033      1.0000        -5.1530
NaSO4-              4.560e-006      0.5426      0.9165        -5.3789
CaHCO3+             3.730e-006      0.3769      0.9165        -5.4662
HSiO3-              2.803e-006      0.2160      0.9165        -5.5903
OH-                 2.540e-006      0.04317     0.9155        -5.6336
MgF+                2.004e-006      0.08674     0.9165        -5.7360
CaSO4(aq)           1.650e-006      0.2245      1.0000        -5.7826
Br-                 1.236e-006      0.09871     0.9145        -5.9468
NaCl(aq)            8.243e-007      0.04815     1.0000        -6.0839
NaCO3-              5.848e-007      0.04852     0.9165        -6.2708
NaHSiO3(aq)         4.924e-007      0.04926     1.0000        -6.3077
KSO4-               3.140e-007      0.04242     0.9165        -6.5409
MgCl+               2.681e-007      0.01601     0.9165        -6.6095
CaF+                1.271e-007      0.007503    0.9165        -6.9338
NaF(aq)             1.207e-007      0.005066    1.0000        -6.9183
CaNO3+              4.361e-008      0.004450    0.9165        -7.3982
CaCl+               2.190e-008      0.001653    0.9165        -7.6974
 (only species > 1e-8 molal listed)

Mineral saturation states
```

	log Q/K		log Q/K
Antigorite	19.9232s/sat	Cristobalite(alp	-0.5505
Talc	2.4329s/sat	Coesite	-0.8100
Dolomite-ord	1.7111s/sat	Monohydrocalcite	-0.8337
Dolomite	1.7111s/sat	Cristobalite(bet	-0.9940
Chrysotile	0.4444s/sat	Fluorite	-1.1333
Dolomite-dis	0.1667s/sat	Sellaite	-1.2588
Magnesite	0.0823s/sat	SiO2(am)	-1.2857
Quartz	0.0000 sat	Huntite	-1.3247
Calcite	0.0000 sat	Sepiolite	-1.6820
Ice	-0.1387	Tremolite	-1.9592
Aragonite	-0.1444	Enstatite	-2.1367
Tridymite	-0.1715	Lansfordite	-2.4651
Chalcedony	-0.2712	Nesquehonite	-2.6197

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

Gases	fugacity	log fug.
O2(g)	0.2100	-0.678
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	9.356e-014	-13.029
HCl(g)	2.466e-018	-17.608
NO2(g)	1.342e-020	-19.872
N2(g)	3.885e-021	-20.411
HBr(g)	6.459e-024	-23.190
Br2(g)	3.919e-025	-24.407
NO(g)	1.963e-026	-25.707
Cl2(g)	4.041e-028	-27.393
SiF4(g)	3.378e-037	-36.471
H2(g)	6.115e-042	-41.214
CO(g)	1.910e-048	-47.719
SO2(g)	3.186e-057	-56.497
NH3(g)	7.186e-070	-69.144
Na(g)	1.061e-074	-73.974
K(g)	1.220e-076	-75.914
F2(g)	4.568e-082	-81.340
Mg(g)	5.347e-128	-127.272
H2S(g)	1.799e-144	-143.745
CH4(g)	1.116e-145	-144.952
Ca(g)	2.358e-151	-150.627
C(g)	9.776e-190	-189.010
Si(g)	4.226e-221	-220.374
S2(g)	1.931e-231	-230.714
C2H4(g)	6.568e-238	-237.183

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Br-	1.24e-006	1.24e-006	0.0987			
Ca++	0.00999	0.000134	5.37			
Cl-	0.00125	0.00125	44.4			
F-	0.000307	0.000307	5.83			
H+	-0.0100	-0.000144	-0.145			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.0139	0.00400	244.			
K+	0.000283	0.000283	11.1			
Mg++	0.000439	0.000439	10.7			
NH3(aq)	0.000100	0.000100	1.71			
Na+	0.00473	0.00473	109.			
O2(aq)	0.000466	0.000466	14.9			
SO4--	0.000226	0.000226	21.7			
SiO2(aq)	0.0166	0.000103	6.21			

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Bromine	1.236e-006	1.236e-006	0.09873		
Calcium	0.009991	0.0001340	5.369		

Carbon	0.01385	0.003997	47.98
Chlorine	0.001254	0.001254	44.43
Fluorine	0.0003068	0.0003068	5.825
Hydrogen	111.0	111.0	1.118e+005
Magnesium	0.0004389	0.0004389	10.66
Nitrogen	0.0001004	0.0001004	1.405
Oxygen	55.59	55.52	8.879e+005
Potassium	0.0002830	0.0002830	11.06
Silicon	0.01664	0.0001035	2.904
Sodium	0.004726	0.004726	108.6
Sulfur	0.0002262	0.0002262	7.250

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 8.280 log fO2 = -0.678
Eh = 0.7292 volts pe = 12.3265
Ionic strength = 0.005794
Activity of water = 0.999955
Solvent mass = 1.000006 kg
Solution mass = 1.000432 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.001254 molal
Dissolved solids = 425 mg/kg sol'n
Rock mass = 0.002011 kg
Carbonate alkalinity= 164.06 mg/kg as CaCO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.009378	-2.028	0.9386	0.3464
Dolomite	0.0004269	-3.370	0.07872	0.02748
Quartz	0.01654	-1.781	0.9938	0.3753
(total)		2.011	0.7491	

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.004701	108.0	0.9223	-2.3629
HCO3-	0.003177	193.8	0.9223	-2.5331
Cl-	0.001253	44.40	0.9205	-2.9381
F-	0.0003064	5.818	0.9214	-3.5493
K+	0.0002826	11.04	0.9205	-3.5848
O2(aq)	0.0002654	8.489	1.0000	-3.5761
SO4--	0.0002181	20.94	0.7223	-3.8027
Ca++	0.0001724	6.906	0.7326	-3.8986
NO3-	0.0001003	6.216	0.9205	-4.0347
SiO2(aq)	0.0001002	6.016	1.0000	-3.9993
CO3--	3.616e-005	2.169	0.7249	-4.5815
CO2(aq)	3.397e-005	1.494	1.0000	-4.4689
NaHCO3(aq)	1.812e-005	1.521	1.0000	-4.7420
Mg++	1.114e-005	0.2707	0.7422	-5.0825
CaCO3(aq)	7.031e-006	0.7034	1.0000	-5.1530
NaSO4-	4.893e-006	0.5822	0.9223	-5.3456
CaHCO3+	4.468e-006	0.4515	0.9223	-5.3851
CaSO4(aq)	2.569e-006	0.3496	1.0000	-5.5902
HSiO3-	2.311e-006	0.1781	0.9223	-5.6713
OH-	2.094e-006	0.03559	0.9214	-5.7146
Br-	1.236e-006	0.09872	0.9205	-5.9440
NaCl(aq)	8.357e-007	0.04882	1.0000	-6.0780
NaHSiO3(aq)	4.114e-007	0.04115	1.0000	-6.3858
NaCO3-	4.029e-007	0.03342	0.9223	-6.4300
KSO4-	3.367e-007	0.04549	0.9223	-6.5079
MgSO4(aq)	3.361e-007	0.04044	1.0000	-6.4735
MgHCO3+	2.852e-007	0.02432	0.9223	-6.5800
MgCO3(aq)	2.065e-007	0.01740	1.0000	-6.6851
CaF+	1.858e-007	0.01097	0.9223	-6.7662
NaF(aq)	1.231e-007	0.005166	1.0000	-6.9098
CaNO3+	6.336e-008	0.006466	0.9223	-7.2333
MgF+	5.698e-008	0.002466	0.9223	-7.2794
CaCl+	3.183e-008	0.002403	0.9223	-7.5323

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.0000 sat	Coesite	-0.8100
Calcite	0.0000 sat	Monohydrocalcite	-0.8337

Dolomite	0.0000 sat	Fluorite	-0.9602
Dolomite-ord	0.0000 sat	Cristobalite(bet	-0.9940
Ice	-0.1387	SiO2(am)	-1.2857
Aragonite	-0.1444	Dolomite-dis	-1.5444
Tridymite	-0.1715	Magnesite	-1.6288
Chalcedony	-0.2712	Talc	-2.7003
Cristobalite(alp	-0.5505	Sellaite	-2.7968

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

Gases	fugacity	log fug.
O2(g)	0.2100	-0.678
H2O(g)	0.02598	-1.585
CO2(g)	0.001000	-3.000
HF(g)	1.142e-013	-12.942
HCl(g)	2.992e-018	-17.524
NO2(g)	1.628e-020	-19.788
N2(g)	5.715e-021	-20.243
HBr(g)	7.835e-024	-23.106
Br2(g)	5.768e-025	-24.239
NO(g)	2.381e-026	-25.623
Cl2(g)	5.950e-028	-27.225
SiF4(g)	7.496e-037	-36.125
H2(g)	6.115e-042	-41.214
CO(g)	1.910e-048	-47.719
SO2(g)	4.962e-057	-56.304
NH3(g)	8.716e-070	-69.060
Na(g)	8.863e-075	-74.052
K(g)	1.019e-076	-75.992
F2(g)	6.804e-082	-81.167
Mg(g)	1.040e-129	-128.983
H2S(g)	2.802e-144	-143.552
CH4(g)	1.116e-145	-144.952
Ca(g)	2.358e-151	-150.627
C(g)	9.777e-190	-189.010
Si(g)	4.226e-221	-220.374
S2(g)	4.683e-231	-230.329
C2H4(g)	6.568e-238	-237.183

		In fluid	Sorbed	Kd	
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Br-	1.24e-006	1.24e-006	0.0987			
Ca++	0.00999	0.000187	7.48			
Cl-	0.00125	0.00125	44.4			
F-	0.000307	0.000307	5.83			
H+	-0.0103	-0.000115	-0.116			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.0135	0.00328	200.			
K+	0.000283	0.000283	11.1			
Mg++	0.000439	1.20e-005	0.292			
NH3(aq)	0.000100	0.000100	1.71			
Na+	0.00473	0.00473	109.			
O2(aq)	0.000466	0.000466	14.9			
SO4--	0.000226	0.000226	21.7			
SiO2(aq)	0.0166	0.000103	6.18			

Elemental composition	In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Bromine	1.236e-006	1.236e-006	0.09874		
Calcium	0.009991	0.0001867	7.481		
Carbon	0.01351	0.003278	39.35		
Chlorine	0.001254	0.001254	44.43		
Fluorine	0.0003068	0.0003068	5.825		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0004389	1.203e-005	0.2924		
Nitrogen	0.0001004	0.0001004	1.405		
Oxygen	55.58	55.52	8.879e+005		
Potassium	0.0002830	0.0002830	11.06		

Silicon	0.01664	0.0001029	2.888
Sodium	0.004726	0.004726	108.6
Sulfur	0.0002262	0.0002262	7.251

For sample ESF-HD-PERM-1, the script is as follows:

```
Temperature is 25 C
    Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
    Working directory:  d:\gwb\test runs
    Options: Debye-Huckel

    Basis is:
     H2O                          1 free kg
     Na+                         61 mg/l
     K+                          6 mg/l
     Mg++                          25.7 mg/l
     Calcite  (swapped for Ca++)     1 gram
     Cl-                        123 mg/l
     SO4--                         124 mg/l
     NO3-  (swapped for NH3(aq))     22 mg/l
     F-                         .36 mg/l
     Br-                        .6 mg/l
     Quartz  (swapped for SiO2(aq))  1 gram
     CO2(g)  (swapped for HCO3-)     -3 log fugacity
     H+                           charge balance
     O2(g)  (swapped for O2(aq))     .21 fugacity
    Reactants:
     Fix fugacity of CO2(g)
```

For sample ESF-HD-PERM-2, the script is as follows:

```
    Temperature is 25 C
    Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
    Working directory:  d:\gwb\test runs
    Options: Debye-Huckel

    Basis is:
     H2O                          1 free kg
     Na+                         61 mg/l
     K+                          7 mg/l
     Mg++                          16.6 mg/l
     Calcite  (swapped for Ca++)     1 gram
     Cl-                        110 mg/l
     SO4--                         111 mg/l
     NO3-  (swapped for NH3(aq))     3 mg/l
     F-                         .96 mg/l
     Br-                        .76 mg/l
     Quartz  (swapped for SiO2(aq))  1 gram
     CO2(g)  (swapped for HCO3-)     -3 log fugacity
     H+                           charge balance
     O2(g)  (swapped for O2(aq))     .21 fugacity
    Reactants:
     Fix fugacity of CO2(g)
```

For sample ESF-HD-PERM-3, the script is as follows:

```
    Temperature is 25 C
    Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
    Working directory:  d:\gwb\test runs
    Options: Debye-Huckel

    Basis is:
     H2O                          1 free kg
     Na+                         62 mg/l
     K+                          9 mg/l
     Mg++                          17.4 mg/l
     Calcite  (swapped for Ca++)     1 gram
```

```
 Cl-                          123 mg/l
 SO4--                          120 mg/l
 NO3-  (swapped for NH3(aq))     10 mg/l
 F-                           .76 mg/l
 Br-                          1.2 mg/l
 Quartz  (swapped for SiO2(aq))  1 gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 H+                           charge balance
 O2(g)  (swapped for O2(aq))     .21 fugacity
Reactants:
 Fix fugacity of CO2(g)
```

For sample ECRB-SYS-CS1250/5.0-5.7/UC, the script is as follows:

```
Temperature is 25 C
Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
Working directory:  d:\gwb\test runs
Options: Debye-Huckel

Basis is:
 H2O                           1 free kg
 Na+                          79 mg/l
 K+                           11.2 mg/l
 Mg++                          7.9 mg/l
 Calcite  (swapped for Ca++)     1 gram
 Cl-                          50 mg/l
 SO4--                          21 mg/l
 NO3-  (swapped for NH3(aq))     25 mg/l
 F-                           3 mg/l
 Br-                          .2 mg/l
 Quartz  (swapped for SiO2(aq))  1 gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 H+                           charge balance
 O2(g)  (swapped for O2(aq))     .21 fugacity
Reactants:
 Fix fugacity of CO2(g)
```

For sample ECRB-SYS-CS400/3.8-4.3/UC, the script is as follows:

```
Temperature is 25 C
Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
Working directory:  d:\gwb\test runs
Options: Debye-Huckel

Basis is:
 H2O                           1 free kg
 Na+                          120 mg/l
 K+                           12.5 mg/l
 Mg++                          35.1 mg/l
 Calcite  (swapped for Ca++)     1 free gram
 Cl-                          29 mg/l
 SO4--                          94 mg/l
 NO3-  (swapped for NH3(aq))     .25 mg/l
 F-                           3.7 mg/l
 Quartz  (swapped for SiO2(aq))  1 free gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 H+                           charge balance
 O2(g)  (swapped for O2(aq))     .21 fugacity
Reactants:
 Fix fugacity of CO2(g)
```

For sample ECRB-SYS-CS700/5.5-5.8/UC, the script is as follows:

```
      Temperature is 25 C
Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
Working directory:  d:\gwb\test runs
Options: Debye-Huckel
```

```
Basis is:
 H2O                          1 free kg
 Na+                         91 mg/l
 K+                         13.7 mg/l
 Mg++                         33 mg/l
 Calcite  (swapped for Ca++)     1 free gram
 Cl-                        64 mg/l
 SO4--                        146 mg/l
 NO3-  (swapped for NH3(aq))     2.8 mg/l
 F-                         6.2 mg/l
 Quartz  (swapped for SiO2(aq))  1 free gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 H+                           charge balance
 O2(g)  (swapped for O2(aq))     .21 fugacity
Reactants:
 Fix fugacity of CO2(g)
```

For sample ECRB-SYS-CS900/3.0-3.2/UC, the script is as follows:

```
Temperature is 25 C
 Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
 Working directory:  d:\gwb\test runs
 Options: Debye-Huckel

 Basis is:
 H2O                          1 free kg
 Na+                         127 mg/l
 K+                          13 mg/l
 Mg++                         28.1 mg/l
 Calcite  (swapped for Ca++)     1 free gram
 Cl-                        66 mg/l
 SO4--                        112 mg/l
 NO3-  (swapped for NH3(aq))     5.9 mg/l
 F-                         .73 mg/l
 Quartz  (swapped for SiO2(aq))  1 free gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 H+                           charge balance
 O2(g)  (swapped for O2(aq))     .21 fugacity
 Br-                        1.2 mg/l
Reactants:
 Fix fugacity of CO2(g)
```

For sample SD-9/670.5-670.6/UC, the script is as follows:

```
Temperature is 25 C
Thermo dataset:  C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat
Working directory:  d:\gwb\test runs
Options: Debye-Huckel

Basis is:
 H2O                          1 free kg
 Na+                         72 mg/l
 K+                         8.4 mg/l
 Mg++                         9 mg/l
 Calcite  (swapped for Ca++)     1 free gram
 Cl-                        46 mg/l
 SO4--                        56 mg/l
 NO3-  (swapped for NH3(aq))     28 mg/l
 F-                         2.8 mg/l
 Br-                        .3 mg/l
 Quartz  (swapped for SiO2(aq))  1 free gram
 CO2(g)  (swapped for HCO3-)     -3 log fugacity
 O2(g)  (swapped for O2(aq))     .21 fugacity
 H+                           charge balance
Reactants:
 Fix fugacity of CO2(g)
```

The following table lists the compositions of the 90 porewaters considered by the DOE in the screening of pore water chemistry for the near-field chemistry model:

Sample Name	Lith. Unit	Screening Status	Group # (rep. water[a])	pH	Na (mg/L)	K (mg/L)	Mg (mg/L)	Ca (mg/L)
SD-9/991.7-992.1/UC	Tptpll	In	1	7.9	61	5.4	0.6	27
SD-9/1060.1-1060.5/UC	Tptpll	In	1	7.6	68	8.8	<0.25	21
SD-9/1119.7-1119.9/UC	Tptpll	In	1	7.7	81	12.8	<0.6	34
SD-9/1184.7-1184.8/UC	Tptpll	In	1[a]	8.2	59	4.8	0.7	19
SD-9/1184.8-1185.0/UC	Tptpll	In	1	7.9	62	5.4	<0.4	24
ECRB-SYS-CS1500/10.0-12.1/UC	Tptpll	Out	—	8.1	120	11.1	16.4	130
ECRB-SYS-CS2000/16.3-16.5/UC	Tptpll	Out	—	7.4	120	6.1	3.3	81
ECRB-SYS-CS2000/16.5-21.1/UC	Tptpll	Out	—	7.4	130	10.6	5.3	82
ECRB-SYS-CS2000/3.3-3.8/UC	Tptpll	Out	—	—	204	20.3	7.1	170
ECRB-SYS-CS2000/3.95-4.1/UC	Tptpll	Out	—	7.8	116	11.1	2.8	88
ECRB-SYS-CS2150/5.5-6.1/UC	Tptpll	Out	—	7.6	83	6.9	8.3	98
ECRB-SYS-CS2250/5.2-5.6/UC	Tptpll	Out	—	8	74	9.1	10.1	87
ECRB-SYS-CS2300/4.3-4.9/UC	Tptpll	Out	—	7.9	98	12.5	10.2	73
ECRB-SYS-CS2300/6.1-6.7/UC	Tptpll	Out	—	8.2	96	12.7	9.3	65
ECRB-SYS-CS2350/5.0-5.7/UC	Tptpll	Out	—	—	110	11.2	10.8	58
SD-9/990.4-991.7/UC	Tptpll	Out	—	7.9	84	7.9	0.9	56
SD-9/1184.0-1184.2/UC	Tptpll	Out	—	7.7	92	7.6	1.9	44
SD-12/1053.7-1054.1 UC-1	Tptpll	Out	—	7.7	122	11.9	23.9	75
SD-9/1185.0-1185.3/UC1	Tptpln	In	1	—	70	8.6	0.27	18.4
SD-9/1234.9-1235.1/UC	Tptpln	In	1	7.9	67	8	0.5	18
SD-9/1276.5-1276.8/UC	Tptpln	In	1	7.9	67	6.4	0.6	23
SD-9/1276.8-1277.0/UC	Tptpln	In	1	7.6	69	6.9	0.6	23
SD-9/1303.4-1303.9/UC	Tptpln	In	1	—	95	11.3	2.3	37
SD-9/1236.4-1236.8/UC	Tptpln	Out	—	7.5	100	8.4	4.9	51
SD-9/1275.6-1276.0/UC	Tptpln	Out	—	7.5	81	7.7	2.5	42
SD-9/1330.4-1330.7/UC	Tptpln	Out	—	7.2	130	9.5	7.5	73
ESF-HD-PERM-1	Tptpmn	In	3	7.8	61	6	25.7	98
ESF-HD-PERM-2	Tptpmn	In	3	8.3	61	7	16.6	106
ESF-HD-PERM-3	Tptpmn	In	3[a]	8.3	62	9	17.4	97
HD-PERM-3/22.4-23.0/UC	Tptpmn	In	4	—	103	14.6	17.4	48.7
HD-PERM-3/56.7-57.1/UC	Tptpmn	In	4[a]	—	123	13.8	16.7	59.9
NRG-7/7A/839.3-839.8/UC	Tptpmn	In	1	7.9	67	6.9	1.6	19
ECRB-SYS-CS1000/10.9-11.1/UC	Tptpmn	Out	—	—	72	18.7	53.5	275
ECRB-SYS-CS1000/11.1-11.6/UC	Tptpmn	Out	—	7.3	79	21.3	54.1	280
ECRB-SYS-CS1000/12.9-14.0/UC	Tptpmn	Out	—	7.8	47	9.9	21.9	120

Sample Name	Lith. Unit	Screening Status	Group # (rep. water[a])	pH	Na (mg/L)	K (mg/L)	Mg (mg/L)	Ca (mg/L)
ECRB-SYS-CS1000/15.6-15.8/UC	Tptpmn	Out	—		110	24.8	44.2	240
ECRB-SYS-CS1000/5.4-6.1/UC	Tptpmn	Out	—	8	64	13.5	21.6	105
ECRB-SYS-CS1000/7.3-7.7/UC	Tptpmn	Out	—	7.6	39	7.6	18.1	94
ECRB-SYS-CS1100/3.7-3.8/UC	Tptpmn	Out	—	7.1	110	9	23.3	170
ECRB-SYS-CS1150/3.2-3.8/UC	Tptpmn	Out	—	—	130	8.8	6.3	96
ECRB-SYS-CS1250/3.4-4.0/UC	Tptpmn	Out	—	7.5	83	13.7	23.5	160
ECRB-SYS-CS1250/5.0-5.7/UC	Tptpmn	Out	—	7.7	79	11.2	7.9	55
ESF-SAD-GTB#1/119.4-120.0/UC	Tptpmn	Out	—	—	69	19.2	12	73
ESF-SAD-GTB#1/126.1-126.4/UC	Tptpmn	Out	—	—	100	22.4	23.3	170
ESF-SAD-GTB#1/194.2-195.2/UC	Tptpmn	Out	—	8	97	24.7	35.5	230
ESF-SAD-GTB#1/195.4-196.7/UC	Tptpmn	Out	—	7.6	81	21.2	29	190
ESF-SAD-GTB#1/199.0-199.3/UC	Tptpmn	Out	—	—	161	30.6	38.2	268
HD-PERM-2/19.3-19.7/UC	Tptpmn	Out	—	—	101	15.7	17.2	113
HD-PERM-2/34.5-34.9/UC	Tptpmn	Out	—	—	110	17.1	17.8	143
HD-PERM-2/61.7-62.3/UC	Tptpmn	Out	—	—	86.7	16.9	8.2	89
ECRB-DS3-1616/7.5-7.7/UC	Tptpul	In	1	—	52.9	5.9	0.81	28.7
ECRB-DS3-1616/7.7-7.9/UC	Tptpul	In	1	—	50.9	7.27	0.72	25.4
ECRB-DS3-1616/7.9-8.0/UC	Tptpul	In	1	—	36.5	4.1	0.35	16.7
ECRB-DS3-1616/8.0-8.1/UC	Tptpul	In	1	—	46.9	5.63	0.59	23.4
ECRB-DS3-1616/9.6-9.8/UC	Tptpul	In	1	—	36.8	6.06	0.73	16.5
ECRB-DS3-1616/9.8-10.1/UC	Tptpul	In	1	—	38	5.77	0.76	20.7
ECRB-DS3-1616/10.1-10.4/UC	Tptpul	In	1	—	39.8	6.03	0.91	20.1
ECRB-DS3-1616/10.6-11.0/UC	Tptpul	In	1	—	61	7.68	1.44	34.1
ECRB-DS3-1616/12.5-12.7/UC	Tptpul	In	1	—	32.5	4.21	0.91	23.5
ECRB-DS3-1616/12.7-13.3/UC	Tptpul	In	1	—	51.4	6.81	1.05	28.8
ESF-THERMALK-017/16.6-17.2/UC	Tptpul	In	2	—	51	14.2	9.8	73
ESF-THERMALK-017/22.3-22.9/UC	Tptpul	In	2	—	48	14.1	7.8	60
ESF-THERMALK-017/22.9-23.0/UC	Tptpul	In	2	7.9	37	14.5	9.9	72
ESF-THERMALK-017/26.3-26.5/UC	Tptpul	In	2	—	42	13.6	7.6	58
ESF-THERMALK-017/26.5-26.9/UC	Tptpul	In	2[a]	7.7	45	14.4	7.9	62
ESF-THERMALK-019/19.2-19.5/UC	Tptpul	In	2	—	47	13.7	9	69
ESF-THERMALK-019/19.5-19.7/UC	Tptpul	In	2	—	44	13.2	9.1	71

Sample Name	Lith. Unit	Screening Status	Group # (rep. water[a])	pH	Na (mg/L)	K (mg/L)	Mg (mg/L)	Ca (mg/L)
SD-9/669.1-669.2/UC	Tptpul	In	4	—	61	6.3	6.9	66
ECRB-DS2-1613/13.2-13.4/UC	Tptpul	Out	—	—	75.6	6.04	1.01	38.2
ECRB-DS2-1613/18.6-18.9/UC	Tptpul	Out	—	—	64.2	6.14	0.88	29.9
ECRB-DS3-1616/7.1-7.5/UC	Tptpul	Out	—	—	50.5	6.07	0.51	19.8
ECRB-DS3-1616/8.7-8.9/UC	Tptpul	Out	—	—	89.1	8.32	0.82	38.4
ECRB-DS3-1616/10.4-10.6/UC	Tptpul	Out	—	—	45.5	6.21	0.85	20.2
ECRB-DS3-1616/11.5-12.5/UC	Tptpul	Out	—	—	70.8	7.33	0.88	33
ECRB-SYS-CS400/3.8-4.3/UC	Tptpul	Out	—	7.3	120	12.5	35.1	240
ECRB-SYS-CS400/5.6-6.2/UC	Tptpul	Out	—	7	89	9.7	15.4	85
ECRB-SYS-CS450/5.3-6.0/UC	Tptpul	Out	—	6.7	68	17	22.9	190
ECRB-SYS-CS500/12.0-16.7/UC	Tptpul	Out	—	8	57	10.3	19.3	120
ECRB-SYS-CS600/3.6-4.0/UC	Tptpul	Out	—	7.5	67	10.4	10.6	81
ECRB-SYS-CS700/5.5-5.8/UC	Tptpul	Out	—	—	91	13.7	33	230
ECRB-SYS-CS750/6.2-6.5/UC	Tptpul	Out	—	7.6	70	8.5	12.9	130
ECRB-SYS-CS800/4.9-5.6/UC	Tptpul	Out	—	7.4	53	6.6	11.9	92
ECRB-SYS-CS850 5.1-5.6/UC	Tptpul	Out	—	8.1	59	5.9	13.1	63
ECRB-SYS-CS900/2.8-3.0/UC	Tptpul	Out	—	—	90	8.7	17.7	142
ECRB-SYS-CS900/3.0-3.2/UC	Tptpul	Out	—	7.4	127	13	28.1	229
ECRB-SYS-CS900/3.5-4.1/UC	Tptpul	Out	—	7.5	140	13.6	25.8	210
ECRB-SYS-CS900/5.4-5.9/UC	Tptpul	Out	—	7.7	79	6.9	14	110
ECRB-SYS-CS950/4.8-5.5/UC	Tptpul	Out	—	7.1	84	7.1	22.6	170
ECRB-SYS-CS950/5.2-5.3/UC	Tptpul	Out	—	7.1	66	6.2	13.6	98
SD-9/670.5-670.6/UC	Tptpul	Out	—	—	72	8.4	9	81

The following is a continuation of the composition table:

Sample Name	Cl (mg/L)	SO_4 (mg/L)	HCO_3 (mg/L)	NO_3 (mg/L)	F (mg/L)	Br (mg/L)	SiO_2 (mg/L)
SD-9/991.7-992.1/UC	26	13	—	20	3.3	0.1	55
SD-9/1060.1-1060.5/UC	32	15	140	21	1.5	<0.16	50
SD-9/1119.7-1119.9/UC	32	24	193	19	1.2	<0.18	45
SD-9/1184.7-1184.8/UC	23	16	142	16	2.2	<0.10	42
SD-9/1184.8-1185.0/UC	16	12	196	12	0.84	<0.10	47

Sample Name	Cl (mg/L)	SO_4 (mg/L)	HCO_3 (mg/L)	NO_3 (mg/L)	F (mg/L)	Br (mg/L)	SiO_2 (mg/L)
ECRB-SYS-CS1500/10.0-12.1/UC	97	97	349	0.5	1.4	0.91	45.7
ECRB-SYS-CS2000/16.3-16.5/UC	24	31	362	0.4	6	<0.2	42
ECRB-SYS-CS2000/16.5-21.1/UC	26	39	382	4.2	11	<0.2	48
ECRB-SYS-CS2000/3.3-3.8/UC	38	76	639	0	3.9	0.96	64
ECRB-SYS-CS2000/3.95-4.1/UC	20	35	329	2	7.7	0.22	39
ECRB-SYS-CS2150/5.5-6.1/UC	27	48	265	1.2	5.3	<0.2	52
ECRB-SYS-CS2250/5.2-5.6/UC	24	27	384	1.3	1.1	<0.10	54
ECRB-SYS-CS2300/4.3-4.9/UC	23	34	340	0.9	1.7	<0.1	43
ECRB-SYS-CS2300/6.1-6.7/UC	20	13	434	1.4	1	<0.10	49
ECRB-SYS-CS2350/5.0-5.7/UC	45	22	—	6.3	5.9	<0.10	46.1
SD-9/990.4-991.7/UC	23	10	313	17	2.5	<0.2	50
SD-9/1184.0-1184.2/UC	44	17	221	17	1.7	<0.10	45
SD-12/1053.7-1054.1 UC-1	180	32	308	4.2	3.8	<0.10	43
SD-9/1185.0-1185.3/UC1	42.4	12	145	18	2.4	2.5	—
SD-9/1234.9-1235.1/UC	17	16	156	11	1.1	<0.12	42
SD-9/1276.5-1276.8/UC	29	17	136	10	1.9	<0.16	59
SD-9/1276.8-1277.0/UC	35	17	165	10	2	0.29	67
SD-9/1303.4-1303.9/UC	65	28	194	19	4.8	<0.43	54
SD-9/1236.4-1236.8/UC	77	21	210	12	3.6	<0.10	54
SD-9/1275.6-1276.0/UC	61	20	146	8.5	3.7	<0.10	38
SD-9/1330.4-1330.7/UC	133	35	245	15	5	0.54	55
ESF-HD-PERM-1	123	124	—	22	0.36	0.6	79
ESF-HD-PERM-2	110	111	—	3	0.96	0.76	66
ESF-HD-PERM-3	123	120	—	10	0.76	1.2	75
HD-PERM-3/22.4-23.0/UC	131	123	120	28	1.6	—	—
HD-PERM-3/56.7-57.1/UC	146	126	149	57	1.3	—	—
NRG-7/7A/839.3-839.8/UC	31	24	151	25	2.8	0.1	41
ECRB-SYS-CS1000/10.9-11.1/UC	29	45	700	4.3	0.87	1.4	64
ECRB-SYS-CS1000/11.1-11.6/UC	18	65	714	5.6	0.59	1.1	57
ECRB-SYS-CS1000/12.9-14.0/UC	22	35	405	17	2	<0.1	50
ECRB-SYS-CS1000/15.6-15.8/UC	29	82	741	9.6	1.3	<0.10	61
ECRB-SYS-CS1000/5.4-6.1/UC	48	41	258	5.9	1	2.9	50
ECRB-SYS-CS1000/7.3-7.7/UC	21	36	333	2.6	3.4	<1	42
ECRB-SYS-CS1100/3.7-3.8/UC	17	55	525	24	0.65	<0.10	54
ECRB-SYS-CS1150/3.2-3.8/UC	33	22	323	24	1.9	<0.10	70
ECRB-SYS-CS1250/3.4-4.0/UC	25	60	464	1.3	2.1	—	54
ECRB-SYS-CS1250/5.0-5.7/UC	50	21	—	25	3	0.2	59
ESF-SAD-GTB#1/119.4-120.0/UC	69	46	266	3.9	1.5	0.4	51
ESF-SAD-GTB#1/126.1-126.4/UC	133	66	427	6.2	1.2	0.63	54
ESF-SAD-GTB#1/194.2-195.2/UC	110	115	545	1.5	1.5	0.89	66
ESF-SAD-GTB#1/195.4-196.7/UC	97	79	501	3.7	1.4	0.57	62
ESF-SAD-GTB#1/199.0-199.3/UC	180	112	706	35	1.4	—	—
HD-PERM-2/19.3-19.7/UC	133	129	259	29	1.8	—	—
HD-PERM-2/34.5-34.9/UC	128	128	368	19	1.5	—	—
HD-PERM-2/61.7-62.3/UC	86.5	76.2	236	37	1.7	—	—
ECRB-DS3-1616/7.5-7.7/UC	15.7	25.3	107	34	1.66	0.2	55

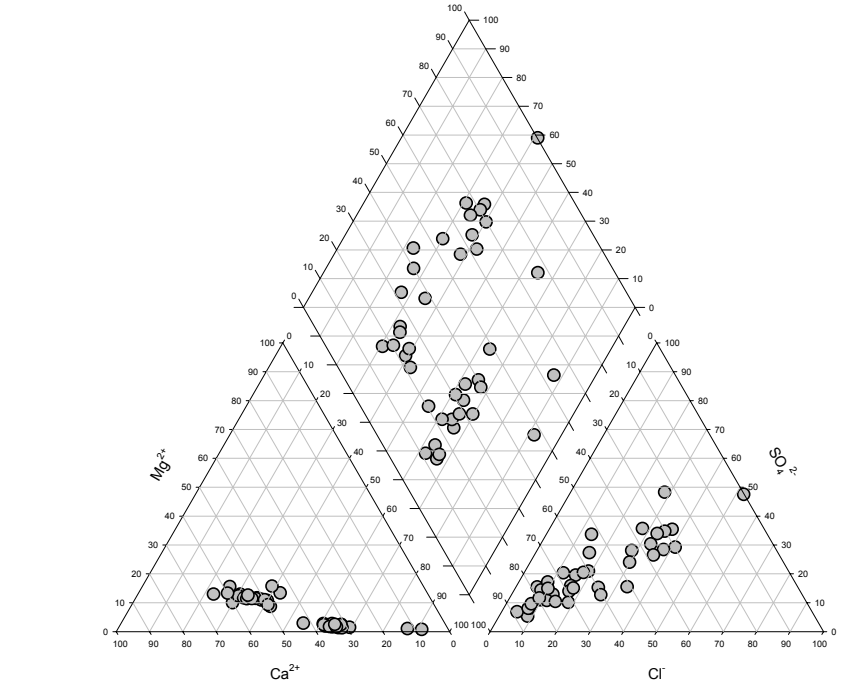
Sample Name	Cl (mg/L)	SO_4 (mg/L)	HCO_3 (mg/L)	NO_3 (mg/L)	F (mg/L)	Br (mg/L)	SiO_2 (mg/L)
ECRB-DS3-1616/7.7-7.9/UC	15.3	19.5	107	30	1.46	<0.03	51
ECRB-DS3-1616/7.9-8.0/UC	7.79	10.5	82	17	1.16	0.1	52
ECRB-DS3-1616/8.0-8.1/UC	11.5	15.4	115	24	1.59	<0.03	58
ECRB-DS3-1616/9.6-9.8/UC	6.89	5.29	113	8.1	1.38	<0.03	42
ECRB-DS3-1616/9.8-10.1/UC	4.98	8.84	149	10	1.35	<0.06	46
ECRB-DS3-1616/10.1-10.4/UC	7.2	9.48	128	15	1.51	<0.03	39
ECRB-DS3-1616/10.6-11.0/UC	20.4	22.3	142	33	2.32	<0.05	46
ECRB-DS3-1616/12.5-12.7/UC	8.99	13.2	123	19	1.15	<0.06	38
ECRB-DS3-1616/12.7-13.3/UC	15	17.8	166	27	1.86	<0.06	44
ESF-THERMALK-017/16.6-17.2/UC	82	105	104	45	1.3	0.33	63
ESF-THERMALK-017/22.3-22.9/UC	65	86	95	41	1.5	0.4	51
ESF-THERMALK-017/22.9-23.0/UC	69	94	116	46	1.1	0.35	55
ESF-THERMALK-017/26.3-26.5/UC	58	76	150	43	1.4	<0.10	58
ESF-THERMALK-017/26.5-26.9/UC	67	82	126	44	1.4	0.33	52
ESF-THERMALK-019/19.2-19.5/UC	84	80	104	47	0.67	<0.19	62
ESF-THERMALK-019/19.5-19.7/UC	82	82	124	50	0.6	0.3	59
SD-9/669.1-669.2/UC	76	75	136	29	1.2	<0.10	49
ECRB-DS2-1613/13.2-13.4/UC	37.3	22.9	97	35	2.84	<0.07	—
ECRB-DS2-1613/18.6-18.9/UC	23.8	19.3	97	31	2.49	<0.04	—
ECRB-DS3-1616/7.1-7.5/UC	14	15.8	91	28	1.76	0.1	55
ECRB-DS3-1616/8.7-8.9/UC	38.3	23.9	146	38	3.89	<0.08	—
ECRB-DS3-1616/10.4-10.6/UC	6.42	8.68	119	14	1.19	<0.03	35
ECRB-DS3-1616/11.5-12.5/UC	23.3	16.6	152	19	2.83	<0.04	69
ECRB-SYS-CS400/3.8-4.3/UC	29	94	—	0.3	3.7	<1	48
ECRB-SYS-CS400/5.6-6.2/UC	21	64	415	8.5	1.7	<1	55
ECRB-SYS-CS450/5.3-6.0/UC	66	147	388	4.8	1.1	0.4	54
ECRB-SYS-CS500/12.0-16.7/UC	54	78	286	6.1	4.8	0.4	49
ECRB-SYS-CS600/3.6-4.0/UC	22	50	346	3.3	2	<1	44
ECRB-SYS-CS700/5.5-5.8/UC	64	146	—	2.8	6.2	<0.1	56
ECRB-SYS-CS750/6.2-6.5/UC	73	78	191	<0.2	1.2	<1	40
ECRB-SYS-CS800/4.9-5.6/UC	20	32	357	0	1.6	—	53
ECRB-SYS-CS850 5.1-5.6/UC	32	30	280	1.6	2.9	<0.2	46
ECRB-SYS-CS900/2.8-3.0/UC	25	63	349	1.2	0.52	0.6	45
ECRB-SYS-CS900/3.0-3.2/UC	66	112	—	5.9	0.73	1.2	43
ECRB-SYS-CS900/3.5-4.1/UC	53	88	775	1.9	2	0.3	65
ECRB-SYS-CS900/5.4-5.9/UC	37	56	216	1.3	1.7	<0.2	54
ECRB-SYS-CS950/4.8-5.5/UC	30	67	286	11	4.9	<0.2	58
ECRB-SYS-CS950/5.2-5.3/UC	19	37	239	0.3	1.9	<0.2	58
SD-9/670.5-670.6/UC	46	56	—	28	2.8	0.3	53

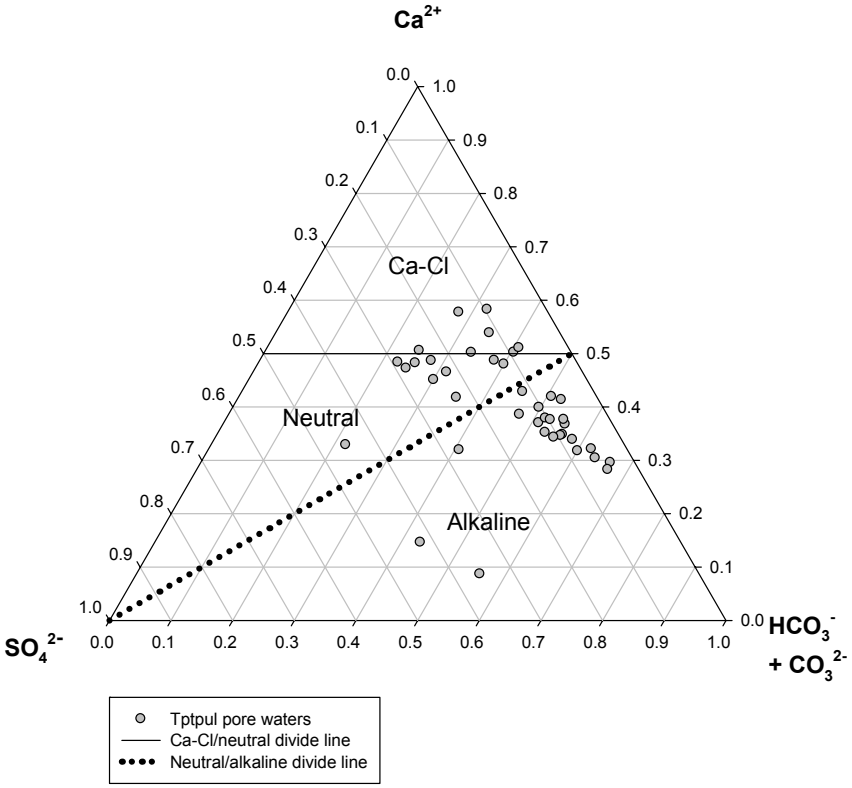
Storage Condition (Column 3) Footnotes:
1-Cleaned split sleeves, shoe, and inner barrel with Liquinox and DI water. Cores handled with sterile gloves.
2 - Core bits, barrels and sleeves cleaned with Liquinox and DI water. Cores handled with sterile gloves.

General Footnote:
a - Representative water used in P&CE model to represent the four water groups (1, 2, 3, and 4).

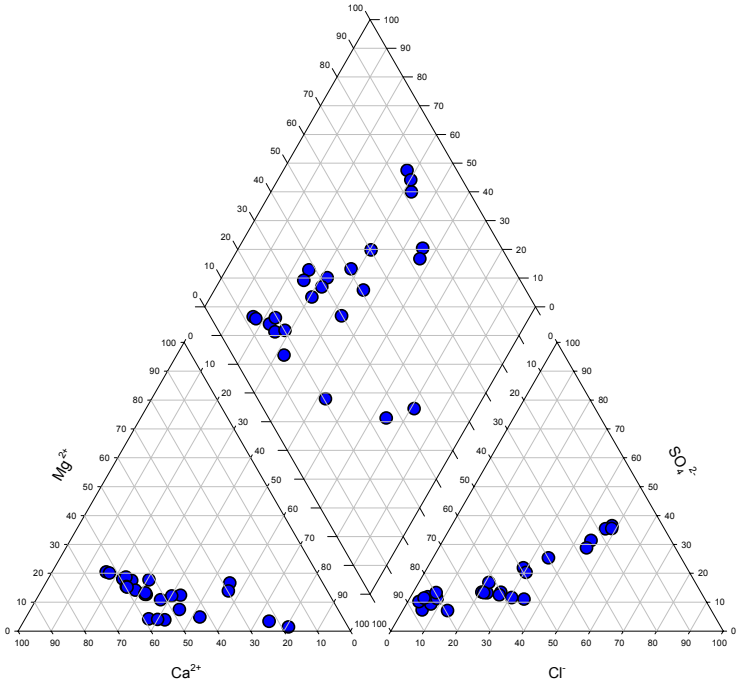
The following are Piper and chemical divide plots of the pore waters from the four TSw lithologies:

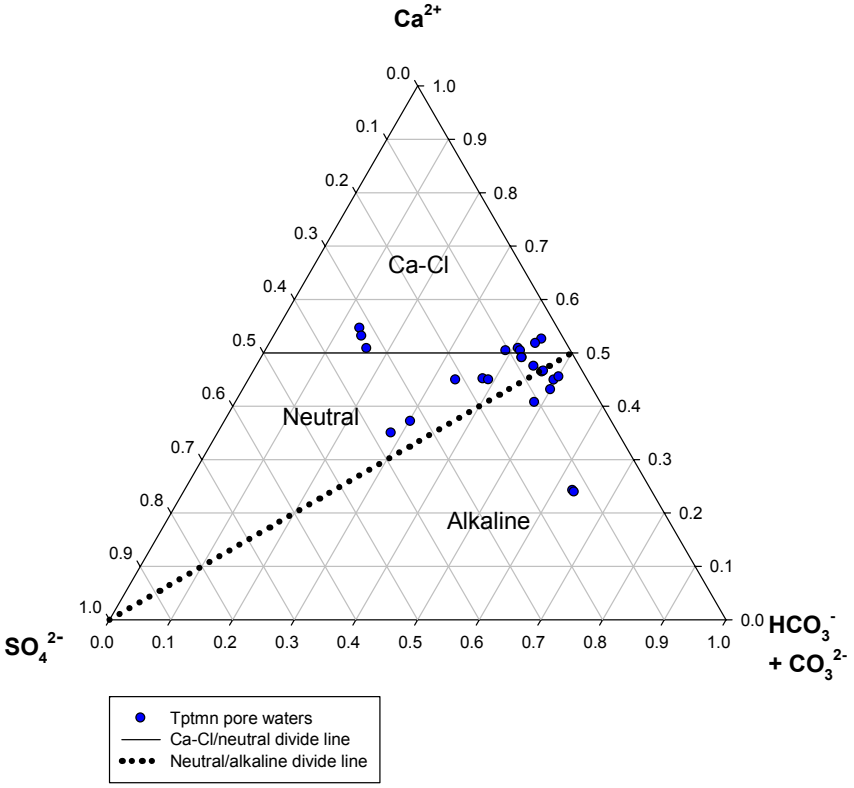
Tptpul Pore Waters



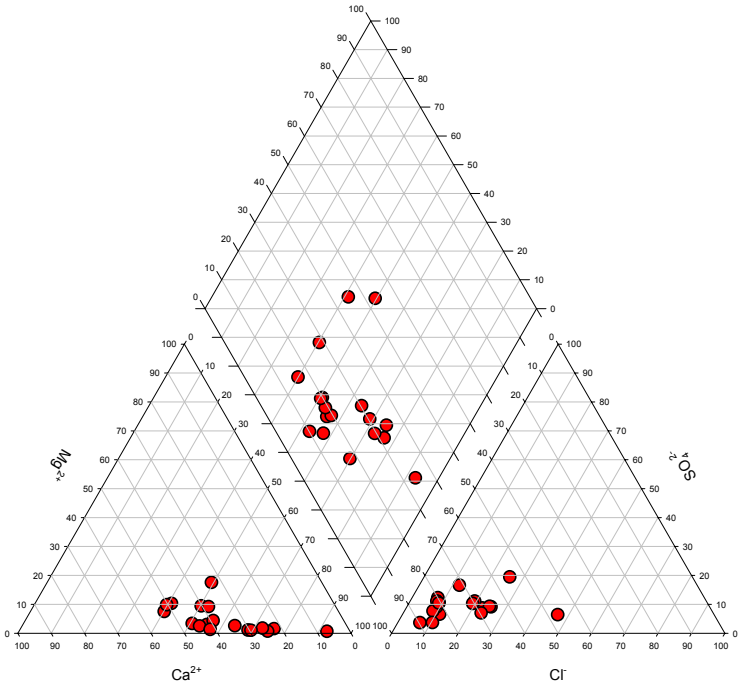


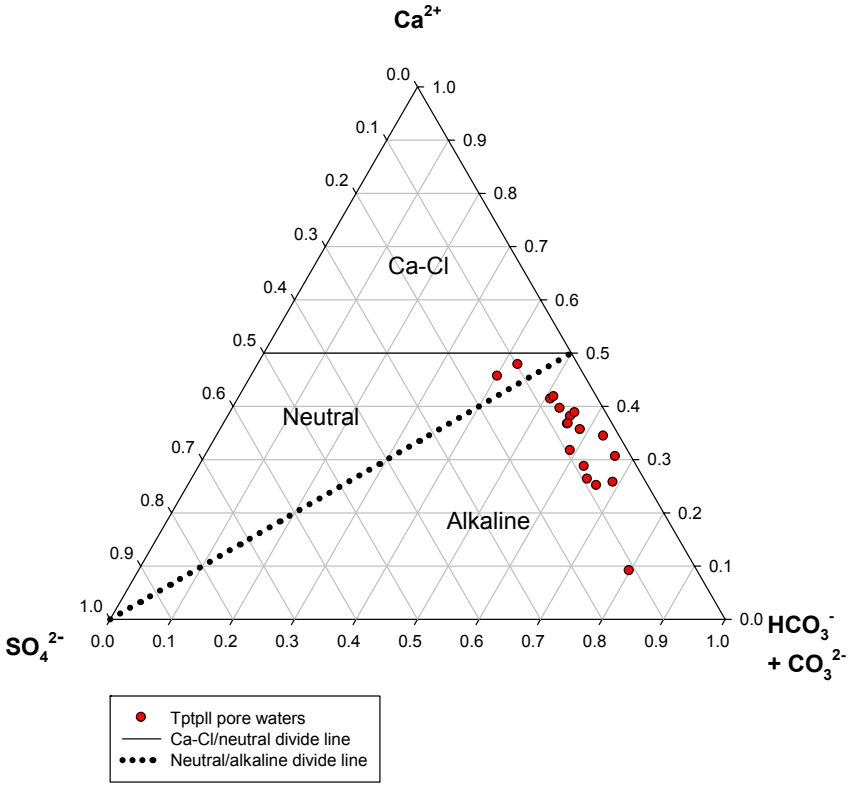
Tptpmn Pore Waters



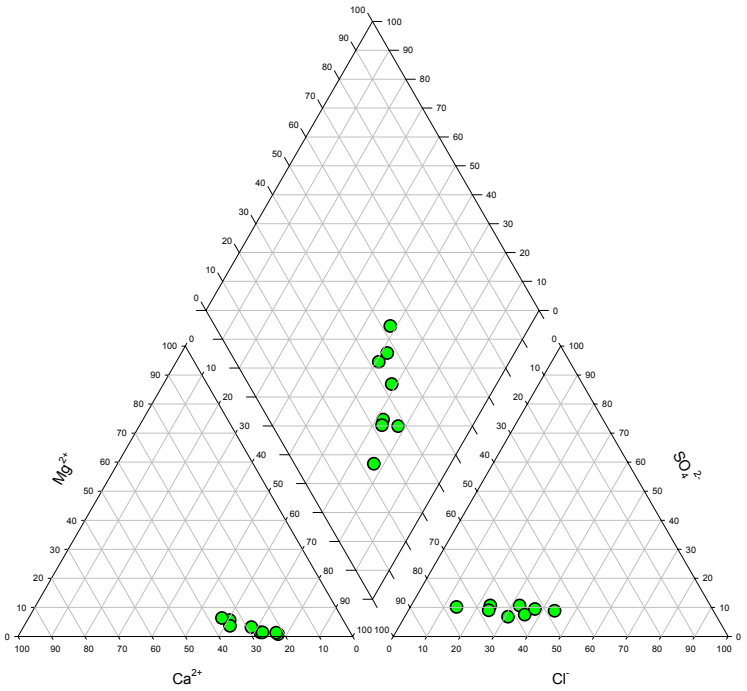


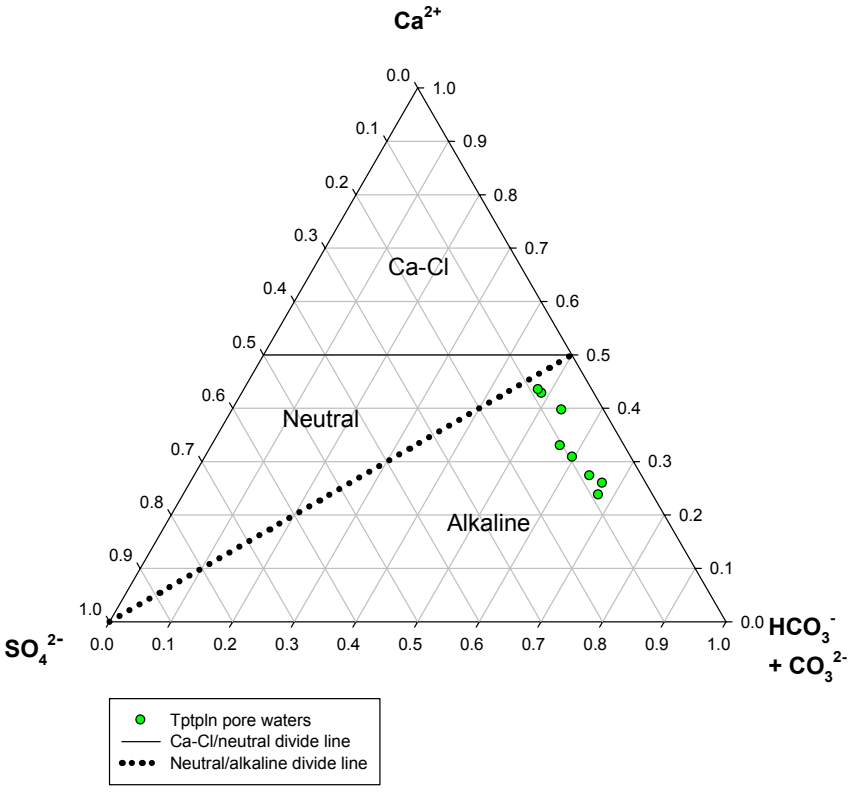
Tptpll Pore Waters





Tptpln Pore Waters





Below is a chemical divide plot of the 90 TSw pore waters. Also plotted are the four representative pore waters used in the DOE near-field chemistry model. Note that the Group 3 representative pore water plots differently in this figure compared to the one on pages 125 and 137 because the composition plotted here was derived from a GWB React calculation, in which quartz and calcite saturation were specified and the log fCO2 was set to -3.0. The figure on pages 125 and 128 used the original data, which did not have HCO3– concentration (and set to zero in the figure).

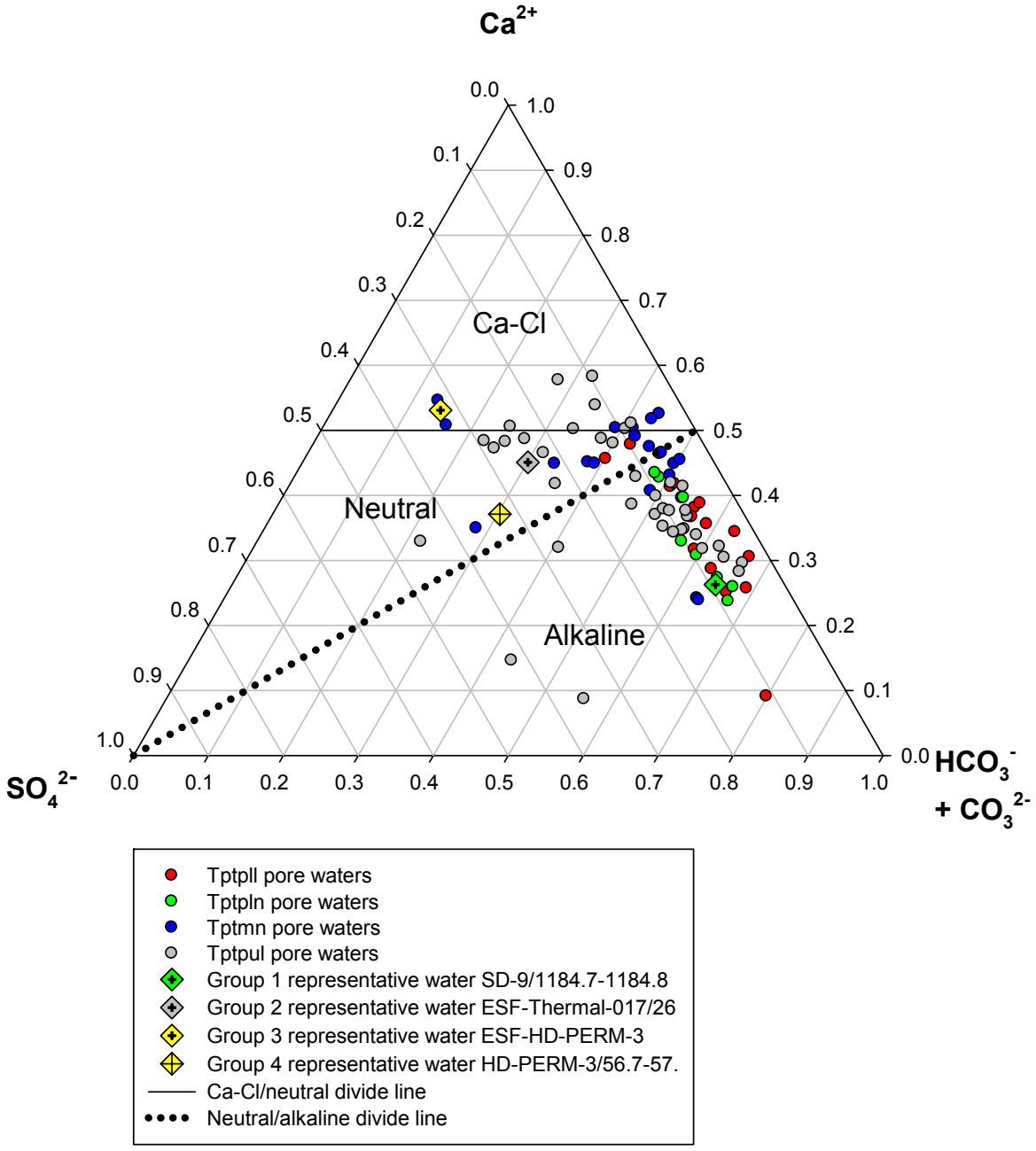


Table 2.3.2-2. Major Hydrogeologic Units, GFM2000 Lithostratigraphy, and Unsaturated Zone Model Layer Correlation

Major Hydrogeologic Units[a,b]	Lithostratigraphic Nomenclature	Hydrogeologic Unit	Unsaturated Zone Flow Model Layer
Tiva Canyon welded (TCw)	Tpcr	CCR, CUC	tcw11
	Tpcp	CUL, CW	tcw12
	TpcLD		
	Tpcpv3	CMW	tcw13
	Tpcpv2		
Paintbrush nonwelded (PTn)	Tpcpv1	CNW	ptn21
	Tpbt4	BT4	ptn22
	Tpy (Yucca)		
		TPY	ptn23
		BT3	ptn24
	Tpbt3		
	Tpp (Pah)	TPP	ptn25
	Tpbt2	BT2	ptn26
	Tptrv3		
	Tptrv2		
Topopah Spring welded (TSw)	Tptrv1	TC	tsw31
	Tptrn		
		TR	tsw32
	Tptrl, Tptf	TUL	tsw33
	Tptpul, RHHtop		
	Tptpmn	TMN	tsw34
	Tptpll	TLL	tsw35
	Tptpln	TM2 (upper 2/3 of Tptpln)	tsw36
		TM1 (lower 1/3 of Tptpln)	tsw37
	Tptpv3	PV3	tsw38

Table 2.3.2-2. Major Hydrogeologic Units, GFM2000 Lithostratigraphy, and Unsaturated Zone Model Layer Correlation (Continued)

Major Hydrogeologic Units[a,b]	Lithostratigraphic Nomenclature	Hydrogeologic Unit	Unsaturated Zone Flow Model Layer
Calico Hills nonwelded (CHn)	Tptpv2	PV2	tsw39 (vitric, zeolitic)
	Tptpv1	BT1 or BT1*a* (altered)	ch1 (vitric, zeolitic)
	Tpbt1		
	Tac (Calico)	CHV (vitric) or CHZ (zeolitic)	ch2 (vitric, zeolitic)
			ch3 (vitric, zeolitic)
			ch4 (vitric, zeolitic)
			ch5 (vitric, zeolitic)
	Tacbt (Calicobt)	BT	ch6 (vitric, zeolitic)
	Tcpuv (Prowuv)	PP4 (zeolitic)	pp4
	Tcpuc (Prowuc)	PP3 (devitrified)	pp3
	Tcpmd (Prowmd)	PP2 (devitrified)	pp2
	Tcplc (Prowlc)		
	Tcplv (Prowlv)	PP1 (zeolitic)	pp1
	Tcpbt (Prowbt)		
	Tcbuv (Bullfroguv)		
Crater Flat undifferentiated (CFu)	Tcbuc (Bullfroguc)	BF3 (welded)	bf3
	Tcbmd (Bullfrogmd)		
	Tcblc (Bullfroglc)		
	Tcblv (Bullfroglv)	BF2 (nonwelded)	bf2
	Tcbbt (Bullfrogbt)		
	Tctuv (Tramuv)		
	Tctuc (Tramuc)	Not Available	tr3
	Tctmd (Trammd)		
	Tctlc (Tramlc)		
	Tctlv (Tramlv)	Not Available	tr2
	Tctbt (Trambt) and below		

NOTE: [a]Montazer and Wilson 1984, Table 1.
[b]At some locations, alluvial and colluvial materials overlie the TCw unit. At other locations, the Rainier Mesa Tuff overlies the TCw unit. These units are not represented in the unsaturated zone flow model.

Source: BSC 2004h, Table 6-5.

May 4, 2009

Below is text taken from the DOE response to RAI: 3.2.2.1.3.3-002 (page 8 of 26):

1.3. AMBIENT WATER COMPOSITIONS PREDICTED BY THE NEAR-FIELD CHEMISTRY MODEL

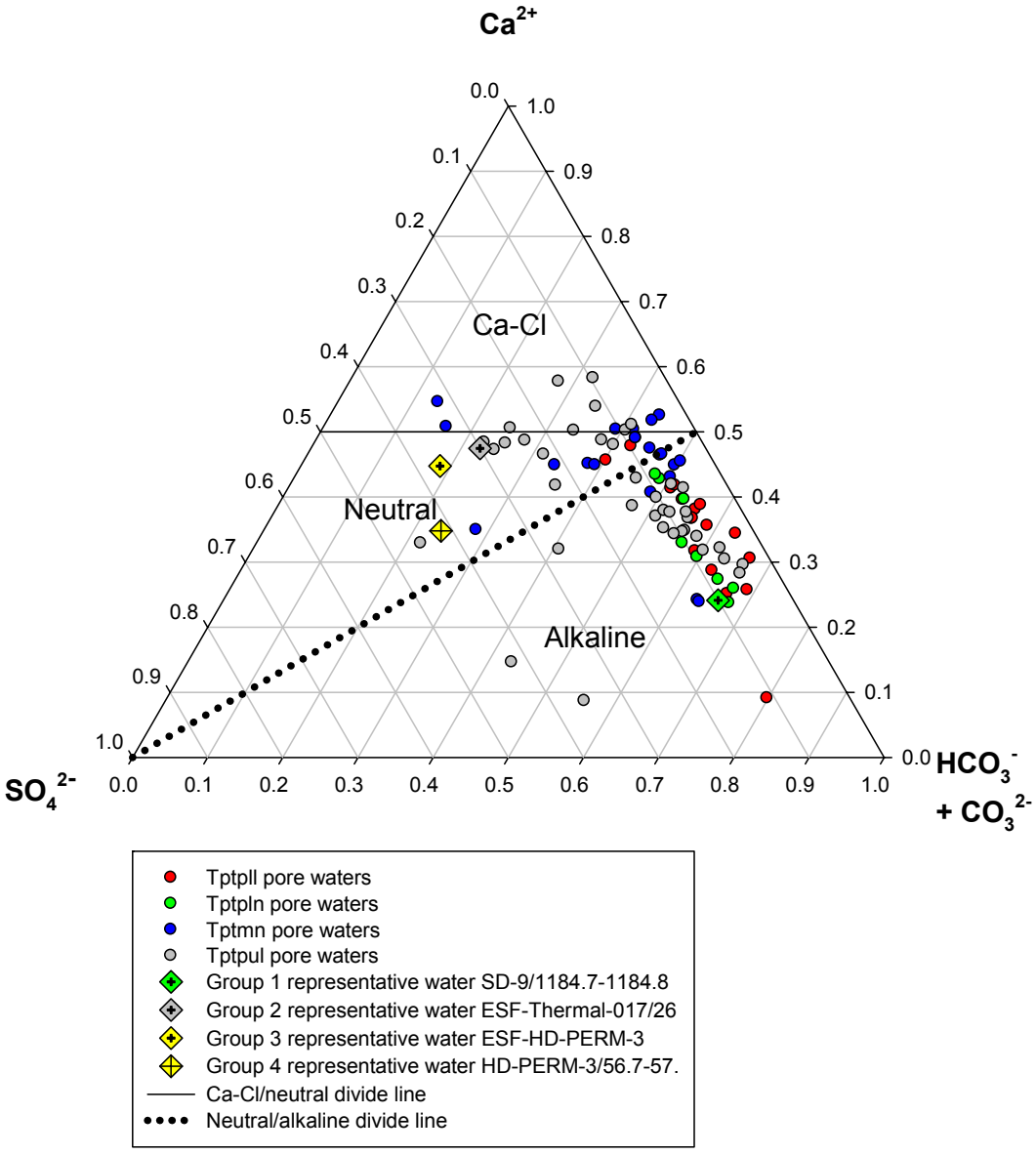
Prior to use in the EQ3/6 simulations which generate the pickup files, the initial pore-water compositions are pre-equilibrated to estimate missing components (e.g., aluminum, and pH, HCO_3^-, or SiO_2(aq)) (SNL 2007a, Section 6.3.2.3). The measured water compositions and the initial pre-equilibrated compositions used in the model are given in Table 1. The pore waters are equilibrated with a pCO_2 of 10^{-3} bars, the assumed value for in situ ambient CO_2 concentrations in the TSw (SNL 2007a, Section 7.1.2.2). This generates a bicarbonate concentration for water ESF-HD-PERM-3/34.8-35.1 and a pH value for ESF-HD-PERM-3/56.7-57.1/UC. It also results in shifts in Ca^{2+} and HCO_3^- concentrations and pH for most of the waters, which appear to have equilibrated at a slightly higher pCO_2 (Ca^{2+} and HCO_3^- both decrease upon equilibration), probably due to minor amounts of microbial activity during core storage. A SiO_2(aq) concentration is calculated for pore water ESF-HD-PERM-3/56.7-57.1/UC by equilibrating with SiO_2(am). Aluminum concentrations are estimated for all samples by first assuming equilibrium with alkali feldspar, resulting in supersaturation with several secondary aluminosilicates, and then in a second simulation, allowing the Al-solubility-limiting phase to precipitate. Stellerite is the solubility-limiting phase for Al for all four waters. The amount of stellerite that precipitates is too small to significantly affect solution concentrations for any other aqueous species.

Table 1. Measured and Pre-equilibrated Compositions for the Representative Group Waters

Pore Water ID	SD-9/1184.7-1184.8/UC		ESF-THERMALK-017/26.5-26.9/UC		ESF-HD-PERM-3/34.8-35.1		ESF-HD-PERM-3/56.7-57.1/UC*	
Group #	1		2		3		4	
	Meas.	Equil.	Meas.	Equil.	Meas.	Equil.	Meas.	Equil.
pH	8.2	8.10	7.7	7.85	8.31	7.83	—	7.91
Na (mg/L)	59	59	45	45	62	62	123	122
K (mg/L)	4.8	4.8	14.4	14.4	9	9	13.8	13.7
Mg (mg/L)	0.7	0.7	7.9	7.9	17.4	17.4	16.7	16.6
Ca (mg/L)	19	16	62	54	97	61	59.9	44
Cl (mg/L)	23	23	67	67	123	123	146	146
SO_4 (mg/L)	16	16	82	82	120	120	126	126
HCO_3 (mg/L)	142	133	126	78	—	77	149	91
NO_3 (mg/L)	16	16	44	44	10	10	57.4	57.4
F (mg/L)	2.2	2.2	1.4	1.4	0.76	0.76	1.3	1.3
SiO_2 (mg/L)	42	42	52	52	75	75	—	111
Equil. pCO_2	−3.06	−3.0	−2.64	−3.0	—	−3.0	—	−3.0

* Na, K, and Mg concentrations differ slightly for measured and equilibrated values because of minor changes in the reported values between the preliminary measured values, used in the EQ3/6 equilibration calculations, and the final, qualified values.

The following Ca–SO4–CO3 ternary plot is similar to that on page 160 of this notebook, except the Group1, 2, 3, and 4 representative water compositions were taken from the above table.



Note that the four representative water compositions plot differently compared to the figure on page 160. For Groups 1, 2, and 4, the difference is due to the EQ3/6 equilibration DOE performed on the water chemistry, as described in the preceding paragraphs and the figure on this page used the equilibrated compositions. For Group 1, the composition plotted on page 160 was equilibrated using GWB React, but the difference with the DOE equilibration is that equilibrium with feldspar was not constrained in the React calculation, in contrast to the DOE EQ3/6 calculation.

The BOTTOM LINE is that the Group 1 representative pore water chemistry used by DOE plots in the neutral water-type field, instead of the Ca-Cl field. The latter could result in potentially

corrosive brines, upon evaporation, whereas the latter (neutral water) tends to form brines benign to Alloy 22.

Note also that the location of the Groups 1 to 4 compositions plotted on page 160 and 164 of this notebook are different from the locations plotted on page 83 of notebook #930E because in the latter, the water compositions were equilibrated using on log fCO2 of -3.0 as the constraint (calcite and quartz were not used as constraint).

Also, note that DOE used amorphous silica to constrain SiO2(aq) concentration, as opposed to quartz which was done here.

From the DOE response to RAI: 3.2.2.1.3.3-009:

1.3. AMBIENT WATER COMPOSITIONS PREDICTED BY THE NEAR-FIELD CHEMISTRY MODEL

Prior to use in the EQ3/6 simulations which generate the pickup files, the initial pore-water compositions are pre-equilibrated to estimate missing components (e.g., aluminum, and pH, HCO_3^-, or SiO_2(aq)) (SNL 2007a, Section 6.3.2.3). The measured water compositions and the initial pre-equilibrated compositions used in the model are given in Table 1. The pore waters are equilibrated with a pCO_2 of 10^{-3} bars, the assumed value for *in situ* ambient CO_2 concentrations in the TSw (SNL 2007a, Section 7.1.2.2). This generates a bicarbonate concentration for the Group 3 representative water and a pH value for the Group 4 representative water (Table 1). It also results in shifts in Ca^{2+} and HCO_3^- concentrations and pH for most of the waters, which equilibrated at a slightly higher pCO_2 (Ca^{2+} and HCO_3^- both decrease upon equilibration), probably due to minor amounts of microbial activity during core storage. An SiO_2(aq) concentration is calculated for the Group 4 representative water by equilibrating with SiO_2(am). Aluminum concentrations are estimated for all samples by first assuming equilibrium with alkali feldspar, resulting in supersaturation with several secondary aluminosilicates, and then, in a second simulation, allowing the Al-solubility-limiting phase to precipitate. Stellerite is the solubility-limiting phase for Al for all four waters. The amount of stellerite that precipitates is too small to significantly affect solution concentrations for any other aqueous species.

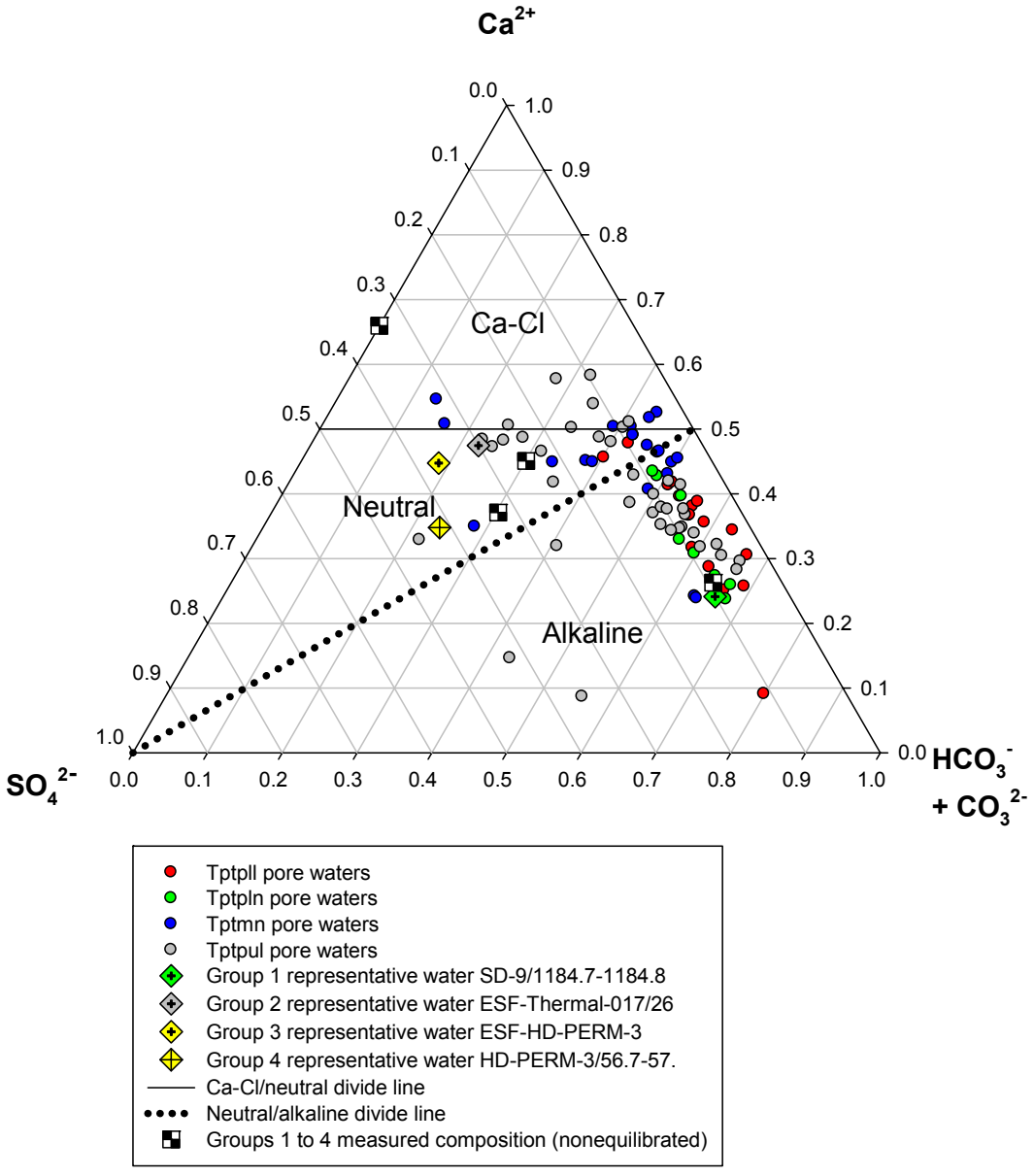
Table 1. Measured and Pre-equilibrated Compositions for the Representative Group Waters

Pore Water ID	SD-9/1184.7-1184.8/UC		ESF-THERMALK-017/26.5-26.9/UC		ESF-HD-PERM-3/34.8-35.1		ESF-HD-PERM-3/56.7-57.1/UC*	
Group #	1		2		3		4	
	Meas.	Equil.	Meas.	Equil.	Meas.	Equil.	Meas.	Equil.
pH	8.2	8.10	7.7	7.85	8.31	7.83	—	7.91
Na (mg/L)	59	59	45	45	62	62	123	122
K (mg/L)	4.8	4.8	14.4	14.4	9	9	13.8	13.7
Mg (mg/L)	0.7	0.7	7.9	7.9	17.4	17.4	16.7	16.6
Ca (mg/L)	19	16	62	54	97	61	59.9	44
Cl (mg/L)	23	23	67	67	123	123	146	146
SO_4 (mg/L)	16	16	82	82	120	120	126	126
HCO_3 (mg/L)	142	133	126	78	—	77	149	91
NO_3 (mg/L)	16	16	44	44	10	10	57.4	57.4
F (mg/L)	2.2	2.2	1.4	1.4	0.76	0.76	1.3	1.3
SiO_2 (mg/L)	42	42	52	52	75	75	—	111
Equil. pCO_2	−3.06	−3.0	−2.64	−3.0	—	−3.0	—	−3.0

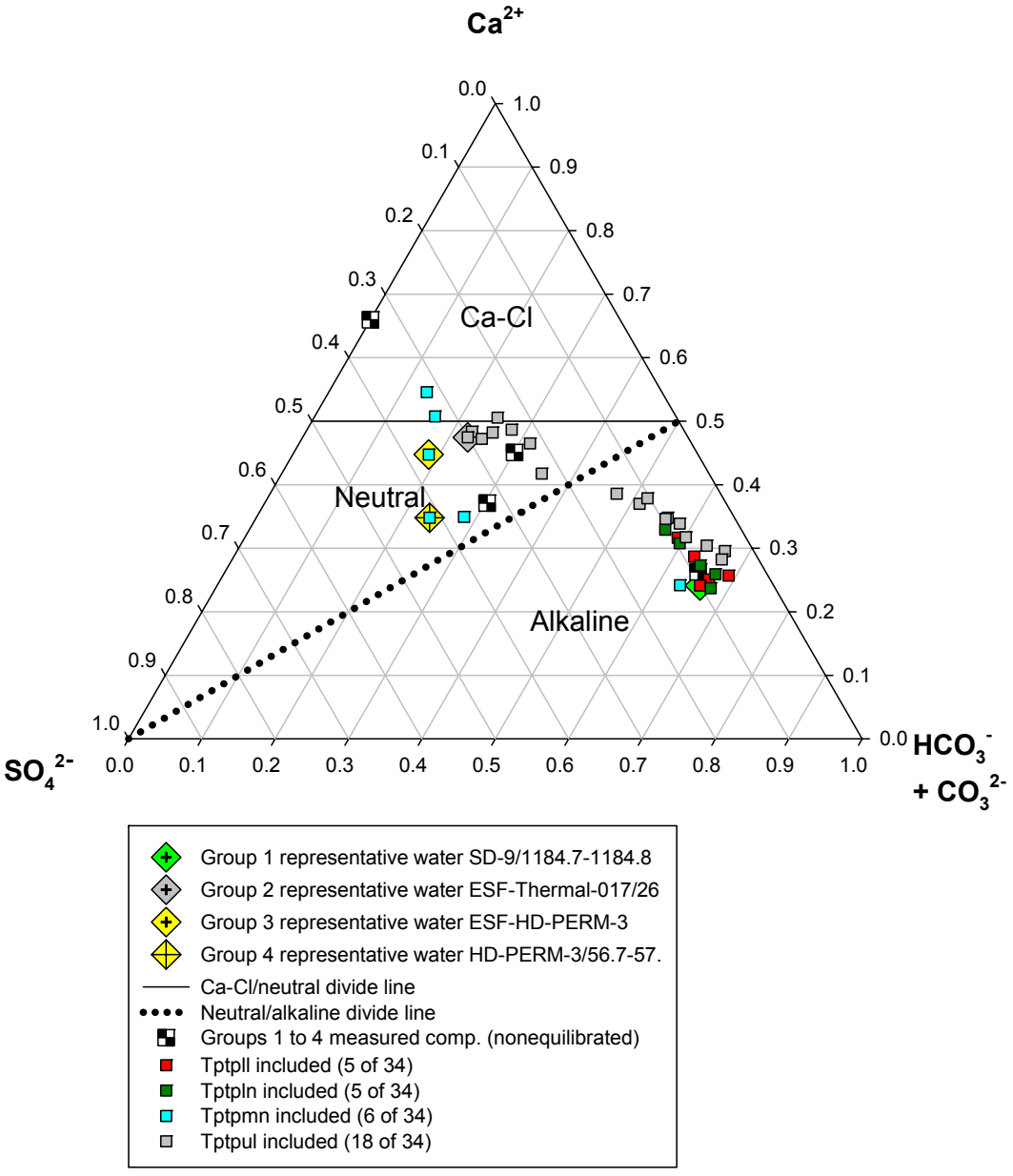
* Na, K, and Mg concentrations differ slightly for measured and equilibrated values because of minor changes in the reported values between the preliminary data used in the EQ3/6 equilibration calculations, and the final, qualified measured values.

In the next step, when the EQ3/6 simulations used to create the pickup files used by the seepage evaporation abstraction are run, calcite and amorphous silica are titrated into each water in excess, in addition to fixed amounts of alkali feldspar. For conditions representing ambient (e.g., at 23°C with no feldspar added), this titration step has no effect on the Ca^{2+} and HCO_3^- concentrations, as the four waters are all saturated with respect to calcite after the equilibration step at a pCO_2 of 10^{-3} bars, but this titration step increases the SiO_2(aq) concentrations to about 110 mg/L in all four waters. Justification for using amorphous silica as the solubility-limiting phase for SiO_2(aq) is provided in *Engineered Barrier System: Physical and Chemical Environment* (SNL 2007a, Section 6.3.2.4.1).

A comparison of pore water compositions (measured and equilibrated) is shown in the following figure. Group 3 water has moved from the Ca-Cl water type to the Neutral water type.



The following shows the 34 pore water compositions included in the DOE near-field chemistry model.

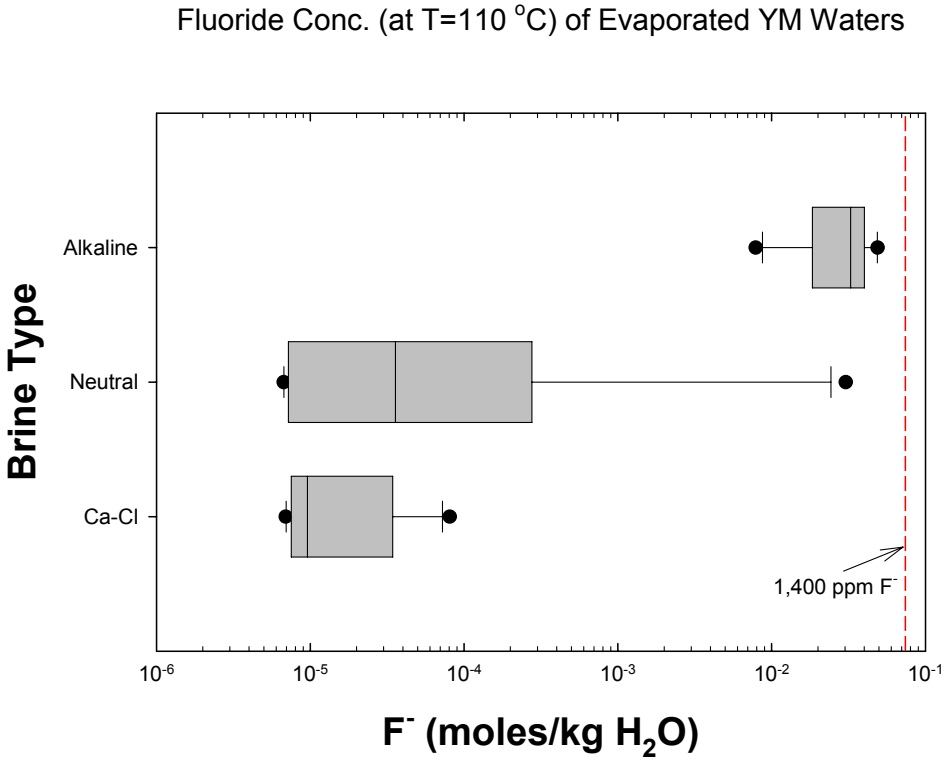


May 5, 2009

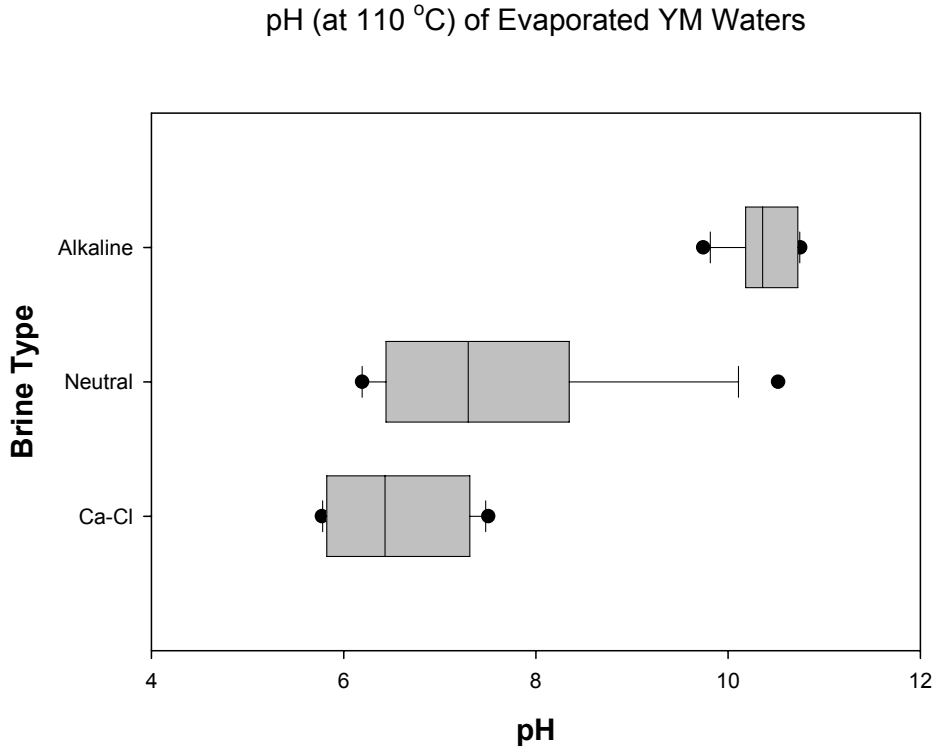
Drip Shield Corrosion

In the draft SER writeup on general corrosion of titanium drip shield, staff described DOE corrosion rate measurements at 90 °C in simulated concentrated water (SCW), which contains 1,400 ppm fluoride ion. Staff indicated the under potential YM repository conditions, fluoride concentration and pH are the primary factors to affect the titanium general corrosion. The DOE test conditions covered pH range of 3 to 10 and fluoride concentration of 0 to 1,400 ppm. Staff concluded that "providing that the fluoride concentration in SCW bounds the possible fluoride concentration in evaporated seepage water and the lowest pH of evaporated seepage water, based on independent, literature, and analog studies, the staff finds that the experimental approach DOE used to obtain the general corrosion rate data of titanium Grade 7 is appropriate."

In notebook #679E, page 154, evaporation simulations of YM unsaturated zone porewaters were described and documented. The evaporation calculations were done for a temperature of 110 °C and a total pressure of 0.85 atm. For pore water samples without a reported fluoride concentration, a value of 2.18 mg/L was used based on the mean value reported for J-13 well water samples. The range in fluoride concentrations of the brines that form upon evaporation is illustrated in the following figure (taken from page 163 of notebook #679E):



The range in pH of the brines that form upon evaporation is illustrated in the following figure (taken from page 158 of notebook #679E):



The mean, standard deviation, and median of fluoride concentrations of the 90 pore waters considered by DOE in its screening for the near-field chemistry model are 2.25, 1.72, and 1.68, respectively. The average value of 2.25 is close to the 2.18 value used in the evaporation simulation of Yucca Mountain pore waters.

Localized Corrosion of the Waste Package

In Section 2.2.1.3.1.3.2.1 of the draft SER, it states:

> The applicant's overall localized corrosion model for the waste package outer barrier is divided into an initiation model and a propagation model… The localized corrosion initiation model is based on experimental testing of Alloy 22 under various environments included mixed ionic solutions, chloride solutions, and mixed chloride and nitrate solutions. These corrosion test solutions bound the range of water chemistries expected for the repository based on NRC staff review of repository chemical environment provided in SER Chapter 2.2.1.3.3.

According to Yiming Pan:

From: Yiming Pan [ypan@cnwra.swri.edu]
Sent: Tuesday, May 05, 2009 1:02 PM
To: 'Roberto Pabalan'
Cc: James Myers; 'Hipolito Gonzalez'
Subject: Review of corrosion test solutions

Bobby,

The compositions of the corrosion test solutions DOE used are provided in SAR Table 2.3.6-1. We do need your support for the review. Please feel free to call me if you have any questions.

Yiming

Table 2.3.6-1 from the DOE SAR is copied below:

Table 2.3.6-1. Target Composition of Standard Test Solutions Based on J-13 Well Water

Ion	SDW (mg/L)	SCW (mg/L)	SAW (mg/L)	SSW (mg/L)	BSW-12 (mg/L)
K^+	3.4×10^1	3.4×10^3	3.4×10^3	1.42×10^5	6.762×10^4
Na^+	4.09×10^2	4.09×10^4	3.769×10^4	4.87×10^5	1.0586×10^5
Mg^{2+}	1	<1	1.00×10^3	0	0
Ca^{2+}	5×10^{-1}	<1	1.00×10^3	0	0
F^-	1.4×10^1	1.4×10^3	0	0	1.331×10^3
Cl^-	6.7×10^1	6.7×10^3	2.425×10^4	1.28×10^5	1.313×10^5
NO_3^-	6.4×10^1	6.4×10^3	2.30×10^4	1.313×10^6	1.395×10^5
SO_4^{2-}	1.67×10^2	1.67×10^4	3.86×10^4	0	1.392×10^4
HCO_3^-	9.47×10^2	7×10^4	0	0	0
Si	27 (60°C); 49 (90°C)	27 (60°C); 49 (90°C)	27 (60°C); 49 (90°C)	0	0
pH	9.8 to 10.2	9.8 to 10.2	2.7	5.5 to 7	12

NOTE: pH measured for actual solutions at room temperature. BSW-12 denotes the specific pH of the water. For certain experiments, the pH of basic saturated water is altered by addition of NaOH.
BSW = basic saturated water.

Source: DTN: LL040803112251.117.

The values were reproduced in the form of a Word table:

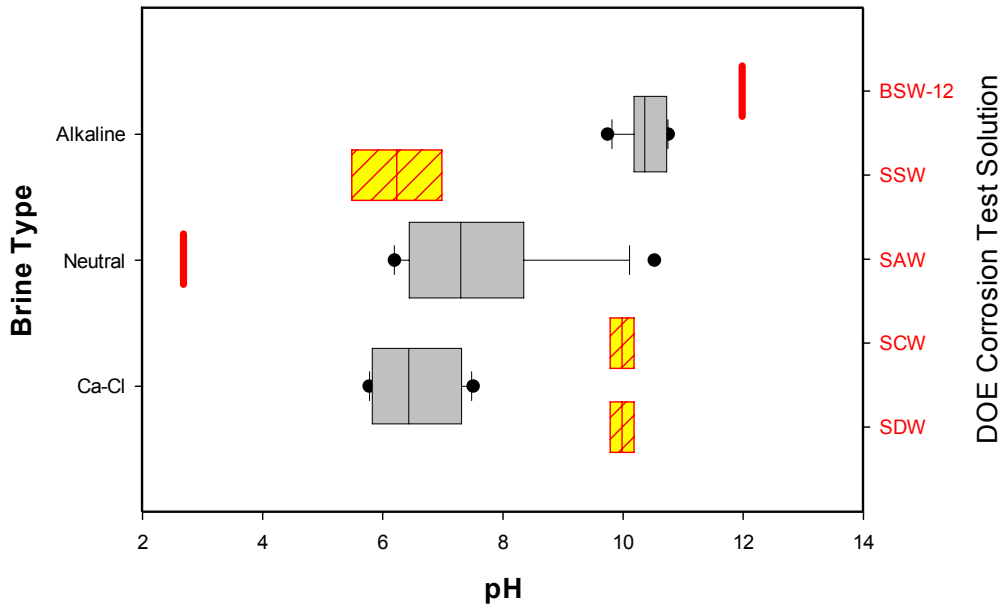
Table 2.3.6-1. Target Composition of Standard Test Solutions Based on J-13 Well Water					
Ion	SDW (mg/L)	SCW (mg/L)	SAW (mg/L)	SSW (mg/L)	BSW-12 (mg/L)
K+	3.40E+01	3.40E+03	3.40E+03	1.42E+05	6.762E+04
Na+	4.09E+02	4.09E+04	3.769E+04	4.87E+05	1.0586E+05
Mg2+	1	<1	1.00E+03	0	0
Ca2+	5.00E-01	<1	1.00E+03	0	0
F−	1.40E+01	1.40E+03	0	0	1.33E+03
Cl−	6.70E+01	6.70E+03	2.425E+04	1.28E+05	1.313E+05
NO3−	6.40E+01	6.40E+03	2.30E+04	1.313E+06	1.395E+05
SO42−	1.67E+02	1.67E+04	3.86E+04	0	1.392E+04
HCO3−	9.47E+02	7.00E+04	0	0	0
Si (60°C)	27	27	27	0	0
Si (90°C)	2.90E+01	2.90E+01	49		
pH	9.8 to 10.2	9.8 to 10.2	2.7	5.5 to 7	12

The compositions were recalculated into units of molality (moles/kgH2O) and are shown below:

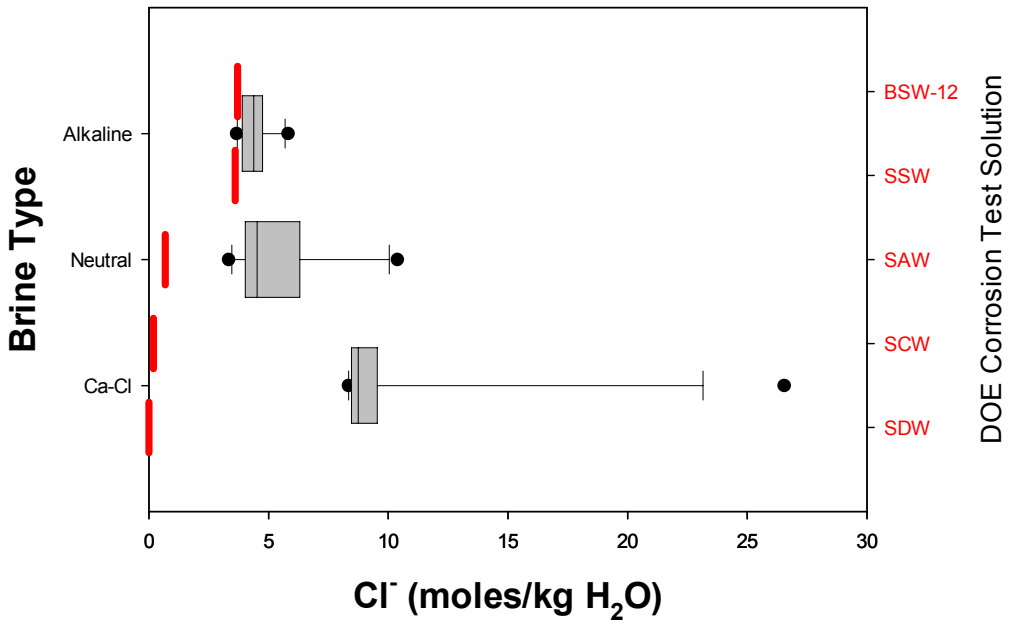
Target Composition (moles/kg H2O) of Standard Test Solutions Based on J-13 Well Water					
Ion	SDW (molal)	SCW (molal)	SAW (molal)	SSW (molal)	BSW-12 (molal)
K+	8.70E-04	8.70E-02	8.70E-02	3.63E+00	1.73E+00
Na+	1.78E-02	1.78E+00	1.64E+00	2.12E+01	4.60E+00
Mg2+	4.11E-05	0.00E+00	4.11E-02	0.00E+00	0.00E+00
Ca2+	1.25E-05	0.00E+00	2.50E-02	0.00E+00	0.00E+00
F−	7.37E-04	7.37E-02	0.00E+00	0.00E+00	7.01E-02
Cl−	1.89E-03	1.89E-01	6.84E-01	3.61E+00	3.70E+00
NO3−	1.03E-03	1.03E-01	3.71E-01	2.12E+01	2.25E+00
SO42−	1.74E-03	1.74E-01	4.02E-01	0.00E+00	1.45E-01
HCO3−	1.55E-02	1.15E+00	0.00E+00	0.00E+00	0.00E+00
SiO2(aq) (60°C)	9.61E-04	9.61E-04	9.61E-04	0.00E+00	0.00E+00
SiO2(aq) (90°C)	1.03E-03	1.03E-03	1.74E-03	0.00E+00	0.00E+00

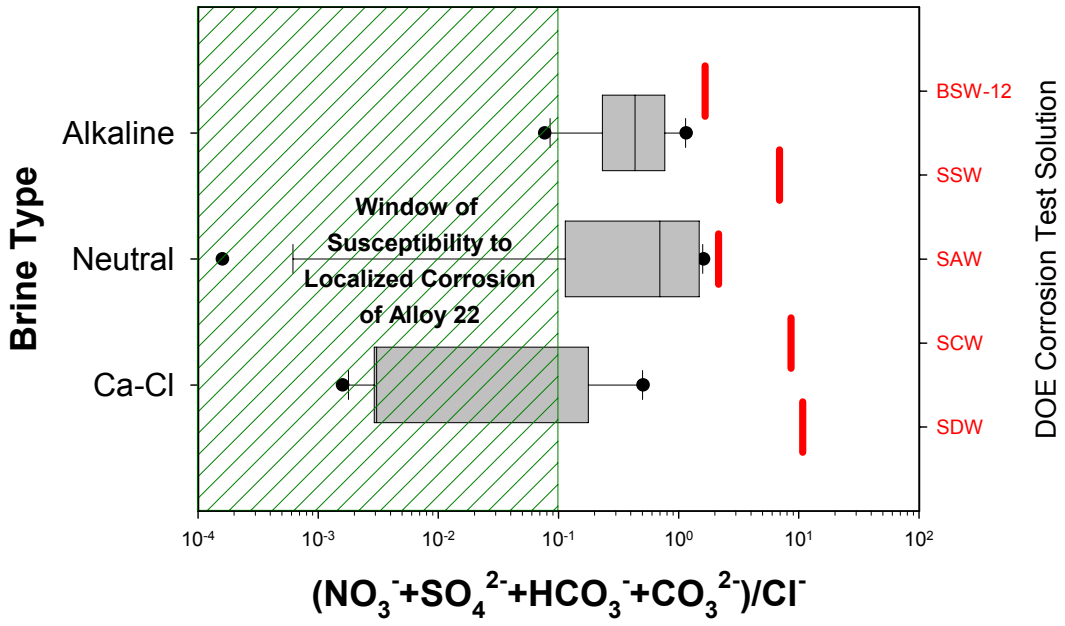
Of particular interest for localized corrosion are the pH, chloride concentration, the ratio of oxyanions (nitrate+sulfate+carbonates) to chloride, and the ratio of nitrate to chloride. A comparison of test solution chemistry versus evaporated seepage water chemistry is shown in the following three figures.

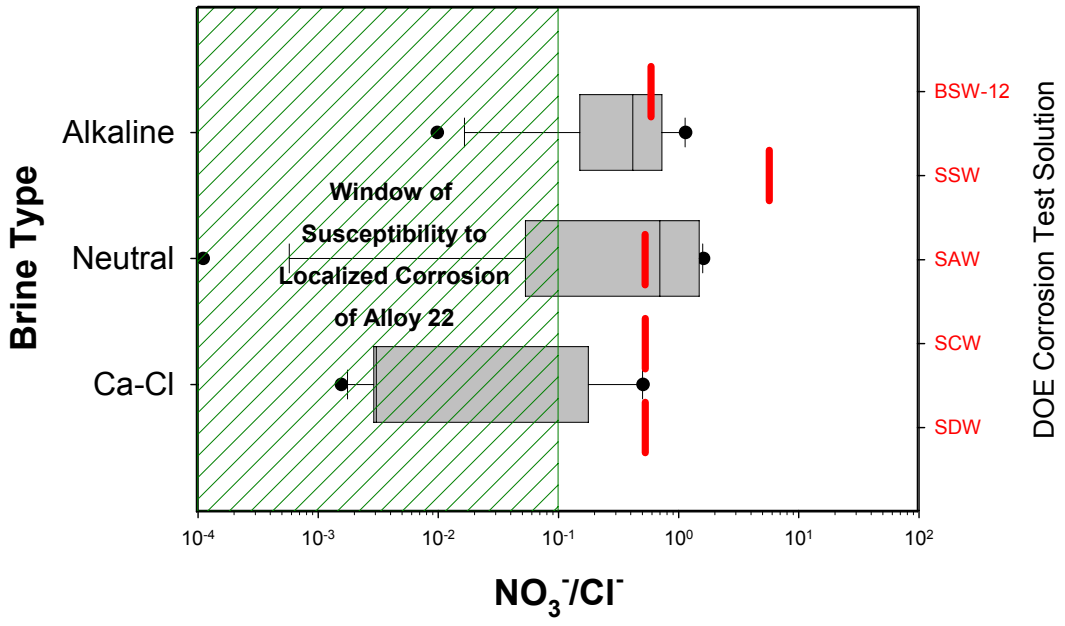
pH (at 110 °C) of Evaporated YM Waters



Chloride Conc. (at T=110 °C) of Evaporated YM Waters




Brine Type
Alkaline
Neutral
Ca-Cl
Window of
Susceptibility to
Localized Corrosion
of Alloy 22
BSW-12
SSW
SAW
SCW
SDW
DOE Corrosion Test Solution
10-4
10-3
10-2
10-1
100
101
102
(NO3-+SO4 2-+HCO3-+CO3 2-)/Cl-


Brine Type
Alkaline
Neutral
Ca-Cl
Window of
Susceptibility to
Localized Corrosion
of Alloy 22
BSW-12
SSW
SAW
SCW
SDW
DOE Corrosion Test Solution
10-4
10-3
10-2
10-1
100
101
102
NO3-/Cl-

May 7, 2009

Thermodynamic simulations were done to assess the chemistry brines that form from evaporation of the DOE Groups 1 to 4 pore waters. The calculations were done using OLIAnalyzer 3.0.5 (Aqueous H+ ion model). The compositions given in Table 1 of the DOE RAI response (RAI 3.2.2.1.3.3-009) was input as water analysis, then charge balance was done using dominant ion as option. The resulting stream was evaporated at 110 °C and 0.85 atm.

The pH and dominant aqueous species for Group 1 brine are tabulated below:

Group 1 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 10.70.			
Na+1	9.224E+00	CaCO3	8.955E-07
Cl-1	5.604E+00	CaHSiO3+1	5.420E-07
NaHSiO3	4.828E+00	CaSiO2(OH)2	4.915E-07
NO3-1	3.750E+00	Ca(NO3)+1	3.894E-07
K+1	2.050E+00	MgSiO2(OH)2	3.722E-07
NaNO3	6.792E-01	CaOH+1	6.192E-08
CO3-2	5.507E-01	CO2	5.953E-08
H3SiO4-1	5.454E-01	MgHSiO3+1	5.221E-08
NaCO3-1	1.951E-01	Ca+2	4.746E-08
Na2F+1	1.078E-01	CaCl+1	3.573E-08
H2SiO4-2	6.136E-02	MgOH+1	2.605E-08
KCl	3.949E-02	CaF+1	2.447E-08
F-1	3.886E-02	MgCO3	2.141E-08
NaF	3.488E-02	CaSO4	9.668E-10
KSO4-1	1.811E-02	CaHCO3+1	9.182E-10
HCO3-1	4.419E-03	MgF+1	3.251E-10
SiO2	2.082E-03	Mg+2	2.672E-10
OH-1	1.569E-03	MgHCO3+1	1.445E-10
NaHCO3	4.575E-04	HF	1.237E-10
SO4-2	1.710E-04		
NO3/Cl	**0.670**	(NO3+SO4+HCO3+CO3)/Cl	0.768

The pH and dominant aqueous species for Group 2 brine are tabulated below:

Group 2 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 7.54.			
Na+1	7.453E+00	NaF	2.893E-05
Cl-1	7.444E+00	MgOH+1	2.777E-05
NO3-1	5.874E+00	MgSO4	6.782E-06
K+1	4.117E+00	OH-1	2.733E-06
Ca(NO3)+1	1.452E+00	HCO3-1	1.518E-06
NaNO3	7.562E-01	CaHCO3+1	1.512E-06
Ca+2	1.194E-01	CaCO3	9.502E-07
KCl	7.589E-02	CaSiO2(OH)2	6.941E-07
CaCl+1	5.737E-02	MgF+1	6.383E-07

NaHSiO3	3.035E-03	SO4-2	4.336E-07
SiO2	2.500E-03	MgSiO2(OH)2	3.949E-07
KSO4-1	1.598E-03	NaHCO3	2.160E-07
CaHSiO3+1	1.147E-03	MgHCO3+1	1.994E-07
H3SiO4-1	4.433E-04	CO3-2	1.553E-07
CaSO4	2.026E-04	NaCO3-1	6.059E-08
Mg+2	1.130E-04	CO2	5.345E-08
CaOH+1	9.174E-05	H2SiO4-2	3.377E-08
MgHSiO3+1	8.304E-05	MgCO3	1.707E-08
Na2F+1	7.427E-05	H+1	1.362E-08
CaF+1	6.425E-05	CaCl2	3.005E-09
F-1	3.217E-05	HSO4-1	1.207E-09
NO3/Cl	**0.79**	(NO3+SO4+HCO3+CO3)/Cl	0.789

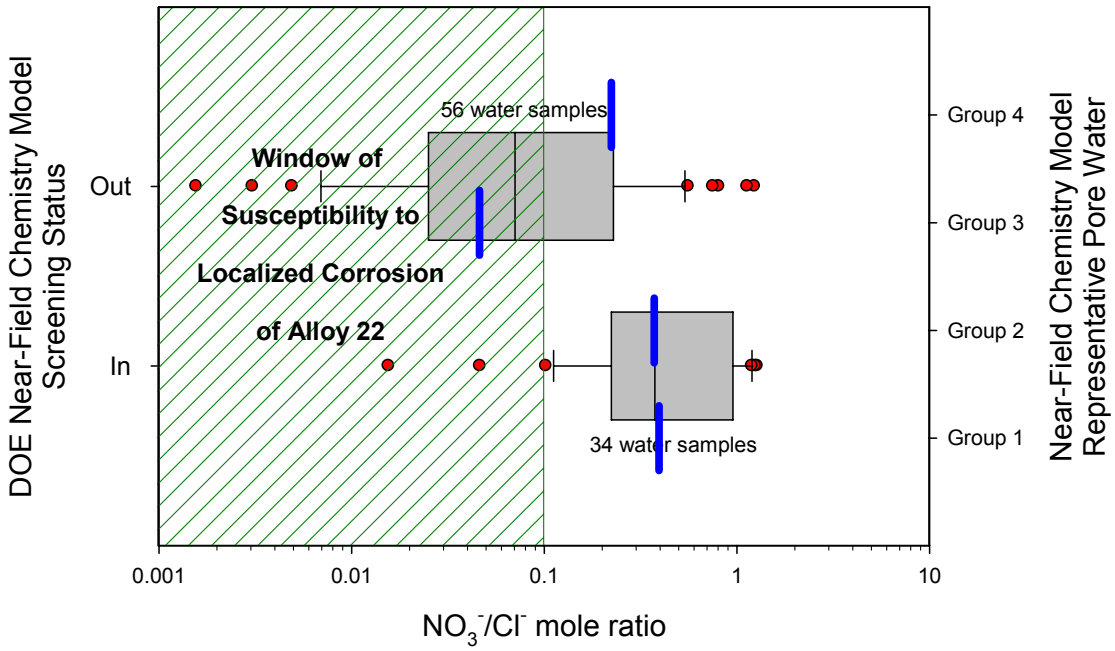
The pH and dominant aqueous species for Group 3 brine are tabulated below:

Group 3 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 5.69.			
Cl-1	1.129E+01	MgHCO3+1	1.210E-05
K+1	2.803E+00	NaHSiO3	9.670E-06
Ca(NO3)+1	**1.907E+00**	F-1	3.536E-06
Na+1	1.819E+00	H3SiO4-1	3.374E-06
Ca+2	1.487E+00	CaHCO3+1	1.130E-06
Mg+2	8.065E-01	Na2F+1	6.160E-07
CaCl+1	2.356E-01	H+1	6.020E-07
KCl	1.089E-01	NaF	3.577E-07
NO3-1	7.336E-02	CaCl2	2.972E-07
NaNO3	5.985E-02	OH-1	2.285E-07
MgHSiO3+1	5.844E-03	MgSiO2(OH)2	2.284E-07
MgOH+1	2.441E-03	CO2	5.184E-08
SiO2	1.870E-03	MgCO3	1.292E-08
MgSO4	7.550E-04	HCO3-1	4.499E-09
CaHSiO3+1	4.194E-04	CaCO3	3.734E-09
SO4-2	2.654E-04	HF	3.425E-09
MgF+1	1.743E-04	CaSiO2(OH)2	2.085E-09
CaSO4	1.171E-04	HSO4-1	1.951E-09
CaF+1	9.113E-05	NaHCO3	9.008E-10
KSO4-1	6.949E-05	HCl	2.555E-10
CaOH+1	4.19E-05		
NO3/Cl	**6.500E-03**	**(NO3+SO4+HCO3+CO3)/Cl**	**6.523E-03**

The pH and dominant aqueous species for Group 4 brine are tabulated below:

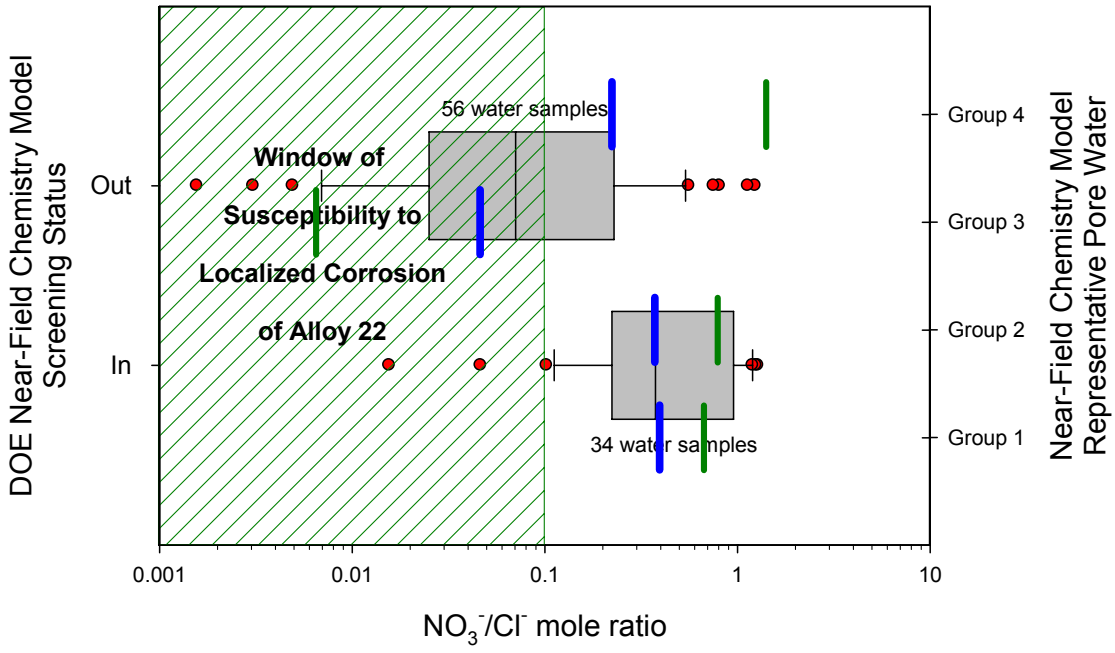
Group 4 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 8.38.			
Na+1	1.012E+01	MgHSiO3+1	1.191E-05
NO3-1	7.695E+00	MgSO4	1.058E-05
Cl-1	5.466E+00	CaOH+1	8.965E-06
K+1	3.099E+00	CaF+1	7.566E-06
NaNO3	8.173E-01	NaCO3-1	4.776E-06
KSO4-1	8.310E-02	MgOH+1	4.024E-06
KCl	4.715E-02	Mg+2	3.445E-06
NaHSiO3	2.443E-02	NaHCO3	2.579E-06
Ca(NO3)+1	1.925E-02	SO4-2	1.947E-06
H3SiO4-1	2.444E-03	H2SiO4-2	1.440E-06
Ca+2	2.390E-03	CaCO3	1.000E-06
SiO2	2.304E-03	CaSiO2(OH)2	4.926E-07
CaCl+1	2.093E-03	MgSiO2(OH)2	4.157E-07
Na2F+1	7.588E-04	CaHCO3+1	1.879E-07
NaF	2.836E-04	MgF+1	1.115E-07
F-1	2.605E-04	CO2	7.342E-08
CaSO4	2.132E-04	MgHCO3+1	5.260E-08
CaHSiO3+1	1.109E-04	MgCO3	2.664E-08
HCO3-1	2.648E-05	HSO4-1	1.291E-08
OH-1	2.135E-05	H+1	2.612E-09
CO3-2	1.288E-05	KHSO4	2.431E-10
NO3/Cl	**1.41**	**(NO3+SO4+HCO3+CO3)/Cl**	**1.41**

Yiming Pan asked if there is a difference in the nitrate to chloride ratio of the pore waters that were screened out by DOE (56 samples) from the near-field chemistry model versus the nitrate to chloride ratio of those that were screened in (34 samples). The following plot compares the NO3/Cl mole ratio of screened in versus screened out pore water samples. Also plotted (blue lines) are the NO3/Cl ratio of the four representative pore waters used by DOE in its near-field chemistry model. These four values for the representative waters are included in the 34 water samples plotted as box plot in the figure.



May 8, 2009

The figure below is the same as the one in the previous page with the exception that the NO3/Cl mole ratios of Groups 1 to 4 representative pore waters after evaporation at 110 °C and 0.85 atm are also plotted (as green lines). The significant decrease in NO3/Cl ratio for Group 3 water is due to the formation of a $CaNO3^+$ aqueous complex (it is the third most dominant aqueous species in evaporated Group 3 water). The increase in NO3/Cl ratio for Groups 1, 2, and 4 is mostly due to the precipitation of NaCl (which decreases the aqueous Cl^- concentration).



The evaporation simulations of Groups 1 to 4 representative pore waters were redone using OLIAnalyzer 3.0.5, but using the mixed-solvent electrolyte (MSE) model. The recalculation was done to eliminate the uncertainty associated with the formation of $CaNO_3^+$ aqueous complex (which decreases the calculated NO3/Cl ratio of evaporation brines).

The calculated pH and dominant aqueous species for Group 1 brine are tabulated below:

Group 1 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 10.87.			
Na+1	1.133E+01	MgF+1	1.959E-06
NO3-1	7.997E+00	MgCO3	7.548E-07
Cl-1	5.105E+00	CaF+1	4.566E-07
K+1	3.805E+00	CaOH+1	1.875E-07
CO3-2	6.261E-01	CO2	7.769E-08
HSiO3-1	4.861E-01	Ca+2	7.159E-08
SO4-2	1.123E-01	CaSO4	6.684E-08
OH-1	2.867E-02	MgOH+1	1.875E-08
F-1	2.362E-02	HF	6.388E-09
SiO2	1.289E-02	CaCl2	3.321E-09
HCO3-1	9.516E-03	NaHF2	5.501E-10
H2SiO4-2	4.279E-03	Mg+2	3.850E-10
CaCO3	1.119E-04	KOH	1.185E-10
NaOH.Na2SO4	2.026E-06		
NO3/Cl	**1.57**	**(NO3+SO4+HCO3+CO3)/Cl**	**1.71**

The pH and dominant aqueous species for Group 2 brine are tabulated below:

Group 2 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 7.15.			
NO3-1	8.140E+00	MgOH+1	9.805E-05
Na+1	7.178E+00	HSiO3-1	9.433E-05
Cl-1	6.448E+00	F-1	8.265E-06
K+1	4.225E+00	OH-1	7.256E-06
Ca+2	1.570E+00	HCO3-1	3.380E-06
CaCl2	4.531E-02	MgSO4	7.172E-07
MgF+1	2.687E-02	MgCO3	6.336E-07
SiO2	1.267E-02	CO2	7.386E-08
CaF+1	9.258E-03	CO3-2	3.605E-08
Mg+2	3.771E-03	H3O+1	1.307E-08
CaSO4	1.851E-03	HF	9.139E-09
CaOH+1	1.154E-03	HNO3	1.622E-09
SO4-2	2.466E-04	HSO4-1	3.071E-10
CaCO3	1.105E-04	H2SiO4-2	1.790E-10
NO3/Cl	**1.26**	**(NO3+SO4+HCO3+CO3)/Cl**	**1.26**

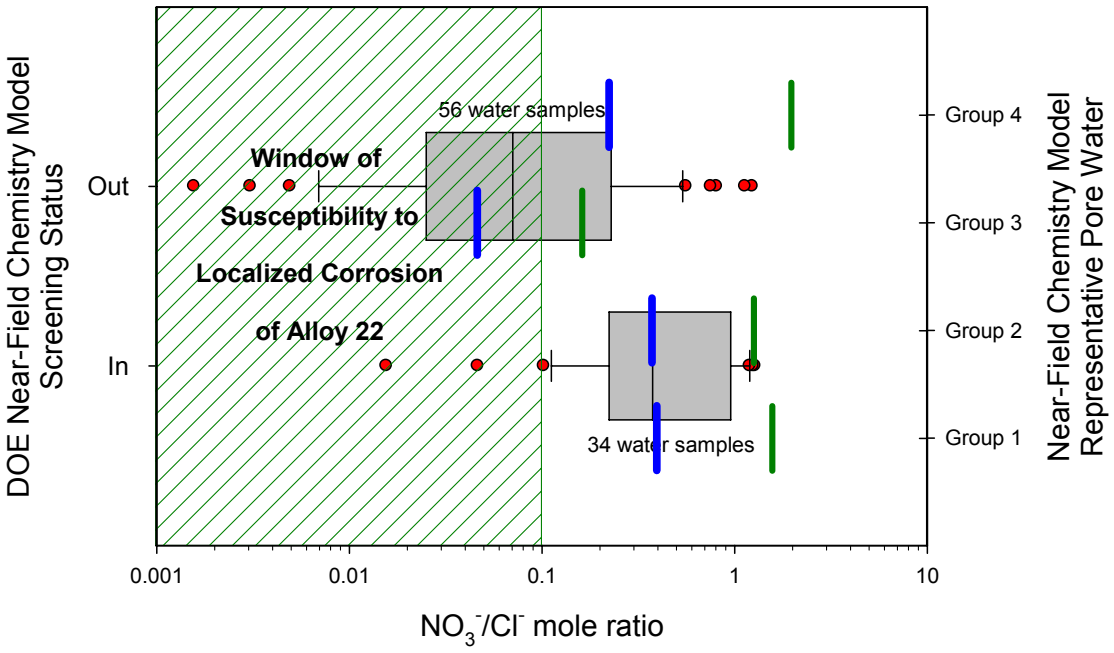
The pH and dominant aqueous species for Group 3 brine are tabulated below:

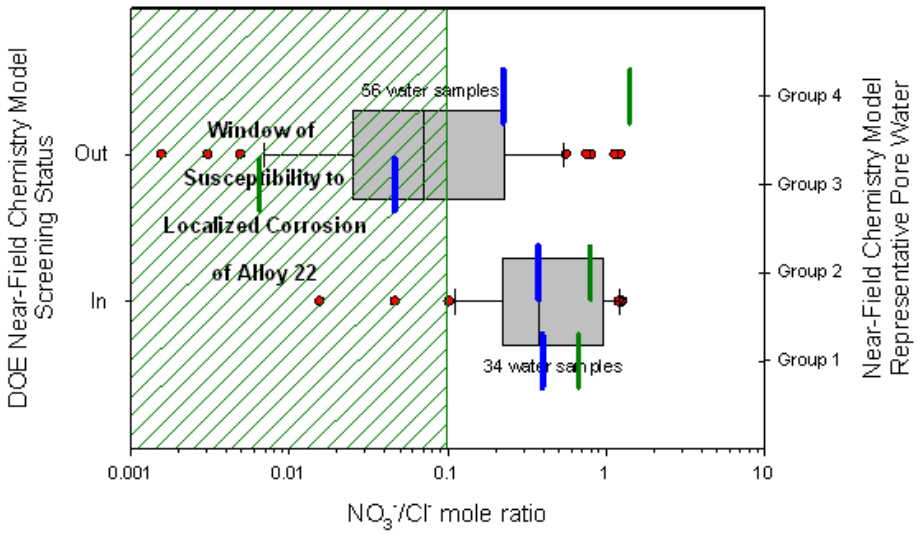
Group 3 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 6.21.			
Cl-1	9.541E+00	MgSO4	1.632E-05
Ca+2	2.642E+00	HSiO3-1	9.780E-06
Na+1	2.335E+00	CaCO3	6.170E-06
K+1	2.205E+00	F-1	2.368E-06
NO3-1	1.544E+00	OH-1	1.264E-06
Mg+2	4.395E-01	MgCO3	8.182E-07
MgF+1	3.724E-01	HCO3-1	8.097E-07
CaCl2	9.476E-02	H3O+1	1.257E-07
SiO2	1.246E-02	CO2	1.155E-07
CaF+1	1.066E-02	HF	9.484E-09
CaSO4	1.378E-03	CO3-2	2.357E-09
MgOH+1	7.966E-04	HNO3	1.713E-09
CaOH+1	4.053E-04	HSO4-1	9.147E-10
SO4-2	6.061E-05	HCl	4.610E-10
NO3/Cl	**1.62E-01**	**(NO3+SO4+HCO3+CO3)/Cl**	**1.62E-01**

The pH and dominant aqueous species for Group 4 brine are tabulated below:

Group 4 pore water evaporation at 110 C and 0.85 atm. Calculated pH is 8.33.			
Na+1	1.160E+01	CaOH+1	5.262E-05
NO3-1	1.012E+01	HCO3-1	3.283E-05
Cl-1	5.135E+00	Mg+2	1.410E-05
K+1	3.832E+00	CO3-2	7.133E-06
SO4-2	9.320E-02	MgOH+1	6.642E-06
SiO2	1.282E-02	MgSO4	1.078E-06
Ca+2	4.632E-03	MgCO3	9.527E-07
CaSO4	2.702E-03	CO2	9.907E-08
MgF+1	2.219E-03	H2SiO4-2	3.980E-08
HSiO3-1	1.455E-03	HF	2.115E-08
CaF+1	4.069E-04	HSO4-1	6.831E-09
CaCl2	2.254E-04	NaOH.Na2SO4	4.700E-09
F-1	1.890E-04	H3O+1	7.864E-10
CaCO3	1.119E-04	HNO3	1.779E-10
NO3/Cl	**1.97**	**(NO3+SO4+HCO3+CO3)/Cl**	**1.99**

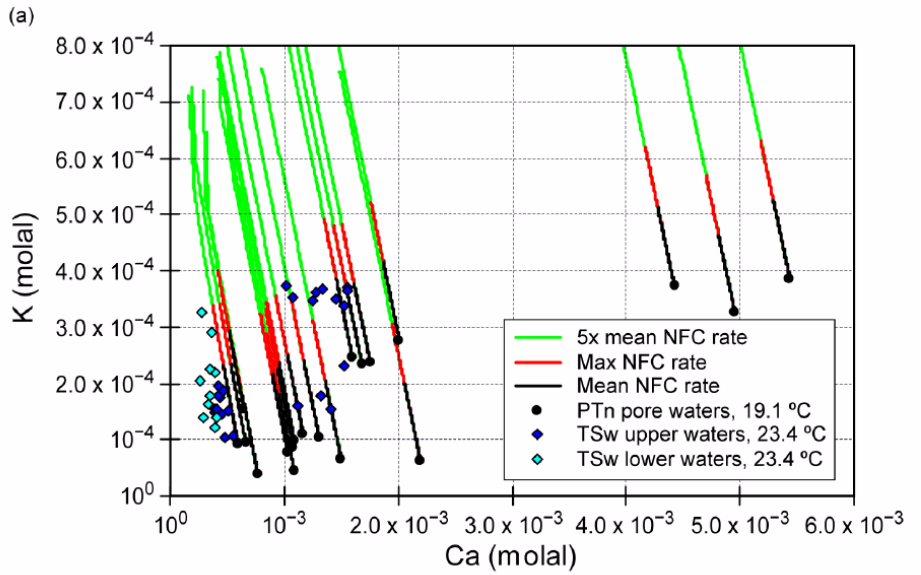
The figure below is similar to the one on page 178, but the green lines (for the NO3/Cl mole ratio of evaporated representative pore waters) were calculated using the Mixed Solvent Electrolyte model (tabulated results on pages 179 and 180). For comparison, the figure from page 178 is copied to the bottom of this page.



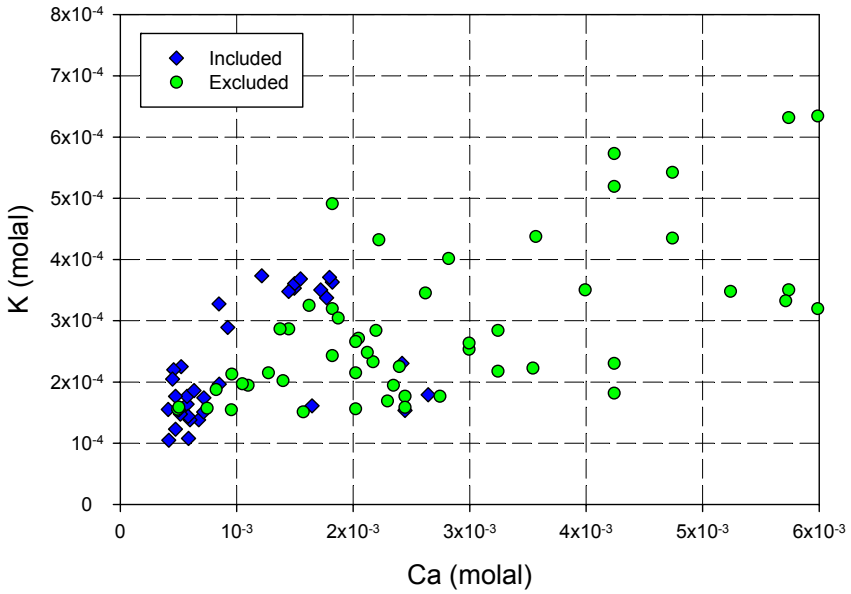


May 11, 2009

The DOE SAR has a plot of K+ versus Ca2+ concentrations for TSw and PTn pore waters showing predicted evolutionary pathways for the PTn waters at three different dissolution rates. The figure is reproduced below:



Using the chemistry information tabulated in a DOE response to RAI 3.2.2.1.3.3-001, I plotted the K+ vs Ca++ for the 90 pore water composition considered in the DOE screening for the near-field chemistry model. The included waters are shown as blue diamonds whereas the excluded waters are shown as green circles in the following figure.



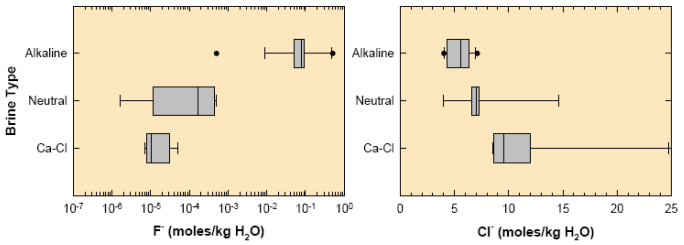
May 12, 2009

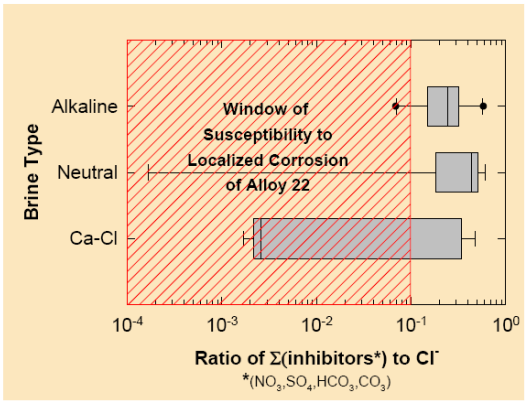
Revised Thermodynamic Simulations of Evaporation of Yucca Mountain Pore Waters

The thermodynamic calculations documented in notebook #697E, page 154–166, formed the basis for the NRC Total-system Performance Assessment (TPA) Version 5.1 abstraction of near-field water chemistry and the NRC/CNWRA staff understanding of the chemistry of water contacting drip shields and waste packages at the proposed Yucca Mountain repository. The results of those calculations indicate that initially dilute, calcium-chloride type waters would form brines, upon evaporation, that have low nitrate to chloride ratio. These brines could be corrosive to the Alloy 22 waste package material. The low nitrate to chloride ratio arises from the formation of $CaNO_3^+$ and $NaNO_3$ aqueous complexes, which ties up most of the nitrate and causes the ratio of aqueous nitrate species to aqueous chloride to be low. This uncertainty is mentioned by R. Pabalan in his Nuclear Waste Technical Review Board presentation on September 25, 2006. A copy of R. Pabalan's slide #11 is reproduced below:

Thermodynamic Modeling of Seepage Water Evaporation — Results (Cont'd.)

CNWRA A center of excellence in earth sciences and engineering





- Some brines have high Cl^- and F^- concentration
- Most have high ratio of corrosion inhibitors (NO_3^-, SO_4^{2-}, HCO_3^-, CO_3^{2-}) to corrosive Cl^-
- Chemistry information abstracted into NRC TPA code (O. Pensado, this workshop)

Note: Low ratio of Σ(inhibitors) to Cl^- is partly due to formation of $CaNO_3^+$ and $NaNO_3$ aqueous complexes, which have uncertain thermodynamic data

11

The uncertainty in the thermodynamic data (stability constant) for the $CaNO_3^+$ complex was acknowledged by Dr. Andre Anderko of OLI Systems, Inc., the company that developed the software (StreamAnalyzer) that was used in the thermodynamic calculations. A copy of his email to R. Pabalan is copied below:

From: Andre Anderko [aanderko@olisystems.com]
Sent: Friday, November 17, 2006 11:22 AM
To: rpabalan@cnwra.swri.edu
Subject: Re: CaNO3+ aqueous complex
Bobby,

When fitting the parameters for Ca(NO3)2 based on both recent and older data, Ron found out that it was not necessary to include the CaNO3+ ion pair. In general, we try to be very conservative when it comes to including ion pairs. We include them only when they are absolutely necessary to reproduce the data or when there is strong evidence from spectroscopic data for their existence. Our experience shows that inclusion of ion pairs whose properties are not very well known is dangerous for concentrated multicomponent systems. The danger stems from the fact that, if the effect of the ion pair and activity coefficients on overall nonideality are not correctly separated, the predictivity of the model may suffer for multicomponent systems.

Best regards,
Andre

----- Original Message -----
From: Bobby Pabalan
To: 'Andre Anderko'
Sent: Thursday, November 16, 2006 11:52 AM
Subject: CaNO3+ aqueous complex

Andre,

I noticed that the MSE model does not include the aqueous species CaNO3+. Was it excluded based on recent thermodynamic data?

Thanks.

bobby

Because of the uncertainty in the thermodynamic data for the nitrate-bearing aqueous complexes, the evaporation simulations will be redone using OLIAnalyzer Version 3.0.6, an updated version of the OLI software. The Mixed-Solvent Electrolyte (MSE) chemistry option of the software will be used. MSE was developed by OLI Systems for electrolyte solutions (aqueous and nonaqueous) with concentrations ranging from dilute conditions to the pure molten salts or pure acids. Thermodynamic properties calculated with this software have been shown to agree very well with experimental data (e.g., Gruszkiewicz, et al., 2007; Journal of Solution Chemistry 36: 723-765). As indicated in Andre Anderko's email, the $CaNO_3^+$ aqueous complex is not included in the MSE thermodynamic database The $NaNO_3$(aq) complex also is not included in the database.

Prior to entering the pore water compositions into OLIAnalyzer, the analytical data will be equilibrated and charge balanced using Geochemist's Workbench REACT Version 7.0. Following the approach used by Browning et al. (2000; Materials Research Society Symposium Proceedings 608, 237-242), the carbonate species will be constrained by equilibrium with a log f CO_2(g) equal to –2.991, and log f O_2(g) will be set to -0.7706. The reason REACT will be used for equilibration with those values of fCO_2 and fO_2 is because OLIAnalyzer does not permit gas fugacities to be fixed at specified values.

In contrast to the Browning et al. approach, however, the K^+ concentration will not be set to a value of 14 mg/L where the USGS chemical analysis did not report a value for K^+ concentration. Instead, it will be set to zero if no value was reported. Browning et al. did not included F^- in their analysis. In this analysis, F^- is included and will be set to 2.18 mg/L if no value is reported in the USGS reports. The inclusion of F^- is needed to assess the potential effect of seepage water evaporation on the corrosion of the titanium drip shield.

The following pages show the REACT script for each of the 33 pore water compositions considered in the evaporation analysis. The compositions are the same as those in the table on pages 155 and 156 of notebook # 679E. The thermodynamic database thermo.com.v8.r6+.dat was used for the REACT calculations. Also listed are the output concentrations of the original basis species for each REACT run. Those concentrations will be used for the OLIAnalyzer 2.0 evaporation simulations.

NRG-6/158.2

SiO2(aq)	1.62100E-03	molal
Na+	1.54850E-03	molal
Mg++	9.58650E-04	molal
Ca++	3.04410E-03	molal
F-	1.14750E-04	molal
Cl-	5.21820E-03	molal
SO4--	1.65510E-03	molal
swap NO3- for NH3(aq)		
NO3-	5.16090E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	3.044100E-03	molal
Cl-	5.218200E-03	molal
F-	1.147500E-04	molal
Mg++	9.586500E-04	molal
Na+	1.548500E-03	molal
NO3-	5.160900E-04	molal
SiO2(aq)	1.621000E-03	molal
SO4--	1.655100E-03	molal
HCO3-	4.226791E-04	molal

NRG-6/160.8

SiO2(aq)	1.398030E-03	molal
Na+	1.522400E-03	molal
Mg++	7.405850E-04	molal
Ca++	2.594930E-03	molal
F-	1.147460E-04	molal
Cl-	4.174520E-03	molal
SO4--	1.446950E-03	molal
swap NO3- for NH3(aq)		
NO3-	5.644690E-04	molal
swap CO2(g) for HCO3-		

log f CO2(g) = -2.9914
swap O2(g) for O2(aq)
log f O2(g) = -.7706
balance on pH
precip off

The output concentrations of the original basis species are as follows:

SiO2(aq)	1.398030E-03	molal
Na+	1.522400E-03	molal
Mg++	7.405850E-04	molal
Ca++	2.594930E-03	molal
F-	1.147460E-04	molal
Cl-	4.174520E-03	molal
SO4--	1.446950E-03	molal
HCO3-1	4.734332E-04	molal
NO3-	5.644690E-04	molal

NRG-6/171.0

SiO2(aq)	1.321345E-03	molal
Na+	1.270111E-03	molal
Mg++	4.730543E-04	molal
Ca++	1.758974E-03	molal
F-	1.147500E-04	molal
Cl-	1.635962E-03	molal
SO4--	9.785914E-04	molal
swap NO3- for NH3(aq)		
NO3-	6.934334E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.758974E-03	molal
Cl-	1.635962E-03	molal
F-	1.147500E-04	molal
HCO3-	1.337820E-03	molal
Mg++	4.730543E-04	molal
Na+	1.270111E-03	molal
NO3-	6.934334E-04	molal
SiO2(aq)	1.321345E-03	molal
SO4--	9.785914E-04	molal

NRG-6/175.6

SiO2(aq)	1.30E-03	molal
Na+	1.28E-03	molal
Mg++	3.54E-04	molal
Ca++	1.23E-03	molal

F-	1.15E-04	molal
Cl-	1.33E-03	molal
SO4--	6.66E-04	molal
swap NO3- for NH3(aq)		
NO3-	6.934334E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.227600E-03	molal
Cl-	1.325700E-03	molal
F-	1.147500E-04	molal
HCO3-1	9.949236E-04	molal
Mg++	3.538400E-04	molal
Na+	1.278800E-03	molal
NO3-	6.934334E-04	molal
SiO2(aq)	1.299800E-03	molal
SO4--	6.662200E-04	molal

SD-12/296.1

SiO2(aq)	1.201600E-03	molal
Na+	9.134400E-04	molal
Mg++	3.291500E-04	molal
Ca++	1.871300E-03	molal
F-	1.147500E-04	molal
Cl-	1.692400E-03	molal
SO4--	2.186000E-04	molal
swap NO3- for NH3(aq)		
NO3-	2.903000E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.871300E-03	molal
Cl-	1.692400E-03	molal
F-	1.147500E-04	molal
HCO3-	2.719370E-03	molal
Mg++	3.291500E-04	molal
Na+	9.134400E-04	molal
NO3-	2.903000E-04	molal
SiO2(aq)	1.201600E-03	molal
SO4--	2.186000E-04	molal

SD-6/471.3

SiO2(aq)	9.736300E-04	molal
Na+	1.953000E-03	molal
K+	6.649900E-05	molal
Mg++	5.060700E-04	molal
Ca++	1.532000E-03	molal
F-	4.526700E-04	molal
Cl-	1.884200E-03	molal
SO4--	7.078600E-04	molal
swap NO3- for NH3(aq)		
NO3-	1.085400E-03	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.532000E-03	molal
Cl-	1.884200E-03	molal
F-	4.526700E-04	molal
K+	6.649900E-05	molal
Mg++	5.060700E-04	molal
Na+	1.953000E-03	molal
NO3-	1.085400E-03	molal
SiO2(aq)	9.736300E-04	molal
SO4--	7.078600E-04	molal
HCO3-	1.268767E-03	molal

SD-9/114.1

SiO2(aq)	1.035210E-03	molal
Na+	2.392340E-03	molal
Mg++	7.405850E-04	molal
Ca++	2.370370E-03	molal
F-	1.147460E-04	molal
Cl-	3.892460E-03	molal
SO4--	1.884160E-03	molal
swap NO3- for NH3(aq)		
NO3-	1.757920E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	2.370370E-03	molal
Cl-	3.892460E-03	molal
F-	1.147460E-04	molal
HCO3-	6.873946E-04	molal
Mg++	7.405850E-04	molal
Na+	2.392340E-03	molal
NO3-	1.757920E-04	molal

SiO2(aq)	1.035210E-03	molal
SO4--	1.884160E-03	molal

SD-9/135.1

SiO2(aq)	9.985900E-04	molal
Na+	2.870800E-03	molal
Mg++	6.171500E-04	molal
Ca++	2.270600E-03	molal
F-	1.147500E-04	molal
Cl-	4.061700E-03	molal
SO4--	1.686400E-03	molal
swap NO3- for NH3(aq)		
NO3-	1.935300E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	2.270600E-03	molal
Cl-	4.061700E-03	molal
F-	1.147500E-04	molal
Mg++	6.171500E-04	molal
Na+	2.870800E-03	molal
NO3-	1.935300E-04	molal
SiO2(aq)	9.985900E-04	molal
SO4--	1.686400E-03	molal
HCO3-	9.224333E-04	molal

SD-9/94.2

SiO2(aq)	1.231600E-03	molal
Na+	1.870400E-03	molal
Mg++	9.874500E-04	molal
Ca++	3.118900E-03	molal
F-	1.147500E-04	molal
Cl-	4.795100E-03	molal
SO4--	2.706500E-03	molal
swap NO3- for NH3(aq)		
NO3-	1.774000E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	3.118900E-03	molal

Cl-	4.795100E-03	molal
F-	1.147500E-04	molal
Mg++	9.874500E-04	molal
Na+	1.870400E-03	molal
NO3-	1.774000E-04	molal
SiO2(aq)	1.231600E-03	molal
SO4--	2.706500E-03	molal
HCO3-	3.470905E-05	molal

UZ-16/1643.4

SiO2(aq)	1.164914E-03	molal
Na+	1.478897E-03	molal
Mg++	4.936220E-04	molal
Ca++	2.270449E-03	molal
F-	1.147500E-04	molal
Cl-	1.974436E-03	molal
SO4--	2.914953E-04	molal
swap NO3- for NH3(aq)		
NO3-	1.290108E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	2.270449E-03	molal
Cl-	1.974436E-03	molal
F-	1.147500E-04	molal
Mg++	4.936220E-04	molal
Na+	1.478897E-03	molal
NO3-	1.290108E-04	molal
SiO2(aq)	1.164914E-03	molal
SO4--	2.914953E-04	molal
HCO3-	4.039828E-03	molal

UZ-14/1,277

SiO2(aq)	6.324400E-04	molal
Na+	1.957400E-03	molal
Mg++	2.098300E-04	molal
Ca++	1.846400E-03	molal
F-	1.147500E-04	molal
Cl-	3.666800E-03	molal
SO4--	3.955700E-04	molal
swap NO3- for NH3(aq)		
NO3-	2.419200E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.846400E-03	molal
Cl-	3.666800E-03	molal
F-	1.147500E-04	molal
Mg++	2.098300E-04	molal
Na+	1.957400E-03	molal
NO3-1	2.419200E-04	molal
SiO2(aq)	6.324400E-04	molal
SO4--	3.955700E-04	molal
HCO3-	1.268380E-03	molal

SD-6/412.2

SiO2(aq)	6.923600E-04	molal
Na+	2.553300E-03	molal
K+	1.662500E-04	molal
Mg++	4.649200E-04	molal
Ca++	1.142800E-03	molal
F-	5.947800E-04	molal
Cl-	1.331300E-03	molal
SO4--	5.517200E-04	molal
swap NO3- for NH3(aq)		
NO3-	1.261200E-03	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.142800E-03	molal
Cl-	1.331300E-03	molal
F-	5.947800E-04	molal
K+	1.662500E-04	molal
Mg++	4.649200E-04	molal
Na+	2.553300E-03	molal
NH3(aq)	1.261200E-03	molal
SiO2(aq)	6.923600E-04	molal
SO4--	5.517200E-04	molal
HCO3-	1.648957E-03	molal

SD-6/443.5

SiO2(aq)	1.404700E-03	molal
Na+	2.849100E-03	molal
K+	1.023100E-04	molal
Mg++	4.813800E-04	molal
Ca++	1.202600E-03	molal
F-	3.316100E-04	molal
Cl-	1.334200E-03	molal
SO4--	1.020200E-03	molal

swap NO3- for NH3(aq)		
NO3-	1.387000E-03	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.202600E-03	molal
Cl-	1.334200E-03	molal
F-	3.316100E-04	molal
K+	1.023100E-04	molal
Mg++	4.813800E-04	molal
Na+	2.849100E-03	molal
NO3-	1.387000E-03	molal
SiO2(aq)	1.404700E-03	molal
SO4--	1.020200E-03	molal
HCO3-	1.235691E-03	molal

SD-6/507.5

SiO2(aq)	1.065200E-03	molal
Na+	2.100900E-03	molal
K+	6.138300E-05	molal
Mg++	1.012100E-03	molal
Ca++	3.118900E-03	molal
F-	1.631700E-04	molal
Cl-	5.725900E-04	molal
SO4--	3.112500E-03	molal
swap NO3- for NH3(aq)		
NO3-	4.144800E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	3.118900E-03	molal
Cl-	5.725900E-04	molal
F-	1.631700E-04	molal
K+	6.138300E-05	molal
Mg++	1.012100E-03	molal
Na+	2.100900E-03	molal
NO3-	4.144800E-04	molal
SiO2(aq)	1.065200E-03	molal
SO4--	3.112500E-03	molal
HCO3-	2.959454E-03	molal

SD-6/1509.9

SiO2(aq)	9.070500E-04	molal
Na+	4.301900E-03	molal
K+	2.122800E-04	molal
Mg++	1.069700E-04	molal
Ca++	1.641800E-03	molal
F-	7.737500E-04	molal
Cl-	2.784000E-03	molal
SO4--	2.914700E-04	molal
swap NO3- for NH3(aq)		
NO3-	2.903000E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.641800E-03	molal
Cl-	2.784000E-03	molal
F-	7.737500E-04	molal
K+	2.122800E-04	molal
Mg++	1.069700E-04	molal
Na+	4.301900E-03	molal
NO3-	2.903000E-05	molal
SiO2(aq)	9.070500E-04	molal
SO4--	2.914700E-04	molal
HCO3-	3.734839E-03	molal

SD-7/370.3

SiO2(aq)	4.310590E-04	molal
Na+	1.696380E-03	molal
Mg++	8.228720E-06	molal
Ca++	7.210910E-03	molal
F-	1.147460E-04	molal
Cl-	3.751430E-03	molal
SO4--	6.766320E-03	molal
swap NO3- for NH3(aq)		
NO3-	9.676610E-06	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	7.210910E-03	molal
Cl-	3.751430E-03	molal
F-	1.147460E-04	molal
Mg++	8.228720E-06	molal

Na+	1.696380E-03	molal
NO3-	9.676610E-06	molal
SiO2(aq)	4.310590E-04	molal
SO4--	6.766320E-03	molal
HCO3-	3.467236E-05	molal

SD-9/176.2

SiO2(aq)	9.736300E-04	molal
Na+	4.132200E-03	molal
Mg++	3.908600E-04	molal
Ca++	1.072900E-03	molal
F-	1.147500E-04	molal
Cl-	1.805200E-03	molal
SO4--	1.290800E-03	molal
swap NO3- for NH3(aq)		
NO3-	3.064300E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.072900E-03	molal
Cl-	1.805200E-03	molal
F-	1.147500E-04	molal
Mg++	3.908600E-04	molal
Na+	4.132200E-03	molal
NO3-	3.064300E-05	molal
SiO2(aq)	9.736300E-04	molal
SO4--	1.290800E-03	molal
HCO3-	2.498334E-03	molal

UZ-14/85.2

SiO2(aq)	1.494600E-03	molal
Na+	1.892100E-03	molal
Mg++	5.431000E-04	molal
Ca++	1.245100E-03	molal
F-	1.147500E-04	molal
Cl-	1.692400E-03	molal
SO4--	6.870400E-04	molal
swap NO3- for NH3(aq)		
NO3-	3.548100E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.245100E-03	molal
Cl-	1.692400E-03	molal
F-	1.147500E-04	molal
Mg++	5.431000E-04	molal
Na+	1.892100E-03	molal
NO3-	3.548100E-04	molal
SiO2(aq)	1.494600E-03	molal
SO4--	6.870400E-04	molal
HCO3-	1.916117E-03	molal

UZ-14/147.7

SiO2(aq)	1.286520E-03	molal
Na+	2.244450E-03	molal
Mg++	4.731520E-04	molal
Ca++	1.367330E-03	molal
F-	1.147460E-04	molal
Cl-	1.692370E-03	molal
SO4--	6.870420E-04	molal
swap NO3- for NH3(aq)		
NO3-	3.548090E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.367330E-03	molal
Cl-	1.692370E-03	molal
F-	1.147460E-04	molal
Mg++	4.731520E-04	molal
Na+	2.244450E-03	molal
NO3-	3.548090E-04	molal
SiO2(aq)	1.286520E-03	molal
SO4--	6.870420E-04	molal
HCO3-	2.355441E-03	molal

NRG-6/244.6

SiO2(aq)	8.488100E-04	molal
Na+	3.131800E-03	molal
Mg++	2.016000E-04	molal
Ca++	8.233900E-04	molal
F-	1.147500E-04	molal
Cl-	1.382100E-03	molal
SO4--	1.197100E-03	molal
swap NO3- for NH3(aq)		
NO3-	6.451100E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		

precip off

The output concentrations of the original basis species are as follows:

Al+++	2.223700E-05	molal
Ca++	8.233900E-04	molal
Cl-	1.382100E-03	molal
F-	1.147500E-04	molal
Mg++	2.016000E-04	molal
Na+	3.131800E-03	molal
NO3-	6.451100E-04	molal
SiO2(aq)	8.488100E-04	molal
SO4--	1.197100E-03	molal
HCO3-	6.729941E-04	molal

NRG-6/255.9

SiO2(aq)	1.131700E-03	molal
Na+	9.351900E-03	molal
Mg++	7.817300E-04	molal
Ca++	4.391400E-03	molal
F-	1.147460E-04	molal
Cl-	3.243700E-03	molal
SO4--	8.744200E-03	molal
swap NO3- for NH3(aq)		
NO3-	5.644700E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	4.391400E-03	molal
Cl-	3.243700E-03	molal
F-	1.147460E-04	molal
Mg++	7.817300E-04	molal
Na+	9.351900E-03	molal
NO3-	5.644700E-04	molal
SiO2(aq)	1.131700E-03	molal
SO4--	8.744200E-03	molal
HCO3-	3.466758E-05	molal

UZ-14/178.1

SiO2(aq)	1.549500E-03	molal
Na+	2.135700E-03	molal
Mg++	4.361200E-04	molal
Ca++	1.596900E-03	molal
F-	1.147500E-04	molal
Cl-	2.736000E-03	molal
SO4--	1.249200E-03	molal
swap NO3- for NH3(aq)		

NO3-	3.386800E-04	molal

swap CO2(g) for HCO3-
log f CO2(g) = -2.9914
swap O2(g) for O2(aq)
log f O2(g) = -.7706
balance on pH
precip off

The output concentrations of the original basis species are as follows:

Ca++	1.596900E-03	molal
Cl-	2.736000E-03	molal
F-	1.147500E-04	molal
HCO3-	5.400607E-04	molal
Mg++	4.361200E-04	molal
Na+	2.135700E-03	molal
NO3-	3.386800E-04	molal
SiO2(aq)	1.549500E-03	molal
SO4--	1.249200E-03	molal

UZ-14/1258.5

SiO2(aq)	5.825120E-04	molal
Na+	2.914300E-03	molal
Mg++	1.522310E-04	molal
Ca++	1.072900E-03	molal
F-	1.147460E-04	molal
Cl-	2.482150E-03	molal
SO4--	1.977850E-04	molal

swap NO3- for NH3(aq)

NO3-	2.580430E-04	molal

swap CO2(g) for HCO3-
log f CO2(g) = -2.9914
swap O2(g) for O2(aq)
log f O2(g) = -.7706
balance on pH
precip off

The output concentrations of the original basis species are as follows:

Ca++	1.072900E-03	molal
Cl-	2.482150E-03	molal
F-	1.147460E-04	molal
Mg++	1.522310E-04	molal
Na+	2.914300E-03	molal
NO3-	2.580430E-04	molal
SiO2(aq)	5.825120E-04	molal
SO4--	1.977850E-04	molal
HCO3-	2.106714E-03	molal

UZ-14/1409.4

SiO2(aq)	9.486630E-04	molal
Na+	3.827740E-03	molal
Mg++	2.880050E-05	molal
Ca++	7.485370E-04	molal

F-	1.147460E-04	molal
Cl-	2.115470E-03	molal
SO4--	1.103430E-03	molal
swap NO3- for NH3(aq)		
NO3-	8.063840E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	7.485370E-04	molal
Cl-	2.115470E-03	molal
F-	1.147460E-04	molal
Mg++	2.880050E-05	molal
Na+	3.827740E-03	molal
NO3-	8.063840E-05	molal
SiO2(aq)	9.486630E-04	molal
SO4--	1.103430E-03	molal
HCO3-	8.879588E-04	molal

UZ-14/1,542

SiO2(aq)	2.380000E-03	molal
Na+	9.003900E-03	molal
Mg++	2.057200E-05	molal
Ca++	8.982400E-05	molal
F-	1.147500E-04	molal
Cl-	5.641200E-04	molal
SO4--	2.914700E-04	molal
swap NO3- for NH3(aq)		
NO3-	6.451100E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	8.982400E-05	molal
Cl-	5.641200E-04	molal
F-	1.147500E-04	molal
Mg++	2.057200E-05	molal
Na+	9.003900E-03	molal
NO3-	6.451100E-05	molal
SiO2(aq)	2.380000E-03	molal
SO4--	2.914700E-04	molal
HCO3-	7.565997E-03	molal

UZ-14/1825.8

SiO2(aq)	7.972100E-04	molal
Na+	5.959100E-03	molal
Mg++	4.114400E-06	molal
Ca++	1.497100E-05	molal
F-	1.147500E-04	molal
Cl-	6.628500E-04	molal
SO4--	1.342900E-04	molal
swap NO3- for NH3(aq)		
NO3-	1.903100E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	1.497100E-05	molal
Cl-	6.628500E-04	molal
F-	1.147500E-04	molal
Mg++	4.114400E-06	molal
Na+	5.959100E-03	molal
NO3-	1.903100E-04	molal
SiO2(aq)	7.972100E-04	molal
SO4--	1.342900E-04	molal
HCO3-	4.687060E-03	molal

UZ-14/2014.7

SiO2(aq)	6.274490E-04	molal
Na+	1.705080E-02	molal
Mg++	8.228720E-06	molal
Ca++	7.984400E-05	molal
F-	1.147460E-04	molal
Cl-	9.054200E-04	molal
SO4--	2.310960E-04	molal
swap NO3- for NH3(aq)		
NO3-	2.902980E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	7.984400E-05	molal
Cl-	9.054200E-04	molal
F-	1.147460E-04	molal
Mg++	8.228720E-06	molal
Na+	1.705080E-02	molal
NO3-	2.902980E-05	molal
SiO2(aq)	6.274490E-04	molal
SO4--	2.310960E-04	molal

HCO3-	1.486746E-02	molal

UZ-16/1343.7

SiO2(aq)	1.033500E-03	molal
Na+	4.306200E-03	molal
Mg++	9.874500E-05	molal
Ca++	4.241700E-04	molal
F-	1.147500E-04	molal
Cl-	1.579500E-03	molal
SO4--	2.394200E-04	molal
swap NO3- for NH3(aq)		
NO3-	2.90E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	4.241700E-04	molal
Cl-	1.579500E-03	molal
F-	1.147500E-04	molal
Mg++	9.874500E-05	molal
Na+	4.306200E-03	molal
NO3-	2.90E-04	molal
SiO2(aq)	1.033500E-03	molal
SO4--	2.394200E-04	molal
HCO3-	2.858556E-03	molal

WT-24/1937.0

SiO2(aq)	7.556000E-04	molal
Na+	2.522800E-03	molal
K+	1.713600E-04	molal
Mg++	2.468600E-05	molal
Ca++	3.967200E-04	molal
F-	2.210700E-04	molal
Cl-	1.009800E-03	molal
SO4--	6.245800E-05	molal
swap NO3- for NH3(aq)		
NO3-	8.063800E-06	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	3.967200E-04	molal
Cl-	1.009800E-03	molal

F-	2.210700E-04	molal
K+	1.713600E-04	molal
Mg++	2.468600E-05	molal
Na+	2.522800E-03	molal
NO3-	8.063800E-06	molal
SiO2(aq)	7.556000E-04	molal
SO4--	6.245800E-05	molal
HCO3-	2.171644E-03	molal

NRG-6/219.9

SiO2(aq)	1.021900E-03	molal
Na+	4.319300E-03	molal
Mg++	1.728000E-04	molal
Ca++	6.063100E-04	molal
F-	1.147500E-04	molal
Cl-	2.171900E-03	molal
SO4--	8.015500E-04	molal
swap NO3- for NH3(aq)		
NO3-	7.580000E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	6.063100E-04	molal
Cl-	2.171900E-03	molal
F-	1.147500E-04	molal
Mg++	1.728000E-04	molal
Na+	4.319300E-03	molal
NO3-	7.580000E-04	molal
SiO2(aq)	1.021900E-03	molal
SO4--	8.015500E-04	molal
HCO3-	1.241657E-03	molal

NRG-7a/460.25

SiO2(aq)	1.497900E-04	molal
Na+	1.826900E-03	molal
K+	1.739200E-04	molal
Ca++	7.485400E-05	molal
F-	1.147500E-04	molal
Cl-	1.974400E-04	molal
SO4--	4.163900E-05	molal
swap NO3- for NH3(aq)		
NO3-	1.612800E-05	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	7.485400E-05	molal
Cl-	1.974400E-04	molal
F-	1.147500E-04	molal
K+	1.739200E-04	molal
Na+	1.826900E-03	molal
NO3-1	1.612800E-05	molal
SiO2(aq)	1.497900E-04	molal
SO4--	4.163900E-05	molal
HCO3-	1.759816E-03	molal

SD-12/1495.5

SiO2(aq)	1.453000E-03	molal
Na+	4.697700E-03	molal
Mg++	8.228700E-06	molal
Ca++	3.992200E-04	molal
F-	1.147500E-04	molal
Cl-	1.607800E-03	molal
SO4--	5.725300E-04	molal
swap NO3- for NH3(aq)		
NO3-	1.306300E-04	molal
swap CO2(g) for HCO3-		
log f CO2(g) = -2.9914		
swap O2(g) for O2(aq)		
log f O2(g) = -.7706		
balance on pH		
precip off		

The output concentrations of the original basis species are as follows:

Ca++	3.992200E-04	molal
Cl-	1.607800E-03	molal
F-	1.147500E-04	molal
Mg++	8.228700E-06	molal
Na+	4.697700E-03	molal
NO3-	1.306300E-04	molal
SiO2(aq)	1.453000E-03	molal
SO4--	5.725300E-04	molal
HCO3-	2.489709E-03	molal

SD-6/522.5

SiO2(aq)	1.060170E-03	molal
Na+	2.566330E-03	molal
K+	1.534590E-04	molal
Mg++	4.073220E-04	molal
Ca++	1.090370E-03	molal
F-	4.052950E-04	molal
Cl-	7.418240E-04	molal
SO4--	5.829450E-04	molal
swap NO3- for NH3(aq)		
NO3-	5.564050E-04	molal
swap CO2(g) for HCO3-		

log f CO2(g) = -2.9914
swap O2(g) for O2(aq)
log f O2(g) = -.7706
balance on pH
precip off

The output concentrations of the original basis species are as follows:

Ca++	1.090370E-03	molal
Cl-	7.418240E-04	molal
F-	4.052950E-04	molal
K+	1.534590E-04	molal
Mg++	4.073220E-04	molal
Na+	2.566330E-03	molal
NO3-	5.564050E-04	molal
SiO2(aq)	1.060170E-03	molal
SO4--	5.829450E-04	molal
HCO3-	2.799928E-03	molal

May 22, 2009

From O. Pensado email:

Restrictions of the thermodynamic analysis:

Water vapor pressure cannot exceed 0.85 atm (boiling temperature 97 °C)

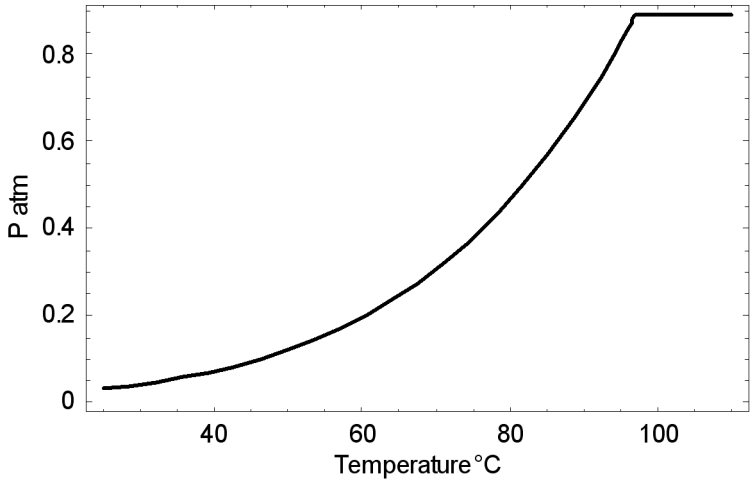
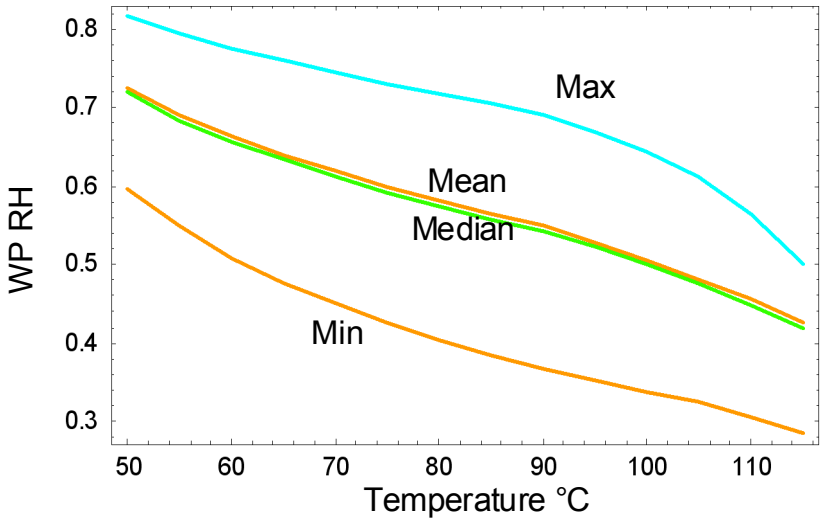


Figure 1

The relative humidity at the WP is less than 100%



T[°C]	Min	Median	Mean	Max	SDev
50	0.597626	0.724841	0.720398	0.817349	0.05031
55	0.550155	0.689885	0.684654	0.794479	0.057122
60	0.508206	0.663233	0.65703	0.776235	0.062347
65	0.477004	0.639953	0.633407	0.75991	0.065822
70	0.450068	0.618355	0.611998	0.744409	0.06849
75	0.426226	0.598958	0.592435	0.730296	0.070967
80	0.404438	0.581175	0.574699	0.717186	0.073141
85	0.385053	0.564995	0.558528	0.705384	0.074932
90	0.367668	0.549577	0.54188	0.690198	0.074547
95	0.352062	0.528459	0.522563	0.668209	0.071773
100	0.338193	0.50475	0.500324	0.644986	0.069115
105	0.323996	0.479821	0.476083	0.611351	0.066954
110	0.303936	0.45498	0.449075	0.56454	0.062066
115	0.284919	0.426621	0.417839	0.500301	0.053188

Data from TPA 5.1betaU, 500 realizations

The water pressure at the WP surface is

$$P_{WP} = P(T)\, RH$$

where *P*(T) is the water pressure as in Figure 1.

The **median RH** is a reasonable value to use in the thermodynamic computations.

At 25%, you may use 100% RH.

May 28, 2009

The thermodynamic calculations of seepage water evaporation using OLIAnalyzer Version 3.0 were done as follows.

Thermodynamic simulations of evaporation were conducted at various waste package temperatures (T_{WP} = 25, 50, 70, 90, and 110 °C) using OLIAnalyzer 3.0.6 (with the MSE H_3O^+ chemistry model) to determine the potential range in chemistry of waters contacting the waste packages. The input chemistry is the same as the GWB React output concentrations listed on pages 185 to 203 of this notebook. It was assumed that evaporation occurs until the median relative humidity given in the table on the previous page is attained (100% RH is used at 25 °C).

The median relative humidity was used as a constraint in the OLIAnalyzer calculation by specifying a total pressure in the input file that would result in an output relative humidity (or water activity) equal to the median relative humidity. That is,

P_{Total} = Median_RH $\times$ pH2O°(T_{WP})

The table below gives the total pressure corresponding to the median relative humidity at different temperatures:

T_{WP}[°C]	Median RH	$pH_2O°$	Total P (atm)
25	1.0	0.031385	0.031385
50	0.724841	0.12207	0.088481
55	0.689885	0.15571	0.107422
60	0.663233	0.196965	0.130634
65	0.639953	0.247171	0.158178
70	0.618355	0.307827	0.190346
75	0.598958	0.380599	0.227963
80	0.581175	0.467334	0.271603
85	0.564995	0.570063	0.322083
90	0.549577	0.69101	0.379763
95	0.528459	0.832599	0.439994
100	0.50475	0.997457	0.503466
105	0.479821	1.18842	0.570229
110	0.45498	1.40854	0.640858
115	0.426621	1.66108	0.708652

In some OLIAnalyzer runs, particularly at 90 and 110 C, the median relative humidity specified in the above table caused the solution to completely evaporate. In those cases, the total pressure specified in the OLIAnalyzer input was reduced such that some amount of aqueous phase remained in the output. For the compositions that required such adjustment, the sample names listed in the tables in the following pages indicate the total pressure used in the input.

The OLIAnalyzer files that have the input and output information are included in a CD that accompanies this notebook. The filenames of the OLIAnalyzer files and the Excel files that summarize the results are:

1. OLIAnalyzer Evaporation of YM Waters temp=110 C P=0.640858 atm Median RH.oad
2. OLIAnalyzer Evaporation of YM Waters temp=90 C P=0.379763 atm Median RH.oad
3. OLIAnalyzer Evaporation of YM Waters temp=70 C P=0.190346 atm Median RH.oad
4. OLIAnalyzer Evaporation of YM Waters temp=50 C P=0.088481 atm Median RH.oad
5. OLIAnalyzer Evaporation of YM Waters temp=25 C P=0.031385 atm Median RH.oad
6. YM Pore Waters Evaporation Results Temp=110C_P=0.640858 atm Median RH.xls
7. YM Pore Waters Evaporation Results Temp=90C_P=0.379763 atm Median RH.xls
8. YM Pore Waters Evaporation Results Temp=70C_P=0.190346 atm Median RH.xls
9. YM Pore Waters Evaporation Results Temp=50C_P=0.088481 atm Median RH.xls
10. YM Pore Waters Evaporation Results Temp=25C_P=0.031385 atm Median RH.xls

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June 9, 2009

For the revised TPA 5.1 abstraction of near-field water chemistry, the following chemistry information was provided to O. Pensado in the file "Revised brine chemistry for TPA 5.1 abstraction.xls". The information in that file is given in the following four tables:

Temperature = 110 °C (P = 0.640858 atm)						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2	Ca-Cl	5.58	1.102E+01	1.535E+00	2.069E-08	1.689E-06
NRG-6/160.8	Ca-Cl	5.60	1.077E+01	2.232E+00	3.975E-08	1.213E-06
NRG-6/171.0	Ca-Cl	6.58	7.214E+00	9.789E+00	9.886E-06	1.160E-07
NRG-6/175.6	Ca-Cl	6.75	5.029E+00	1.443E+01	9.384E-06	1.298E-07
SD-6/471.3	Ca-Cl	6.74	4.259E+00	1.644E+01	1.026E-05	1.901E-07
SD-9/94.2	Ca-Cl	5.47	1.114E+01	6.889E-01	2.390E-10	7.107E-06
SD-9/114.1	Ca-Cl	5.56	1.134E+01	1.313E+00	2.137E-08	2.169E-06
SD-9/135.1	Ca-Cl	5.85	1.177E+01	1.877E+00	5.605E-07	5.041E-07
SD-12/296.1	Ca-Cl	6.38	1.057E+01	3.689E+00	7.941E-06	2.341E-07
UZ-14/1,277	Ca-Cl	6.50	1.165E+01	1.652E+00	4.814E-06	3.217E-07
UZ-16/1643.4	Ca-Cl	6.28	1.121E+01	2.649E+00	8.469E-06	2.867E-07
NRG-6/244.6 - 0.74 atm	Neutral	8.47	2.931E+00	1.864E+01	1.911E-05	6.184E-02
NRG-6/255.9	Neutral	5.73	4.309E+00	2.087E+01	7.915E-10	3.069E-02
SD-6/412.2	Neutral	8.37	2.683E+00	2.895E+01	2.102E-05	4.535E-02
SD-6/443.5	Neutral	8.40	2.683E+00	2.895E+01	1.954E-05	4.535E-02
SD-6/507.5	Neutral	8.22	2.684E+00	2.895E+01	2.866E-05	4.534E-02
SD-6/1509.9	Neutral	10.99	6.107E+00	2.540E+01	1.659E-01	4.669E-02
SD-7/370.3	Neutral	7.21	1.249E+01	6.544E-02	7.903E-07	4.266E-07
SD-9/176.2 - 0.74 atm	Neutral	8.79	2.908E+00	1.840E+01	1.517E-04	2.238E-01
UZ-14/85.2	Neutral	6.88	2.648E+00	2.291E+01	5.716E-06	4.578E-06
UZ-14/147.7 - 0.74 atm	Neutral	8.22	2.932E+00	1.864E+01	2.998E-05	6.181E-02
UZ-14/178.1	Neutral	5.68	9.971E+00	5.081E+00	1.277E-07	5.890E-07
NRG-6/219.9 - 0.74 atm	Alkaline	8.94	2.908E+00	1.840E+01	1.237E-04	2.238E-01
NRG-7a/460.25	Alkaline	11.17	6.083E+00	2.496E+01	1.683E-01	4.765E-02
SD-6/522.5 - 0.74 atm	Alkaline	9.73	2.907E+00	1.834E+01	5.862E-03	2.244E-01
SD-12/1495.5 - 0,74 atm	Alkaline	10.75	2.875E+00	1.730E+01	3.968E-01	7.201E-02
UZ-14/1,542 - 0.74 atm	Alkaline	10.50	2.885E+00	1.750E+01	3.971E-01	7.124E-02
UZ-14/1258.5 - 0.74 atm	Alkaline	8.29	2.931E+00	1.864E+01	2.627E-05	6.182E-02
UZ-14/1409.4 - 0.74 atm	Alkaline	9.06	2.908E+00	1.839E+01	1.090E-04	2.239E-01
UZ-14/1825.8 - 0.74 atm	Alkaline	10.61	2.882E+00	1.742E+01	3.962E-01	7.152E-02
UZ-14/2014.7 - 0,74 atm	Alkaline	10.36	2.889E+00	1.758E+01	4.001E-01	7.098E-02
UZ-16/1343.7 - 0.74 atm	Alkaline	10.71	2.877E+00	1.734E+01	3.965E-01	7.184E-02
WT-24/1937.0 - 0.74 atm	Alkaline	10.78	2.888E+00	1.727E+01	4.011E-01	2.544E-02

Temperature = 90 °C (P = 0.379763 atm)						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	6.19	9.220E+00	1.155E+00	7.749E-08	2.418E-05
NRG-6--160.8	Ca-Cl	6.23	8.991E+00	1.670E+00	1.292E-07	2.265E-05
NRG-6--171.0	Ca-Cl	6.86	6.383E+00	6.721E+00	5.601E-06	1.843E-05
NRG-6--175.6	Ca-Cl	7.00	5.090E+00	9.300E+00	4.986E-06	2.507E-05
SD-6--471.3	Ca-Cl	6.98	4.641E+00	1.034E+01	5.475E-06	3.099E-05
SD-9--94.2	Ca-Cl	6.08	9.337E+00	5.278E-01	1.089E-09	4.070E-05
SD-9--114.1	Ca-Cl	6.18	9.437E+00	9.901E-01	8.756E-08	2.577E-05
SD-9--135.1	Ca-Cl	6.45	9.619E+00	1.387E+00	1.043E-06	1.719E-05
SD-12--296.1	Ca-Cl	6.67	8.715E+00	2.694E+00	5.137E-06	1.589E-05
UZ-14--1,277	Ca-Cl	6.79	9.596E+00	1.218E+00	3.537E-06	1.547E-05
UZ-16--1643.4	Ca-Cl	6.57	9.205E+00	1.942E+00	5.301E-06	1.623E-05
NRG-6--244.6 - 0.388 atm	Neutral	8.61	3.002E+00	1.511E+01	1.894E-05	5.705E-02
NRG-6--255.9	Neutral	6.12	4.867E+00	8.114E+00	7.124E-10	6.369E-02
SD-6--412.2	Neutral	8.45	3.082E+00	1.681E+01	2.580E-05	5.487E-02
SD-6--443.5	Neutral	8.48	2.963E+00	1.661E+01	2.405E-05	5.449E-02
SD-6--507.5	Neutral	8.31	3.117E+00	1.685E+01	3.460E-05	5.501E-02
SD-6--1509.9	Neutral	11.13	6.491E+00	1.044E+01	6.905E-01	4.569E-02
SD-7--370.3	Neutral	7.50	1.030E+01	4.825E-02	6.690E-07	1.536E-05
SD-9--176.2 - 0.385 atm	Neutral	8.91	2.919E+00	1.533E+01	1.378E-04	1.933E-01
UZ-14--85.2	Neutral	7.09	3.453E+00	1.376E+01	4.231E-06	1.004E-04
UZ-14--147.7 - 0.388 atm	Neutral	8.37	3.003E+00	1.511E+01	2.966E-05	5.702E-02
UZ-14--178.1	Neutral	6.35	8.266E+00	3.675E+00	3.150E-07	2.084E-05
NRG-6--219.9 - 0.385 atm	Alkaline	9.03	2.919E+00	1.533E+01	1.168E-04	1.933E-01
NRG-7a--460.25	Alkaline	11.31	6.442E+00	1.004E+01	7.110E-01	4.677E-02
SD-6--522.5 - 0.385 atm	Alkaline	9.88	2.920E+00	1.530E+01	5.931E-03	1.940E-01
SD-12--1495.5	Alkaline	10.98	2.760E+00	1.468E+01	5.328E-01	5.925E-02
UZ-14--1,542	Alkaline	10.74	2.771E+00	1.489E+01	5.314E-01	5.841E-02
UZ-14--1258.5 - 0.388 atm	Alkaline	8.44	3.002E+00	1.511E+01	2.600E-05	5.703E-02
UZ-14--1409.4 - 0.385 atm	Alkaline	9.18	2.918E+00	1.533E+01	9.821E-05	1.934E-01
UZ-14--1825.8	Alkaline	10.85	2.767E+00	1.481E+01	5.310E-01	5.872E-02
UZ-14--2014.7 - 0.385 atm	Alkaline	10.59	2.873E+00	1.416E+01	5.638E-01	5.970E-02
UZ-16--1343.7	Alkaline	10.94	2.762E+00	1.472E+01	5.320E-01	5.906E-02
WT-24--1937.0	Alkaline	11.01	2.774E+00	1.463E+01	5.399E-01	1.811E-02

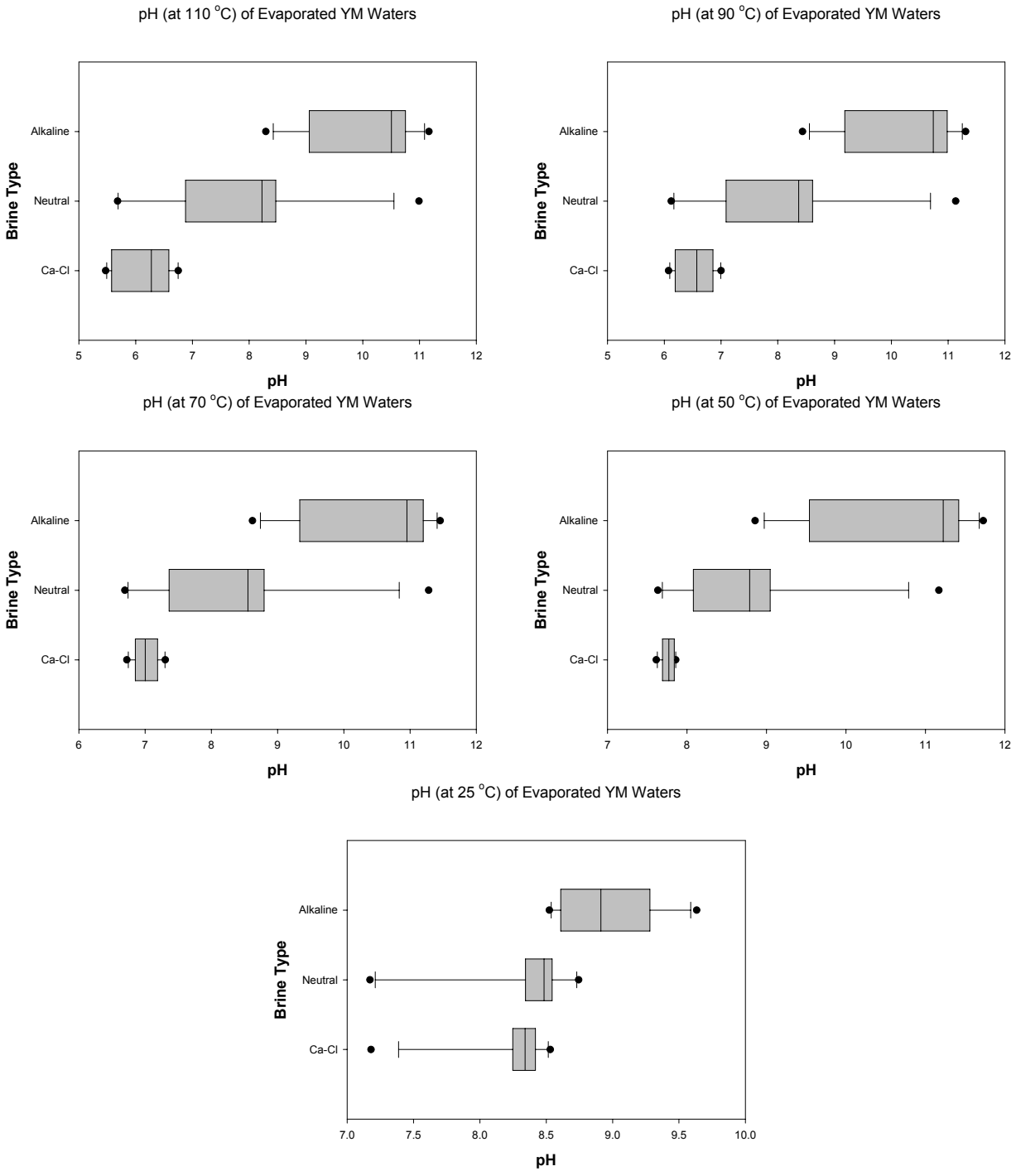
Temperature = 70 °C (P = 0.190346 atm)						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	6.85	7.949E+00	8.873E-01	2.514E-07	1.077E-04
NRG-6--160.8	Ca-Cl	6.89	7.768E+00	1.270E+00	3.745E-07	1.084E-04
NRG-6--171.0	Ca-Cl	7.19	5.986E+00	4.520E+00	3.174E-06	1.447E-04
NRG-6--175.6	Ca-Cl	7.31	5.255E+00	5.936E+00	2.949E-06	1.801E-04
SD-6--471.3	Ca-Cl	7.28	5.008E+00	6.446E+00	3.238E-06	2.021E-04
SD-9--94.2	Ca-Cl	6.73	8.059E+00	4.131E-01	6.662E-09	1.380E-04
SD-9--114.1	Ca-Cl	6.84	8.107E+00	7.612E-01	3.137E-07	1.086E-04
SD-9--135.1	Ca-Cl	7.00	8.053E+00	1.033E+00	1.403E-06	1.008E-04
SD-12--296.1	Ca-Cl	7.03	7.462E+00	1.967E+00	2.776E-06	1.094E-04
UZ-14--1,277	Ca-Cl	7.14	8.148E+00	9.187E-01	2.221E-06	9.846E-05
UZ-16--1643.4	Ca-Cl	6.95	7.785E+00	1.429E+00	2.595E-06	1.063E-04
NRG-6--244.6	Neutral	8.80	3.579E+00	1.001E+01	2.094E-05	6.648E-02
NRG-6--255.9	Neutral	6.70	6.242E+00	2.350E+00	3.038E-09	1.771E-01
SD-6--412.2	Neutral	8.63	3.853E+00	1.014E+01	2.980E-05	7.137E-02
SD-6--443.5	Neutral	8.65	3.725E+00	1.010E+01	2.759E-05	6.902E-02
SD-6--507.5	Neutral	8.49	3.890E+00	1.014E+01	3.934E-05	7.199E-02
SD-6--1509.9	Neutral	11.28	6.317E+00	3.272E+00	1.473E+00	5.279E-02
SD-7--370.3	Neutral	7.84	8.746E+00	3.713E-02	5.557E-07	9.283E-05
SD-9--176.2	Neutral	9.06	3.550E+00	9.789E+00	1.461E-04	2.158E-01
UZ-14--178.1	Neutral	6.93	7.045E+00	2.594E+00	4.565E-07	1.236E-04
UZ-14--147.7	Neutral	8.55	3.582E+00	1.000E+01	3.196E-05	6.643E-02
UZ-14--85.2	Neutral	7.36	4.233E+00	8.277E+00	3.282E-06	3.484E-04
NRG-6--219.9	Alkaline	9.22	3.549E+00	9.788E+00	1.208E-04	2.159E-01
NRG-7a--460.25	Alkaline	11.46	6.246E+00	3.016E+00	1.505E+00	5.396E-02
SD-6--522.5	Alkaline	10.07	3.547E+00	9.742E+00	8.215E-03	2.167E-01
SD-12--1495.5	Alkaline	11.20	3.385E+00	8.082E+00	8.544E-01	7.659E-02
UZ-14--1,542	Alkaline	10.95	3.402E+00	8.260E+00	8.501E-01	7.530E-02
WT-24--1937.0	Alkaline	11.22	3.403E+00	8.037E+00	8.699E-01	2.017E-02
UZ-16--1343.7	Alkaline	11.16	3.389E+00	8.122E+00	8.528E-01	7.629E-02
UZ-14--2014.7	Alkaline	10.80	3.407E+00	8.324E+00	8.529E-01	7.488E-02
UZ-14--1825.8	Alkaline	11.06	3.396E+00	8.194E+00	8.506E-01	7.577E-02
UZ-14--1409.4	Alkaline	9.33	3.549E+00	9.787E+00	1.076E-04	2.159E-01
UZ-14--1258.5	Alkaline	8.62	3.581E+00	1.000E+01	2.820E-05	6.645E-02

Temperature = 50 °C (P = 0.088481 atm)						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	7.69	6.056E+00	5.993E-01	2.098E-06	4.828E-04
NRG-6--160.8	Ca-Cl	7.73	5.949E+00	8.049E-01	2.563E-06	5.221E-04
NRG-6--171.0	Ca-Cl	7.77	5.085E+00	2.156E+00	3.275E-06	8.538E-04
NRG-6--175.6	Ca-Cl	7.86	4.892E+00	2.560E+00	3.009E-06	9.936E-04
SD-6--471.3	Ca-Cl	7.84	4.765E+00	2.746E+00	3.311E-06	1.121E-03
SD-9--94.2	Ca-Cl	7.61	6.304E+00	2.333E-01	7.474E-08	8.748E-04
SD-9--114.1	Ca-Cl	7.79	6.452E+00	2.916E-01	2.304E-06	1.058E-03
SD-9--135.1	Ca-Cl	7.86	6.462E+00	3.358E-01	3.004E-06	1.174E-03
SD-12--296.1	Ca-Cl	7.68	5.820E+00	9.988E-01	3.732E-06	8.158E-04
UZ-14--1,277	Ca-Cl	7.76	6.370E+00	4.200E-01	2.970E-06	7.080E-04
UZ-16--1643.4	Ca-Cl	7.77	6.376E+00	4.289E-01	5.049E-06	1.972E-03
NRG-6--244.6	Neutral	9.05	5.110E+00	2.385E+00	3.205E-05	1.391E-01
NRG-6--255.9	Neutral	7.63	5.569E+00	9.691E-01	3.608E-08	1.993E-01
SD-6--412.2	Neutral	8.91	4.186E+00	3.966E+00	4.675E-05	1.616E-01
SD-6--443.5	Neutral	8.94	4.008E+00	4.167E+00	4.370E-05	1.551E-01
SD-6--507.5	Neutral	8.75	4.593E+00	3.325E+00	5.768E-05	1.591E-01
SD-6--1509.9	Neutral	11.17	5.551E+00	8.115E-02	9.883E-01	7.179E-02
SD-7--370.3	Neutral	8.47	6.704E+00	1.731E-02	1.352E-06	6.408E-04
SD-9--176.2	Neutral	9.27	5.450E+00	1.413E+00	2.095E-04	4.287E-01
UZ-14--85.2	Neutral	8.08	5.809E+00	1.469E+00	6.244E-06	4.888E-03
UZ-14--147.7	Neutral	8.79	5.567E+00	1.703E+00	4.447E-05	1.373E-01
UZ-14--178.1	Neutral	7.91	6.189E+00	7.668E-01	2.325E-06	1.260E-03
NRG-6--219.9	Alkaline	9.44	5.181E+00	1.808E+00	1.837E-04	4.323E-01
NRG-7a--460.25	Alkaline	11.73	2.565E+00	2.095E-01	3.348E+00	9.936E-02
SD-6--522.5	Alkaline	10.37	4.220E+00	3.165E+00	1.928E-02	4.511E-01
SD-12--1495.5	Alkaline	11.40	4.358E+00	3.541E-01	1.609E+00	2.201E-01
UZ-14--1,542	Alkaline	11.22	3.940E+00	4.500E-01	2.024E+00	2.010E-01
UZ-14--1258.5	Alkaline	8.86	5.563E+00	1.709E+00	3.998E-05	1.373E-01
UZ-14--1409.4	Alkaline	9.54	5.447E+00	1.414E+00	1.658E-04	4.289E-01
UZ-14--1825.8	Alkaline	11.35	3.517E+00	1.010E+00	2.044E+00	1.476E-01
UZ-14--2014.7	Alkaline	11.07	4.223E+00	1.354E-01	2.013E+00	1.982E-01
UZ-16--1343.7	Alkaline	11.42	3.751E+00	6.887E-01	1.955E+00	2.078E-01
WT-24--1937.0	Alkaline	11.48	4.160E+00	3.322E-02	2.087E+00	4.552E-02

Temperature = 25 °C (P = 0.031385 atm)						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	8.22	5.220E-03	5.160E-04	3.348E-04	1.310E-03
NRG-6--160.8	Ca-Cl	8.25	4.176E-03	5.647E-04	3.525E-04	1.168E-03
NRG-6--171.0	Ca-Cl	8.37	1.640E-03	6.951E-04	4.479E-04	8.509E-04
NRG-6--175.6	Ca-Cl	8.42	1.328E-03	6.944E-04	4.954E-04	5.920E-04
SD-6--471.3	Ca-Cl	8.39	1.888E-03	1.088E-03	4.769E-04	6.245E-04
SD-9--94.2	Ca-Cl	7.18	4.795E-03	1.774E-04	3.055E-05	2.160E-03
SD-9--114.1	Ca-Cl	8.29	3.896E-03	1.759E-04	3.849E-04	1.571E-03
SD-9--135.1	Ca-Cl	8.30	4.067E-03	1.938E-04	3.998E-04	1.423E-03
SD-12--296.1	Ca-Cl	8.45	1.722E-03	2.953E-04	5.299E-04	1.999E-04
UZ-14--1,277	Ca-Cl	8.34	3.675E-03	2.424E-04	4.207E-04	3.378E-04
UZ-16--1643.4	Ca-Cl	8.53	2.041E-03	1.333E-04	6.402E-04	2.796E-04
NRG-6--244.6	Neutral	8.48	1.383E-03	6.453E-04	5.868E-04	1.098E-03
NRG-6--255.9	Neutral	7.17	3.244E-03	5.645E-04	3.079E-05	7.191E-03
SD-6--412.2	Neutral	8.52	1.335E-03	1.265E-03	6.402E-04	5.137E-04
SD-6--443.5	Neutral	8.46	1.337E-03	1.390E-03	5.567E-04	9.290E-04
SD-6--507.5	Neutral	8.35	5.813E-04	4.208E-04	4.419E-04	2.745E-03
SD-6--1509.9	Neutral	8.74	2.842E-03	2.963E-05	1.084E-03	2.894E-04
SD-7--370.3	Neutral	7.37	3.751E-03	9.676E-06	3.212E-05	4.732E-03
SD-9--176.2	Neutral	8.67	1.820E-03	3.090E-05	9.276E-04	1.255E-03
UZ-14--85.2	Neutral	8.52	1.703E-03	3.571E-04	6.259E-04	6.401E-04
UZ-14--147.7	Neutral	8.54	1.710E-03	3.585E-04	6.699E-04	6.485E-04
UZ-14--178.1	Neutral	8.34	2.737E-03	3.388E-04	4.299E-04	1.073E-03
NRG-6--219.9	Alkaline	8.61	2.175E-03	7.590E-04	7.948E-04	7.642E-04
NRG-7a--460.25	Alkaline	8.95	1.975E-04	1.614E-05	1.652E-03	4.115E-05
SD-6--522.5	Alkaline	8.71	7.455E-04	5.591E-04	9.722E-04	5.664E-04
SD-12--1495.5	Alkaline	8.91	1.620E-03	1.316E-04	1.621E-03	5.695E-04
UZ-14--1,542	Alkaline	9.41	5.902E-04	6.750E-05	6.025E-03	3.046E-04
UZ-14--1258.5	Alkaline	8.59	2.494E-03	2.593E-04	7.440E-04	1.879E-04
UZ-14--1409.4	Alkaline	8.52	2.117E-03	8.070E-05	6.464E-04	1.027E-03
UZ-14--1825.8	Alkaline	9.28	6.733E-04	1.933E-04	4.088E-03	1.362E-04
UZ-14--2014.7	Alkaline	9.63	9.667E-04	3.099E-05	1.243E-02	2.467E-04
UZ-16--1343.7	Alkaline	8.98	1.593E-03	2.926E-04	1.889E-03	2.392E-04
WT-24--1937.0	Alkaline	8.87	1.012E-03	8.083E-06	1.403E-03	6.154E-05

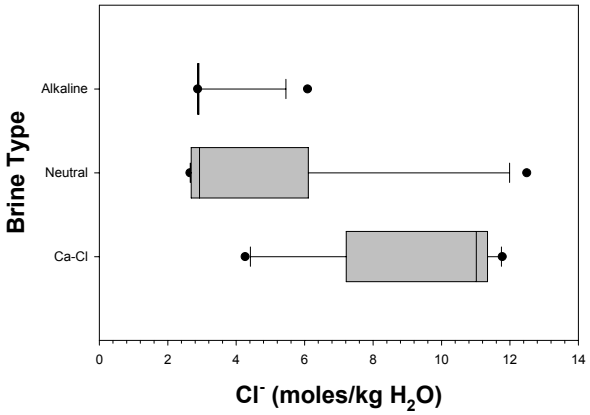
June 10, 2009

The following figures compare the calculated pH of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

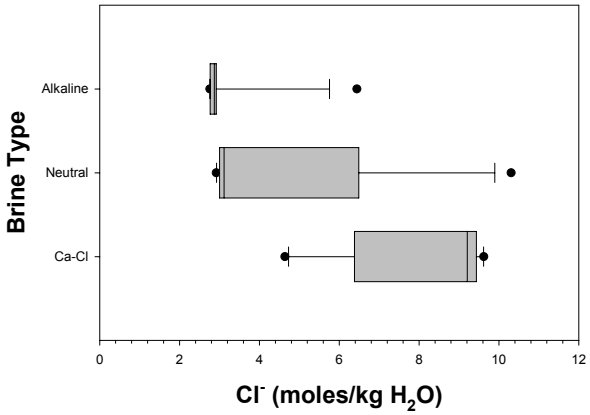


The following figures compare the calculated chloride concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

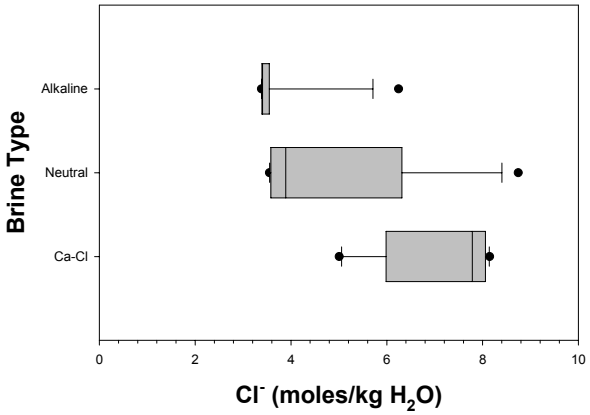
Chloride Conc. (at T=110 °C) of Evaporated YM Waters



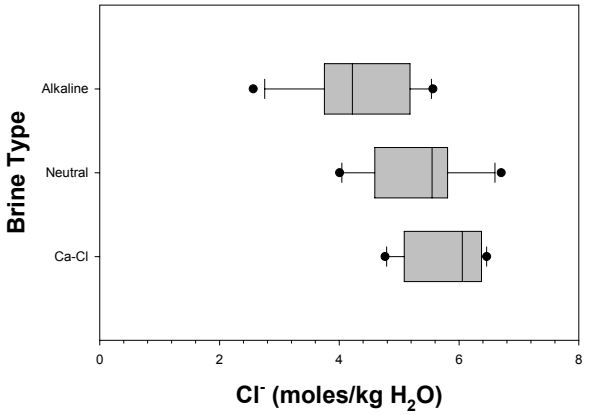
Chloride Conc. (at T=90 °C) of Evaporated YM Waters



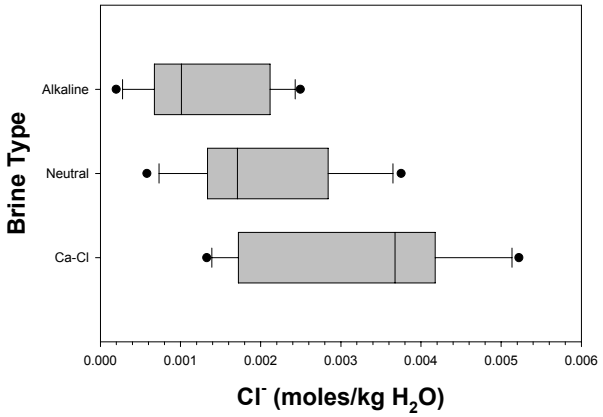
Chloride Conc. (at T=70 °C) of Evaporated YM Waters



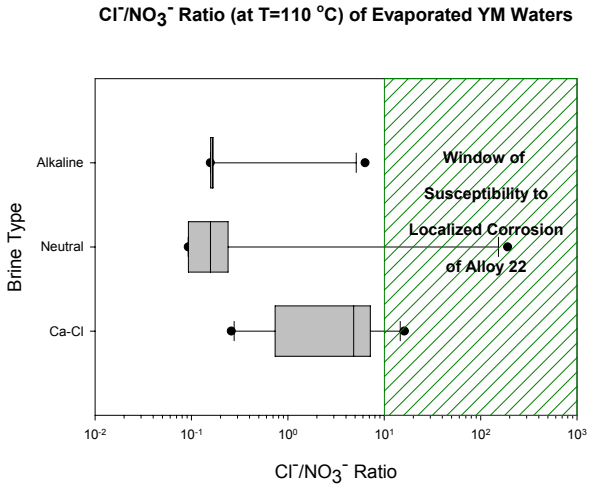
Chloride Conc. (at T=50 °C) of Evaporated YM Waters

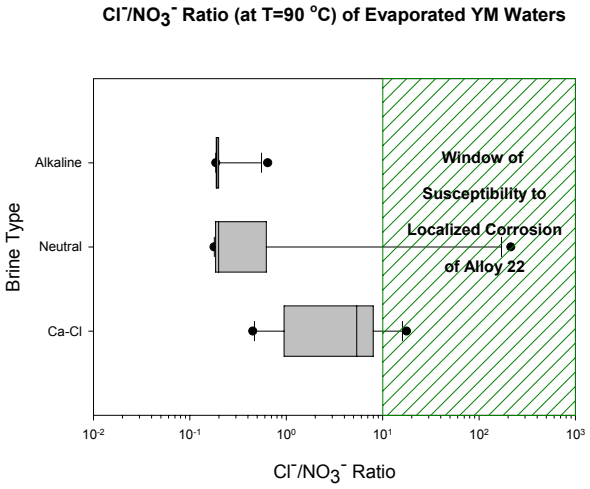


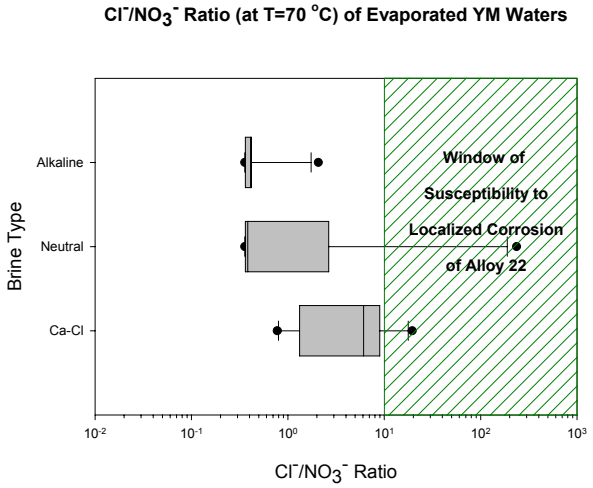
Chloride Conc. (at T=25 °C) of Evaporated YM Waters

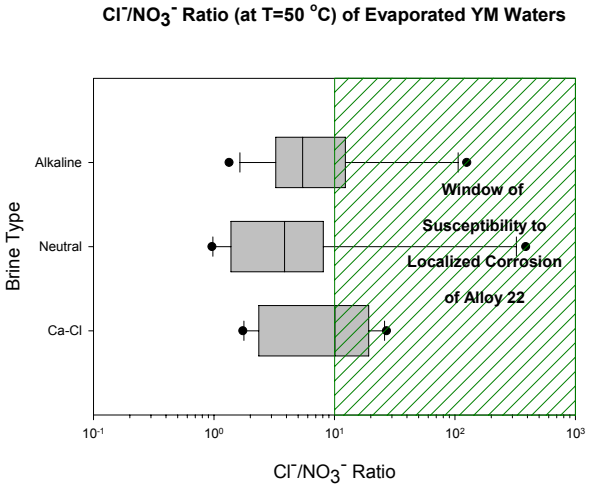


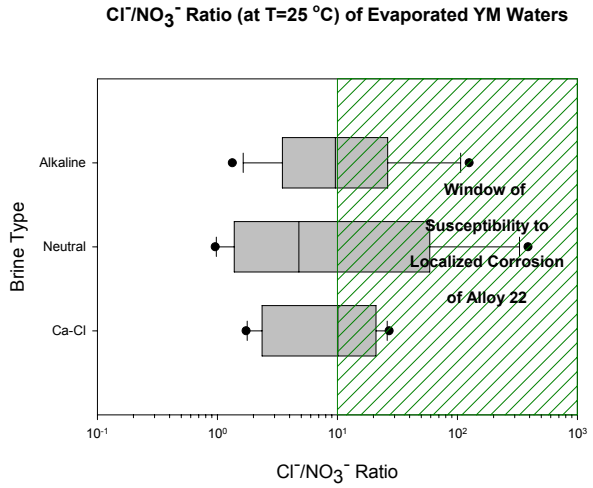
The following figures compare the calculated chloride to nitrate ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).



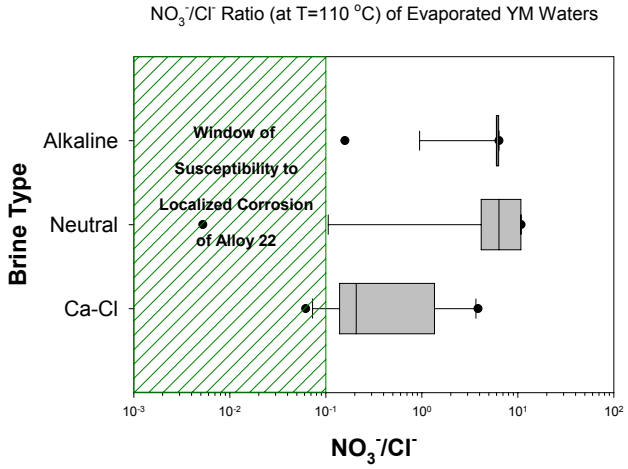


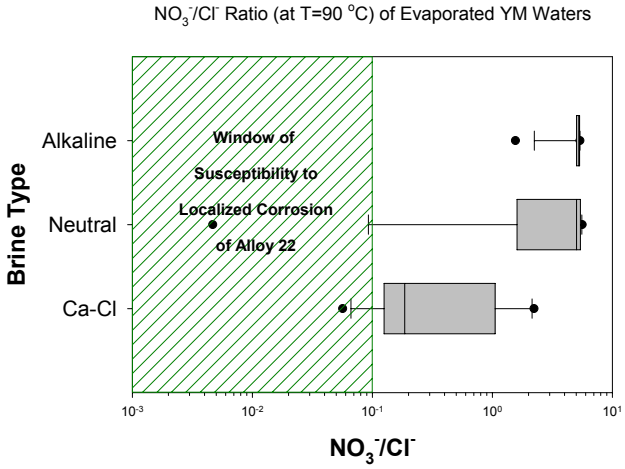


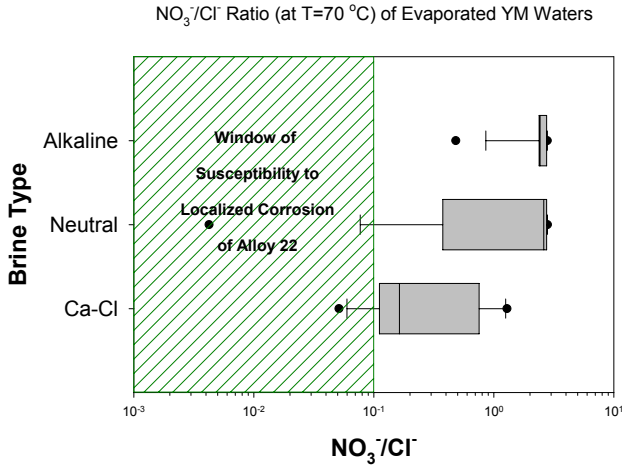


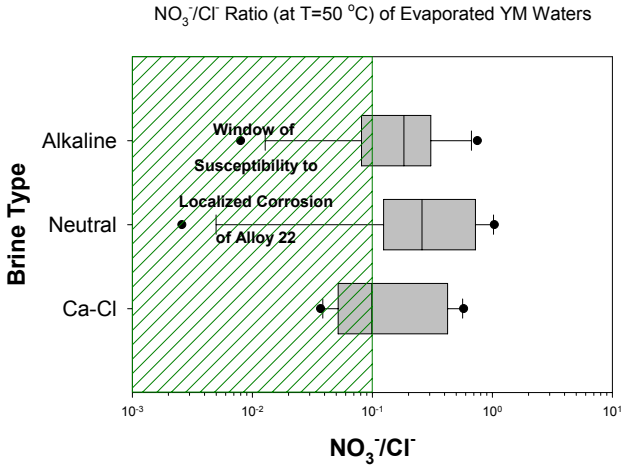


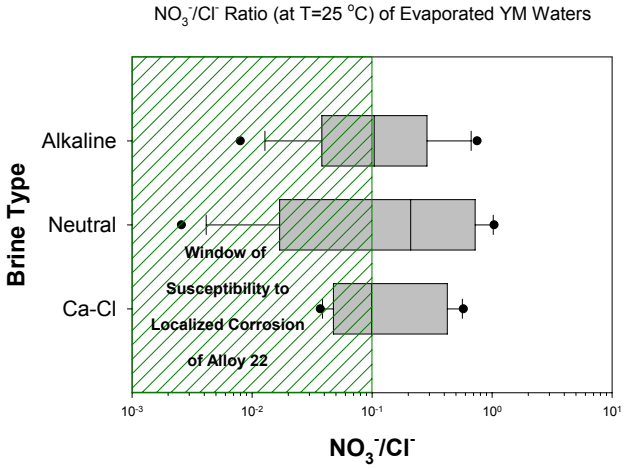
The following figures compare the calculated nitrate to chloride ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).



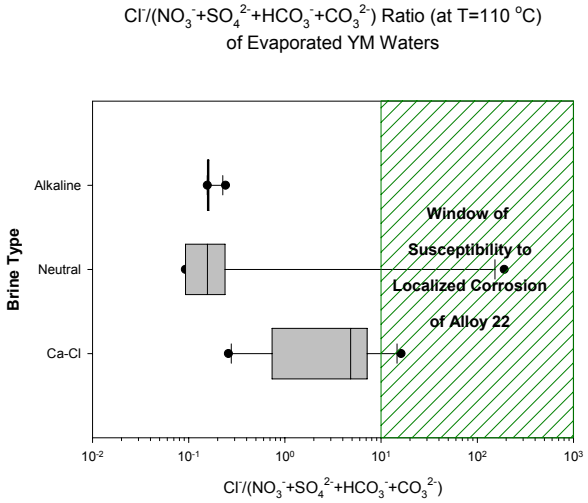


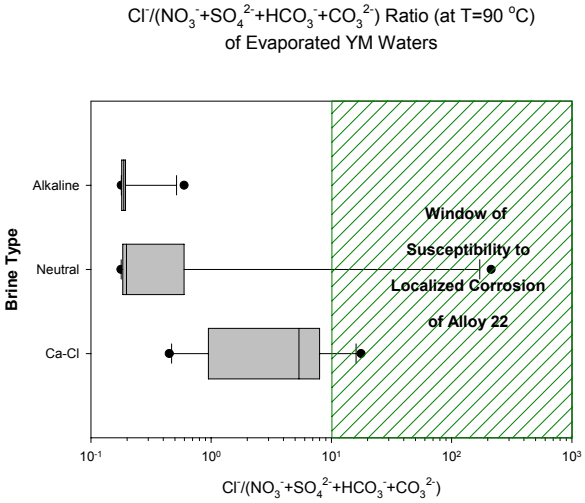


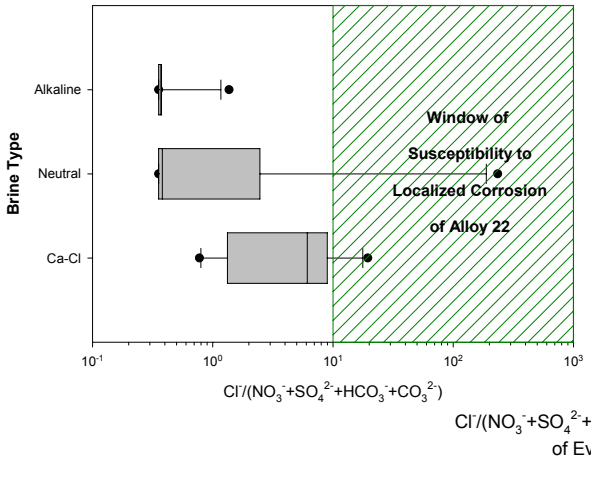


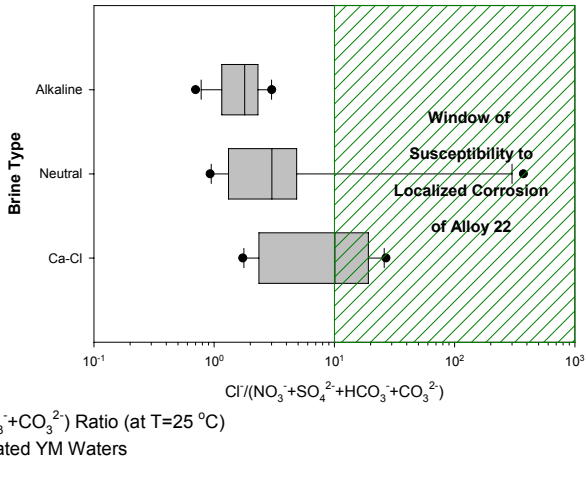


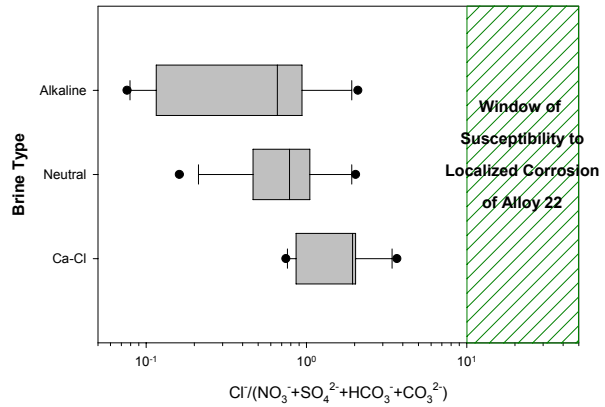
The following figures compare the calculated chloride to corrosion-inhibiting oxyanion ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).



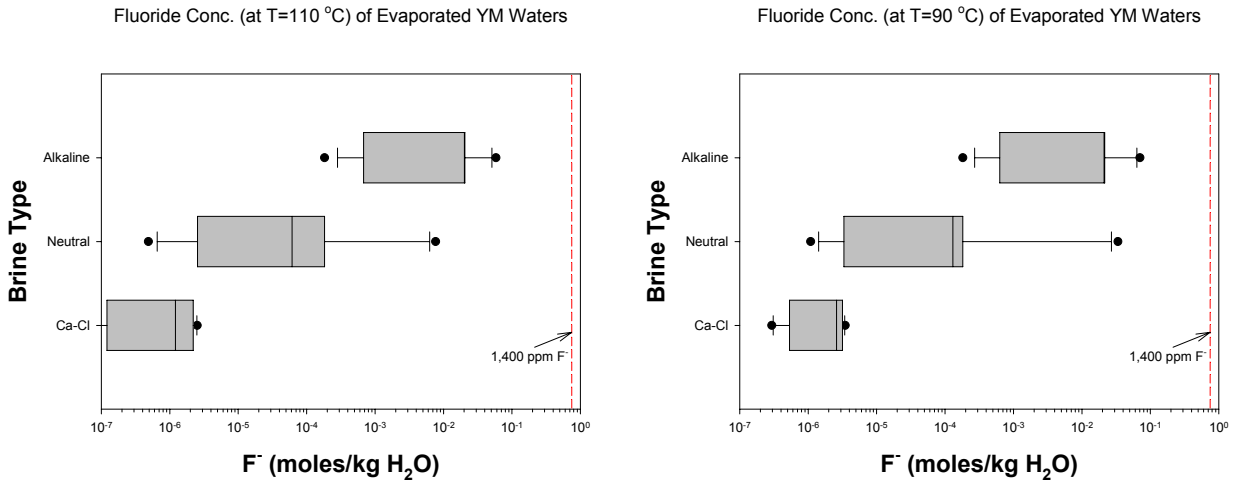


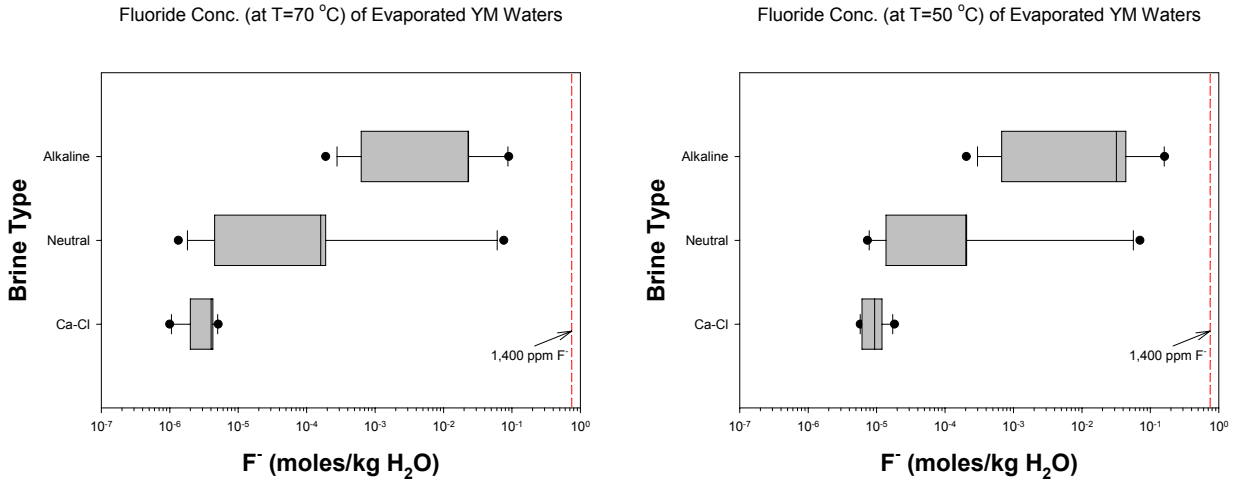


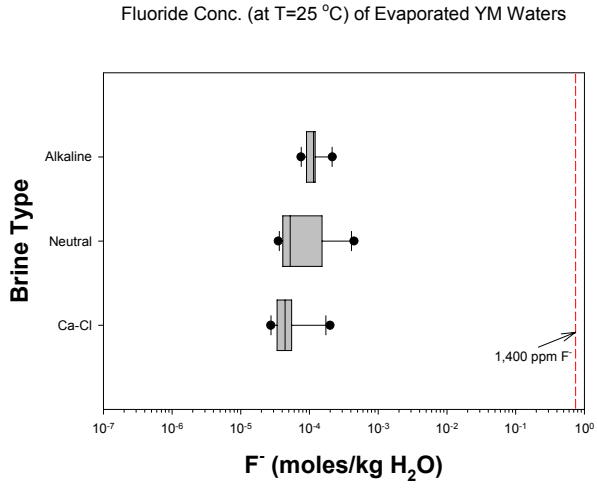




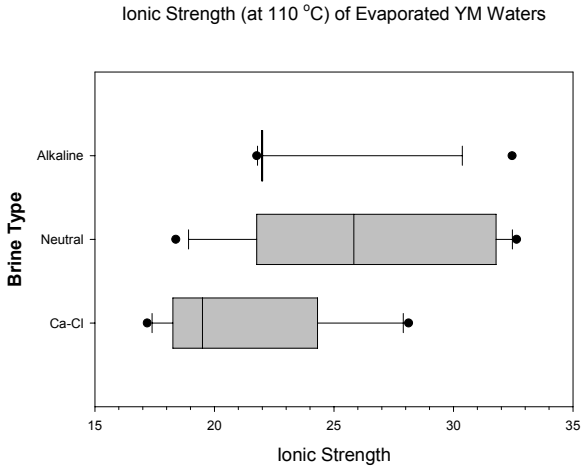
The following figures compare the calculated fluoride concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH). The 1,400 ppm F^- value is the maximum value in DOE titanium corrosion tests reported in the SER.

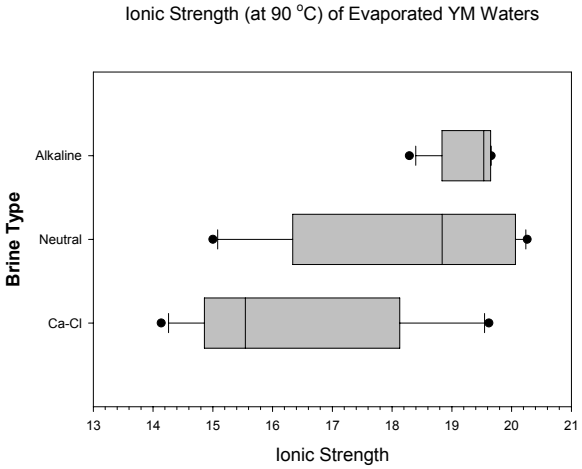


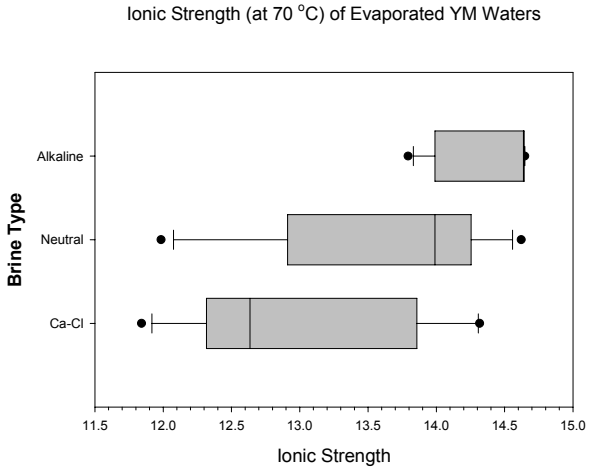


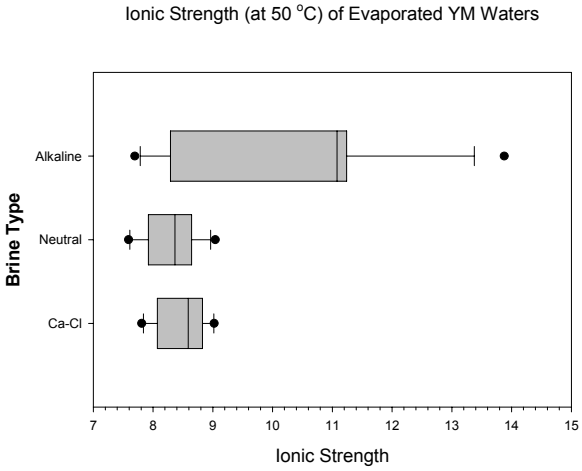


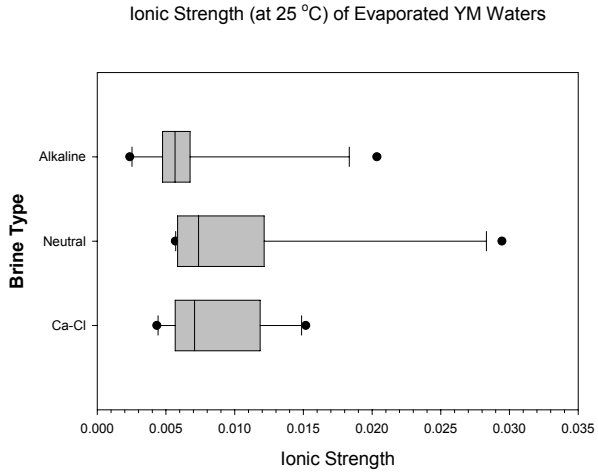
The following figures compare the calculated ionic strength of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).



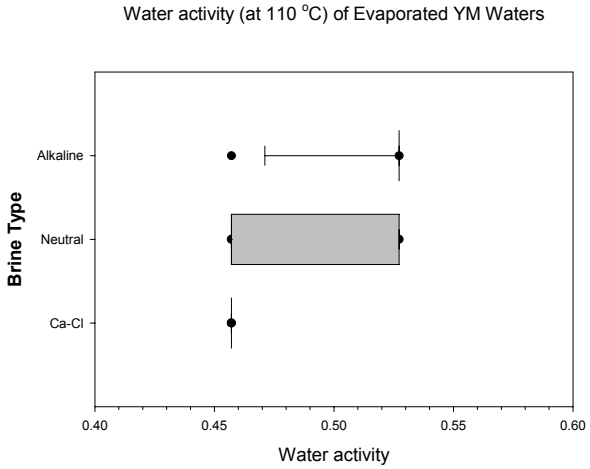


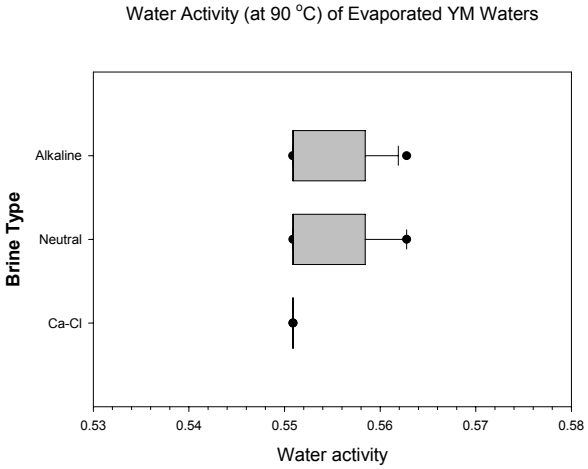


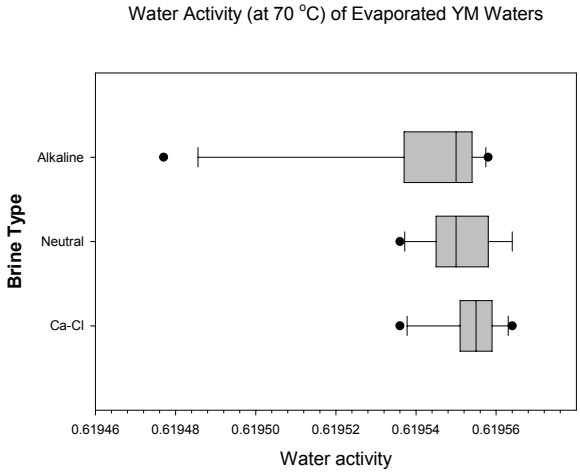


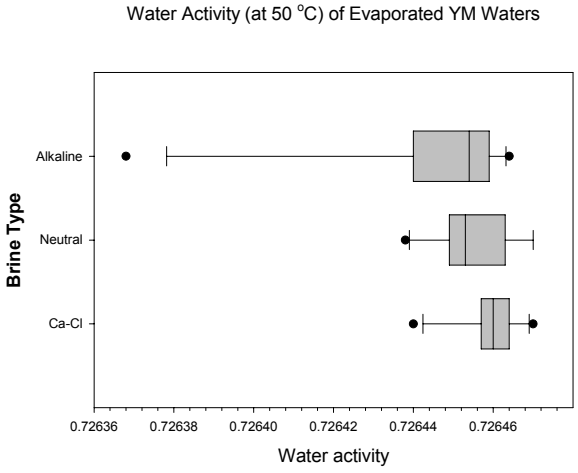


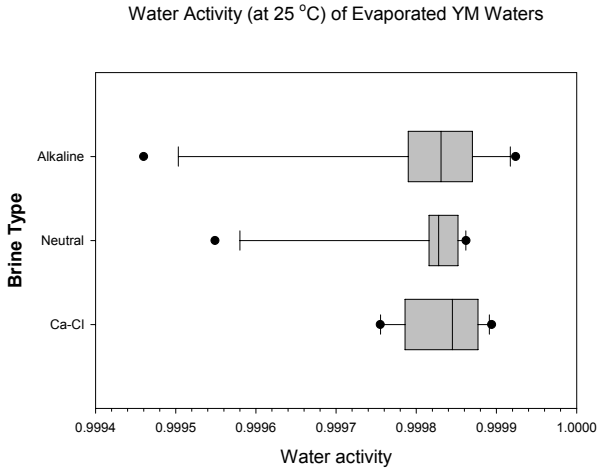
The following figures compare the calculated water activity of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).





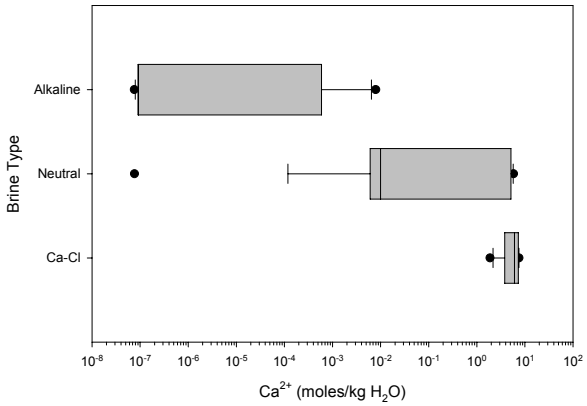




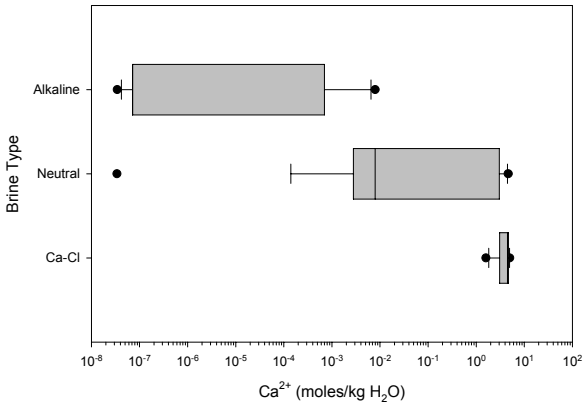


The following figures compare the calculated calcium concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

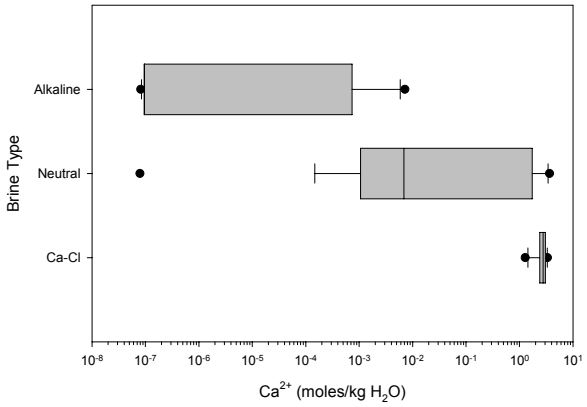
Calcium Conc. (at T=110 °C) of Evaporated YM Waters



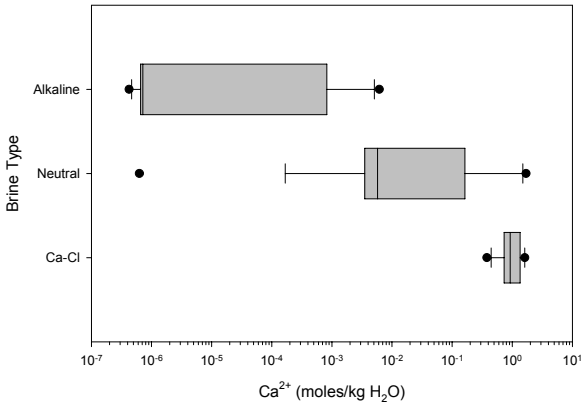
Calcium Conc. (at T=90 °C) of Evaporated YM Waters



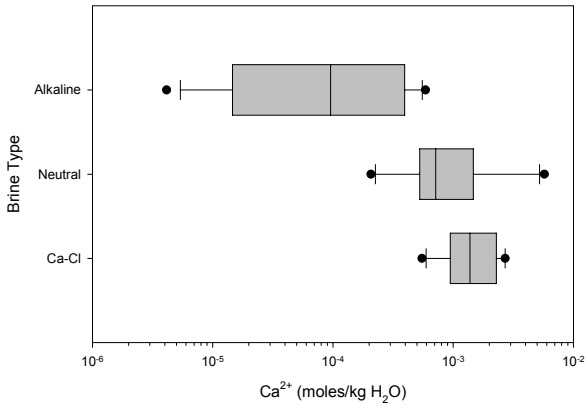
Calcium Conc. (at T=70 °C) of Evaporated YM Waters



Calcium Conc. (at T=50 °C) of Evaporated YM Waters

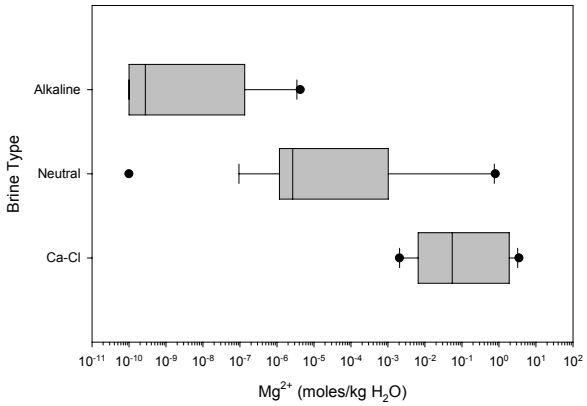


Calcium Conc. (at T=25 °C) of Evaporated YM Waters

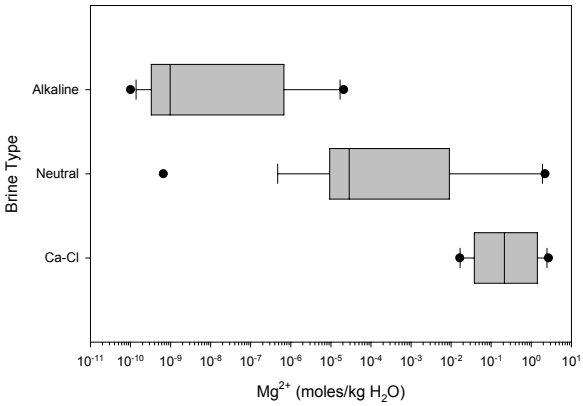


The following figures compare the calculated magnesium concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

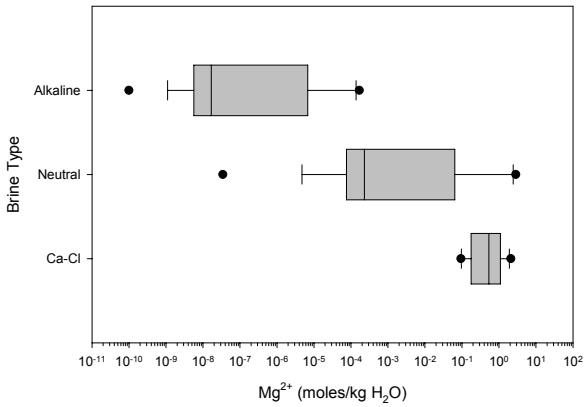
Magnesium Conc. (at T=110 °C) of Evaporated YM Waters



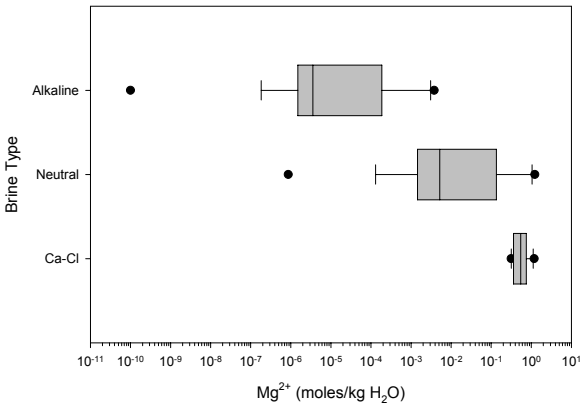
Magnesium Conc. (at T=90 °C) of Evaporated YM Waters



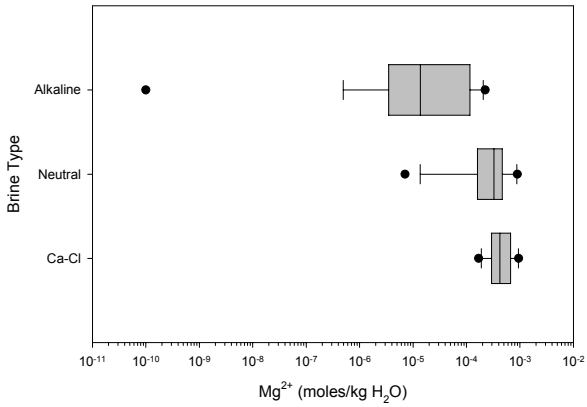
Magnesium Conc. (at T=70 °C) of Evaporated YM Waters



Magnesium Conc. (at T=50 °C) of Evaporated YM Waters

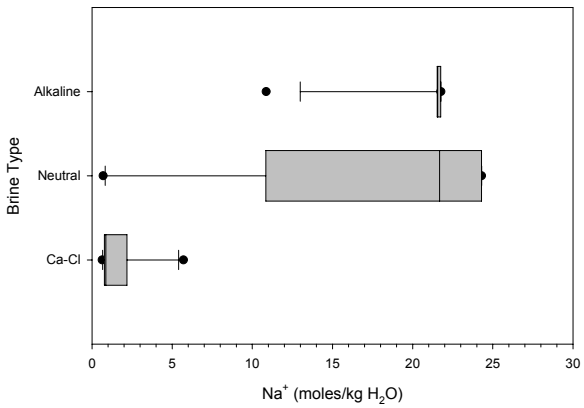


Magnesium Conc. (at T=25 °C) of Evaporated YM Waters

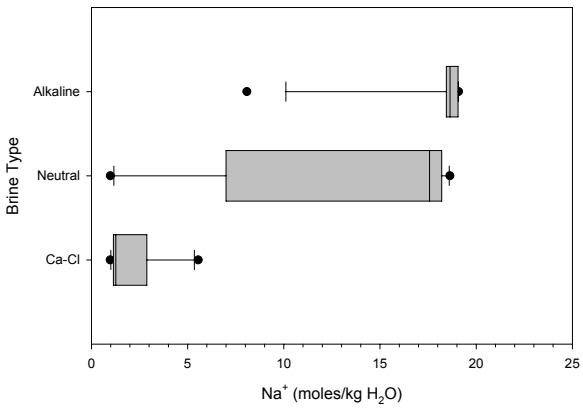


The following figures compare the calculated sodium concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

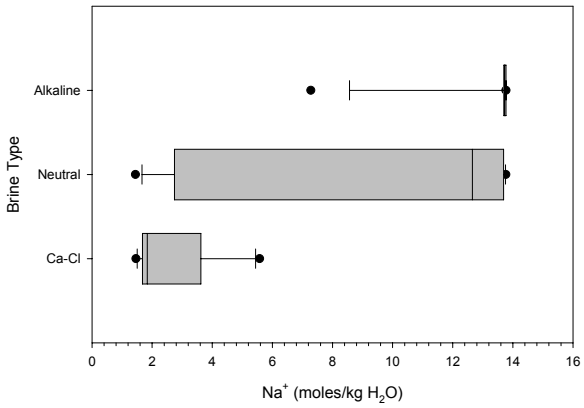
Sodium Conc. (at T=110 °C) of Evaporated YM Waters



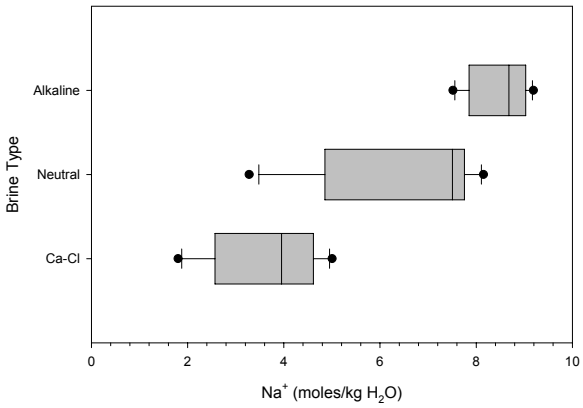
Sodium Conc. (at T=90 °C) of Evaporated YM Waters



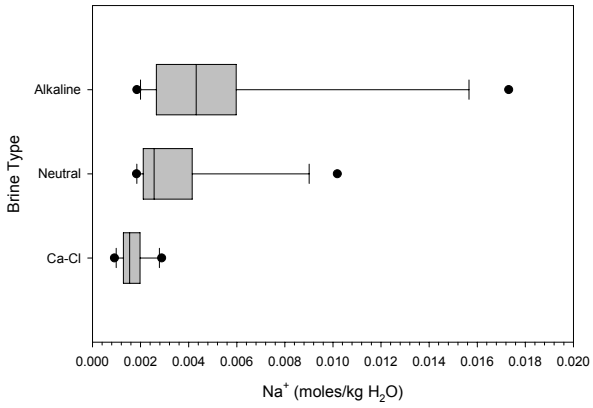
Sodium Conc. (at T=70 °C) of Evaporated YM Waters



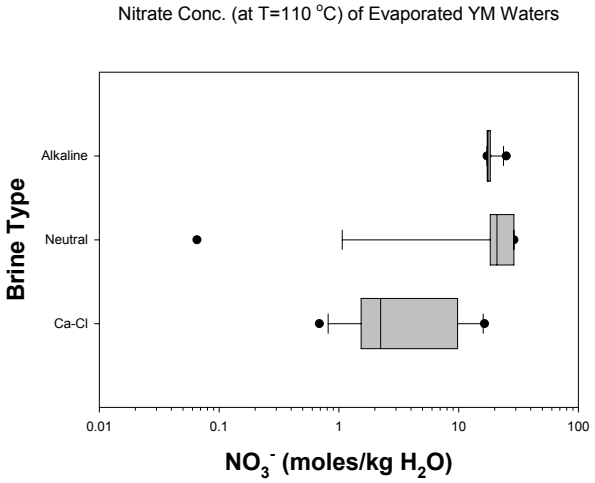
Sodium Conc. (at T=50 °C) of Evaporated YM Waters

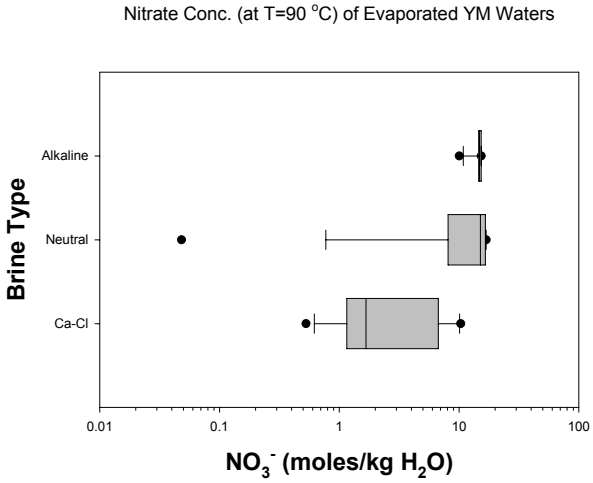


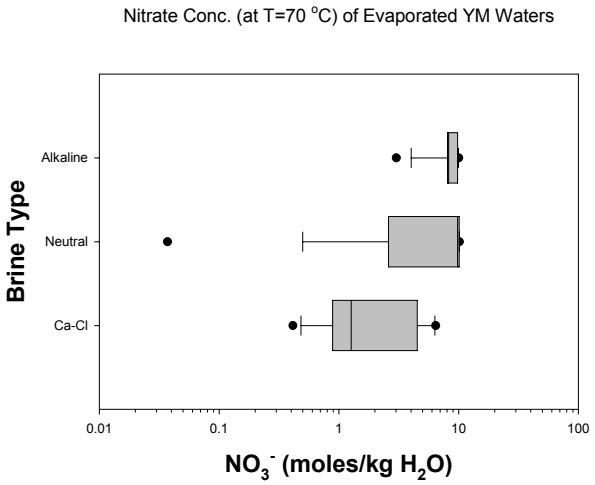
Sodium Conc. (at T=25 °C) of Evaporated YM Waters

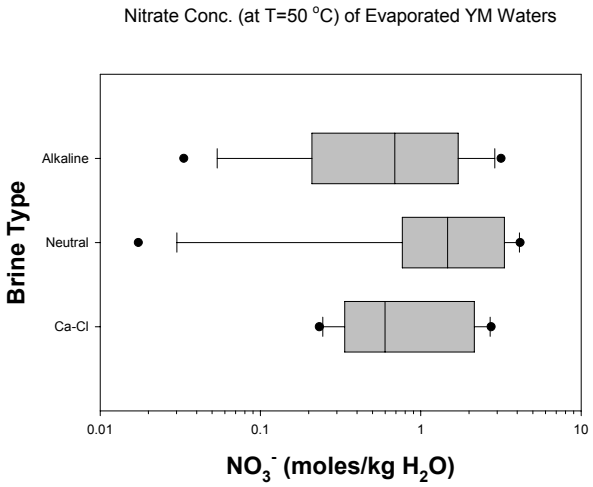


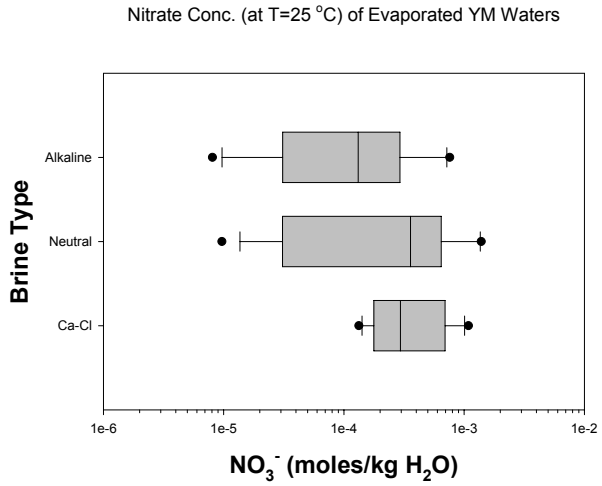
The following figures compare the calculated nitrate concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).





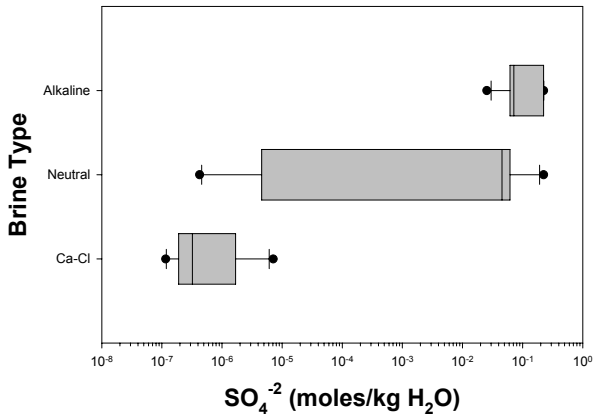




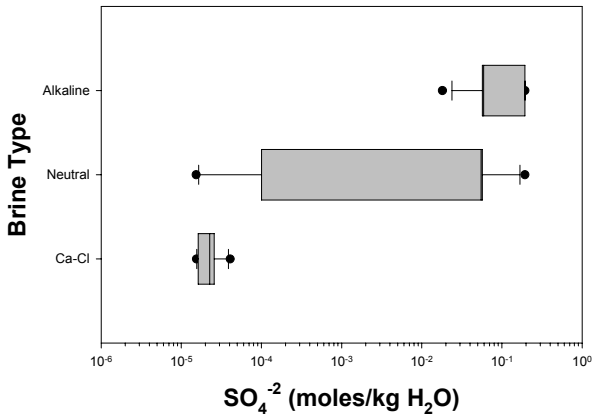


The following figures compare the calculated sulfate concentration of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50 °C (total pressure corresponding to median RH), and at 25 °C (total pressure corresponding to 100% RH).

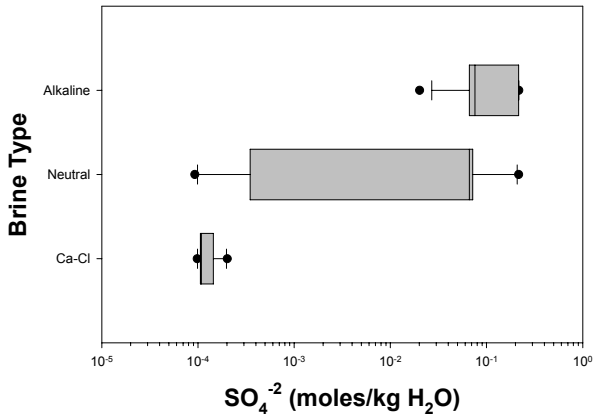
SO_4^{-2} Conc. (at T=110 °C) of Evap. YM Waters



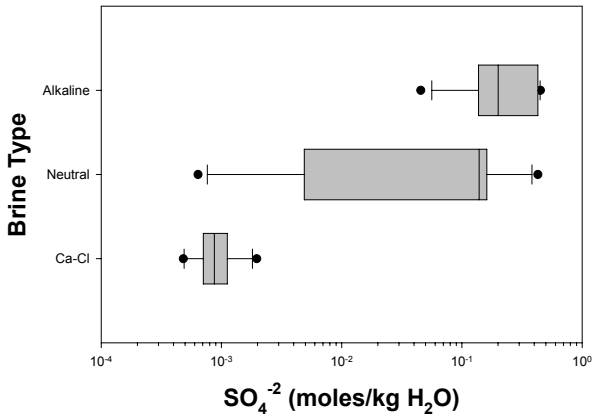
SO_4^{-2} Conc. (at T=90 °C) of Evap. YM Waters



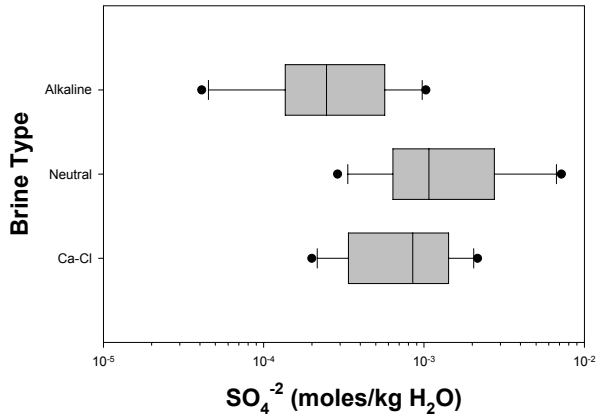
SO_4^{-2} Conc. (at T=70 °C) of Evap. YM Waters



SO_4^{-2} Conc. (at T=50 °C) of Evap. YM Waters



SO_4^{-2} Conc. (at T=25 °C) of Evap. YM Waters



June 15, 2009

O. Pensado requested additional OLIAnalyzer calculations be done at the following temperature and median RH values:

T[°C]	Median RH
25	0.975774
30	0.912202
40	0.807974

The corresponding vapor pressure of pure water (pH2O°) and total pressure are as follows:

T[°C]	Median RH	$pH_2O°$	Total P (atm)
25	0.975774	0.031385	0.030625
30	0.912202	0.042033	0.038343
40	0.807974	0.073037	0.059012

The OLIAnalyzer files that have the input and output information are included in a CD that accompanies this notebook. The TPA 5.1 localized corrosion abstraction uses concentration units of molarity (moles per liter of solution). To be consistent with the TPA abstraction, O. Pensado requested that values of chloride, nitrate, total carbonate, and sulfate of the brines formed by evaporation of initially dilute pore waters be given in molar unit [as opposed to the molal units (moles per kg H2O) for the values given on pages 208 through 212 of this notebook). Thus, the Excel files summarizing the evaporation results at 25, 30, and 40 °C have concentration units of molarity. The filenames of the OLIAnalyzer files and the Excel files that summarize the results are:

1. OLIAnalyzer Evaporation of YM Waters temp=25 C P=0.030625 atm Median RH.oad
2. OLIAnalyzer Evaporation of YM Waters temp=30 C P=0.038343 atm Median RH.oad
3. OLIAnalyzer Evaporation of YM Waters temp=40 C P=0.059012 atm Median RH.oad
4. YM Pore Waters Evaporation Results Temp=25 C P=0.030625 atm Median RH molar unit.xls
5. YM Pore Waters Evaporation Results Temp=30 C P=0.038343 atm Median RH molar unit.xls
6. YM Pore Waters Evaporation Results Temp=40 C P=0.059012 atm Median RH molar unit.xls

The summary of results for temperatures of 25, 50, 70, 90, and 110 °C were recast into molar units and were saved with the following filenames:

1. YM Pore Waters Evaporation Results Temp=110C_P=0.640858 atm Median RH molar unit.xls
2. YM Pore Waters Evaporation Results Temp=90C_P=0.379763 atm Median RH molar unit.xls
3. YM Pore Waters Evaporation Results Temp=70C_P=0.190346 atm Median RH molar unit.xls
4. YM Pore Waters Evaporation Results Temp=50C_P=0.088481 atm Median RH molar unit.xls
5. YM Pore Waters Evaporation Results Temp=25C_P=0.031385 atm Median RH molar unit.xls

The tables in the next several pages provide the pH and species molar concentrations calculated using OLIAnalyzer at temperatures of 110, 90, 70, 50, 40, 30, and 25 °C and total P corresponding to the median relative humidity at the waste package surface (from TPA calculation).

Temperature = 110 °C (P = 0.640858 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2	Ca-Cl	5.58	8.755	1.220E+00	1.647E-08	1.342E-06
NRG-6/160.8	Ca-Cl	5.60	8.475	1.757E+00	3.131E-08	9.549E-07
NRG-6/171.0	Ca-Cl	6.58	5.003	6.789E+00	6.856E-06	8.042E-08
NRG-6/175.6	Ca-Cl	6.75	3.227	9.255E+00	6.021E-06	8.330E-08
SD-6/471.3	Ca-Cl	6.74	2.631	1.016E+01	6.337E-06	1.174E-07
SD-9/94.2	Ca-Cl	5.47	9.121	5.643E-01	2.139E-10	5.821E-06
SD-9/114.1	Ca-Cl	5.56	9.117	1.055E+00	1.719E-08	1.743E-06
SD-9/135.1	Ca-Cl	5.85	9.179	1.463E+00	4.370E-07	3.930E-07
SD-12/296.1	Ca-Cl	6.38	7.949	2.775E+00	5.974E-06	1.761E-07
UZ-14/1,277	Ca-Cl	6.50	8.931	1.266E+00	3.690E-06	2.465E-07
UZ-16/1643.4	Ca-Cl	6.28	8.544	2.018E+00	6.452E-06	2.185E-07
NRG-6/244.6 - 0.74 atm	Neutral	8.47	1.678	1.068E+01	1.095E-05	3.541E-02
NRG-6/255.9	Neutral	5.73	2.579	1.249E+01	5.140E-10	1.837E-02
SD-6/412.2	Neutral	8.37	1.188	1.281E+01	9.303E-06	2.007E-02
SD-6/443.5	Neutral	8.40	1.188	1.281E+01	7.124E-07	2.007E-02
SD-6/507.5	Neutral	8.22	1.188	1.281E+01	1.269E-05	2.007E-02
SD-6/1509.9	Neutral	10.99	2.568	2.604E-03	6.486E-02	1.000E-10
SD-7/370.3	Neutral	7.21	9.683	5.072E-02	6.125E-07	3.306E-07
SD-9/176.2 - 0.74 atm	Neutral	8.79	1.664	1.053E+01	8.681E-05	1.280E-01
UZ-14/85.2	Neutral	6.88	1.423	1.231E+01	3.072E-06	2.460E-06
UZ-14/147.7 - 0.74 atm	Neutral	8.22	1.679	1.068E+01	1.449E-05	3.540E-02
UZ-14/178.1	Neutral	5.68	7.631	3.888E+00	9.776E-08	4.508E-07
NRG-6/219.9 - 0.74 atm	Alkaline	8.94	1.664	1.053E+01	7.078E-05	1.281E-01
NRG-7a/460.25	Alkaline	11.17	2.578	1.058E+01	7.134E-02	2.020E-02
SD-6/522.5 - 0.74 atm	Alkaline	9.73	1.665	1.051E+01	3.358E-03	1.286E-01
SD-12/1495.5 - 0,74 atm	Alkaline	10.75	1.680	1.010E+01	2.318E-01	4.207E-02
UZ-14/1,542 - 0.74 atm	Alkaline	10.50	1.682	1.020E+01	2.315E-01	4.153E-02
UZ-14/1258.5 - 0.74 atm	Alkaline	8.29	1.679	1.068E+01	1.505E-05	3.540E-02
UZ-14/1409.4 - 0.74 atm	Alkaline	9.06	1.664	1.052E+01	6.239E-05	1.281E-01
UZ-14/1825.8 - 0.74 atm	Alkaline	10.61	1.681	1.016E+01	2.311E-01	4.172E-02
UZ-14/2014.7 - 0,74 atm	Alkaline	10.36	1.685	1.025E+01	2.333E-01	4.138E-02
UZ-16/1343.7 - 0.74 atm	Alkaline	10.71	1.680	1.013E+01	2.315E-01	4.194E-02
WT-24/1937.0 - 0.74 atm	Alkaline	10.78	1.691	1.011E+01	2.348E-01	1.489E-02

Temperature = 90 °C (P = 0.379763 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	6.19	7.761	9.722E-01	6.523E-08	2.036E-05
NRG-6--160.8	Ca-Cl	6.23	7.514	1.396E+00	1.080E-07	1.893E-05
NRG-6--171.0	Ca-Cl	6.86	4.906	5.166E+00	4.305E-06	1.417E-05
NRG-6--175.6	Ca-Cl	7.00	3.730	6.815E+00	3.654E-06	1.837E-05
SD-6--471.3	Ca-Cl	6.98	3.329	7.415E+00	3.928E-06	2.224E-05
SD-9--94.2	Ca-Cl	6.08	8.002	4.523E-01	9.335E-10	3.489E-05
SD-9--114.1	Ca-Cl	6.18	7.998	8.391E-01	7.420E-08	2.184E-05
SD-9--135.1	Ca-Cl	6.45	8.023	1.157E+00	8.702E-07	1.433E-05
SD-12--296.1	Ca-Cl	6.67	7.109	2.198E+00	4.191E-06	1.296E-05
UZ-14--1,277	Ca-Cl	6.79	7.944	1.008E+00	2.928E-06	1.280E-05
UZ-16--1643.4	Ca-Cl	6.57	7.592	1.602E+00	4.373E-06	1.339E-05
NRG-6--244.6 - 0.388 atm	Neutral	8.61	1.861	9.365E+00	1.174E-05	3.536E-02
NRG-6--255.9	Neutral	6.12	3.707	6.179E+00	4.664E-10	4.851E-02
SD-6--412.2	Neutral	8.45	1.808	9.862E+00	1.514E-05	3.220E-02
SD-6--443.5	Neutral	8.48	1.760	9.867E+00	1.428E-05	3.236E-02
SD-6--507.5	Neutral	8.31	1.823	9.858E+00	2.024E-05	3.219E-02
SD-6--1509.9	Neutral	11.13	3.899	6.270E+00	4.147E-01	2.744E-02
SD-7--370.3	Neutral	7.50	8.608	4.031E-02	5.589E-07	1.283E-05
SD-9--176.2 - 0.385 atm	Neutral	8.91	1.792	9.412E+00	8.457E-05	1.187E-01
UZ-14--85.2	Neutral	7.09	2.275	9.067E+00	2.788E-06	6.617E-05
UZ-14--147.7 - 0.388 atm	Neutral	8.37	1.862	9.365E+00	1.839E-05	3.535E-02
UZ-14--178.1	Neutral	6.35	6.761	3.005E+00	2.577E-07	1.704E-05
NRG-6--219.9 - 0.385 atm	Alkaline	9.03	1.792	9.411E+00	7.168E-05	1.187E-01
NRG-7a--460.25	Alkaline	11.31	3.902	6.082E+00	4.307E-01	2.833E-02
SD-6--522.5 - 0.385 atm	Alkaline	9.88	1.793	9.390E+00	3.645E-03	1.192E-01
SD-12--1495.5	Alkaline	10.98	1.704	9.064E+00	3.290E-01	3.659E-02
UZ-14--1,542	Alkaline	10.74	1.707	9.172E+00	3.274E-01	3.599E-02
UZ-14--1258.5 - 0.388 atm	Alkaline	8.44	1.861	9.365E+00	1.612E-05	3.535E-02
UZ-14--1409.4 - 0.385 atm	Alkaline	9.18	1.792	9.410E+00	6.029E-05	1.187E-01
UZ-14--1825.8	Alkaline	10.85	1.706	9.130E+00	3.274E-01	3.620E-02
UZ-14--2014.7 - 0.385 atm	Alkaline	10.59	1.801	8.875E+00	3.534E-01	3.742E-02
UZ-16--1343.7	Alkaline	10.94	1.705	9.087E+00	3.283E-01	3.645E-02
WT-24--1937.0	Alkaline	11.01	1.717	9.052E+00	3.342E-01	1.121E-02

Temperature = 70 °C (P = 0.190346 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	6.85	6.883	7.684E-01	2.514E-07	2.177E-07
NRG-6--160.8	Ca-Cl	6.89	6.687	1.093E+00	3.745E-07	3.224E-07
NRG-6--171.0	Ca-Cl	7.19	4.862	3.671E+00	3.174E-06	2.578E-06
NRG-6--175.6	Ca-Cl	7.31	4.140	4.676E+00	2.949E-06	2.323E-06
SD-12--296.1	Ca-Cl	7.03	6.343	1.672E+00	3.238E-06	2.360E-06
SD-6--471.3	Ca-Cl	7.28	3.899	5.018E+00	6.662E-09	2.521E-06
SD-9--114.1	Ca-Cl	6.84	7.052	6.622E-01	3.137E-07	2.729E-07
SD-9--135.1	Ca-Cl	7.00	6.937	8.896E-01	1.403E-06	1.209E-06
SD-9--94.2	Ca-Cl	6.73	7.067	3.623E-01	2.776E-06	5.843E-09
UZ-14--1,277	Ca-Cl	7.14	7.007	7.901E-01	2.221E-06	1.910E-06
UZ-16--1643.4	Ca-Cl	6.95	6.686	1.227E+00	2.595E-06	2.229E-06
NRG-6--244.6	Neutral	8.80	2.479	6.931E+00	2.094E-05	1.450E-05
NRG-6--255.9	Neutral	6.70	5.336	2.008E+00	3.038E-09	2.597E-09
SD-6--1509.9	Neutral	11.28	4.579	2.372E+00	2.980E-05	1.068E+00
SD-6--412.2	Neutral	8.63	2.622	6.901E+00	2.759E-05	2.028E-05
SD-6--443.5	Neutral	8.65	2.555	6.923E+00	3.934E-05	1.892E-05
SD-6--507.5	Neutral	8.49	2.644	6.891E+00	1.473E+00	2.673E-05
SD-7--370.3	Neutral	7.84	7.577	3.217E-02	5.557E-07	4.814E-07
SD-9--176.2	Neutral	9.06	2.460	6.784E+00	1.461E-04	1.013E-04
UZ-14--147.7	Neutral	8.55	2.481	6.929E+00	4.565E-07	2.214E-05
UZ-14--178.1	Neutral	6.93	5.956	2.193E+00	3.196E-05	3.860E-07
UZ-14--85.2	Neutral	7.36	3.130	6.120E+00	3.282E-06	2.427E-06
NRG-6--219.9	Alkaline	9.22	2.460	6.783E+00	1.208E-04	8.373E-05
NRG-7a--460.25	Alkaline	11.46	4.555	2.200E+00	1.505E+00	1.097E+00
SD-12--1495.5	Alkaline	11.20	2.409	5.752E+00	8.215E-03	6.081E-01
SD-6--522.5	Alkaline	10.07	2.460	6.757E+00	8.544E-01	5.698E-03
UZ-14--1,542	Alkaline	10.95	2.415	5.863E+00	8.501E-01	6.034E-01
UZ-14--1258.5	Alkaline	8.62	2.480	6.930E+00	8.699E-01	1.953E-05
UZ-14--1409.4	Alkaline	9.33	2.460	6.782E+00	8.528E-01	7.454E-05
UZ-14--1825.8	Alkaline	11.06	2.412	5.821E+00	8.529E-01	6.042E-01
UZ-14--2014.7	Alkaline	10.80	2.418	5.907E+00	8.506E-01	6.053E-01
UZ-16--1343.7	Alkaline	11.16	2.410	5.776E+00	1.076E-04	6.065E-01
WT-24--1937.0	Alkaline	11.22	2.427	5.733E+00	2.820E-05	6.205E-01

Temperature = 50 °C (P = 0.088481 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	7.69	5.421	5.365E-01	1.878E-06	4.322E-04
NRG-6--160.8	Ca-Cl	7.73	5.292	7.161E-01	2.280E-06	4.645E-04
NRG-6--171.0	Ca-Cl	7.77	4.382	1.858E+00	2.823E-06	7.359E-04
NRG-6--175.6	Ca-Cl	7.86	4.161	2.177E+00	2.559E-06	8.451E-04
SD-6--471.3	Ca-Cl	7.84	4.035	2.326E+00	2.803E-06	9.489E-04
SD-9--94.2	Ca-Cl	7.61	5.636	2.086E-01	6.682E-08	7.821E-04
SD-9--114.1	Ca-Cl	7.79	5.674	2.565E-01	2.027E-06	9.302E-04
SD-9--135.1	Ca-Cl	7.86	5.653	2.938E-01	2.628E-06	1.027E-03
SD-12--296.1	Ca-Cl	7.68	5.132	8.808E-01	3.290E-06	7.194E-04
UZ-14--1,277	Ca-Cl	7.76	5.613	3.707E-01	2.625E-06	6.245E-04
UZ-16--1643.4	Ca-Cl	7.77	5.572	3.748E-01	4.413E-06	1.723E-03
NRG-6--244.6	Neutral	9.05	4.224	1.972E+00	2.649E-05	1.150E-01
NRG-6--255.9	Neutral	7.63	4.862	8.461E-01	3.150E-08	1.740E-01
SD-6--412.2	Neutral	8.91	3.349	3.172E+00	3.740E-05	1.293E-01
SD-6--443.5	Neutral	8.94	3.205	3.332E+00	3.495E-05	1.240E-01
SD-6--507.5	Neutral	8.75	3.716	2.690E+00	4.667E-05	1.287E-01
SD-6--1509.9	Neutral	11.17	4.723	6.904E-02	8.409E-01	6.108E-02
SD-7--370.3	Neutral	8.47	5.931	1.532E-02	1.196E-06	5.669E-04
SD-9--176.2	Neutral	9.27	4.549	1.179E+00	1.749E-04	3.578E-01
UZ-14--85.2	Neutral	8.08	4.915	1.243E+00	5.283E-06	4.135E-03
UZ-14--147.7	Neutral	8.79	4.650	1.423E+00	3.715E-05	1.147E-01
UZ-14--178.1	Neutral	7.91	5.366	6.648E-01	2.016E-06	1.093E-03
NRG-6--219.9	Alkaline	9.44	4.299	1.500E+00	1.524E-04	3.587E-01
NRG-7a--460.25	Alkaline	11.73	2.155	1.760E-01	2.813E+00	8.348E-02
SD-6--522.5	Alkaline	10.37	3.428	2.571E+00	1.566E-02	3.664E-01
SD-12--1495.5	Alkaline	11.40	3.713	3.017E-01	1.371E+00	1.875E-01
UZ-14--1,542	Alkaline	11.22	3.349	3.830E-01	1.720E+00	1.707E-01
UZ-14--1258.5	Alkaline	8.86	4.646	1.427E+00	3.339E-05	1.147E-01
UZ-14--1409.4	Alkaline	9.54	4.547	1.180E+00	1.384E-04	3.580E-01
UZ-14--1825.8	Alkaline	11.35	2.968	8.521E-01	1.725E+00	1.246E-01
UZ-14--2014.7	Alkaline	11.07	3.609	1.157E-01	1.721E+00	1.694E-01
UZ-16--1343.7	Alkaline	11.42	3.179	5.837E-01	1.657E+00	1.762E-01
WT-24--1937.0	Alkaline	11.48	3.573	2.853E-02	1.792E+00	3.909E-02

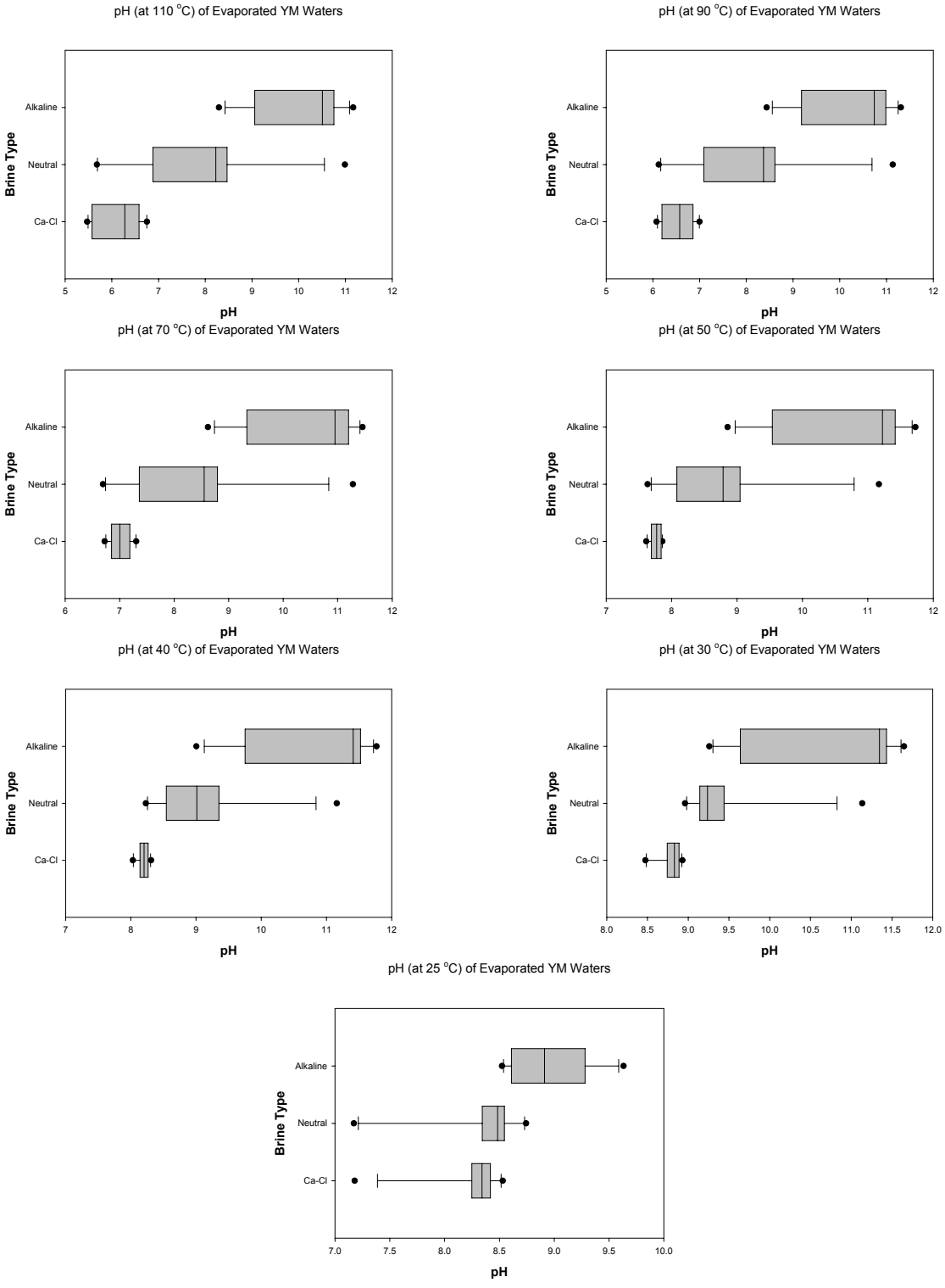
Temperature = 40 °C (P =0.059012 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	8.19	4.168	4.123E-01	7.523E-06	1.299E-03
NRG-6--160.8	Ca-Cl	8.20	4.050	5.476E-01	6.913E-06	1.417E-03
NRG-6--171.0	Ca-Cl	8.20	3.285	1.393E+00	6.404E-06	2.745E-03
NRG-6--175.6	Ca-Cl	8.27	3.108	1.626E+00	5.378E-06	3.004E-03
SD-6--471.3	Ca-Cl	8.27	3.009	1.733E+00	5.929E-06	3.589E-03
SD-9--94.2	Ca-Cl	8.14	4.334	1.604E-01	3.331E-07	2.340E-03
SD-9--114.1	Ca-Cl	8.27	4.299	1.942E-01	5.571E-06	3.136E-03
SD-9--135.1	Ca-Cl	8.31	4.280	2.040E-01	5.583E-06	4.174E-03
SD-12--296.1	Ca-Cl	8.03	3.903	6.696E-01	7.676E-06	2.299E-03
UZ-14--1,277	Ca-Cl	8.07	4.285	2.828E-01	5.692E-06	1.721E-03
UZ-16--1643.4	Ca-Cl	8.25	4.200	2.745E-01	1.237E-05	9.528E-03
NRG-6--244.6	Neutral	9.35	2.957	1.380E+00	5.666E-05	3.201E-01
NRG-6--255.9	Neutral	8.23	3.346	5.822E-01	1.486E-07	4.923E-01
SD-6--412.2	Neutral	9.01	2.459	2.330E+00	4.191E-05	1.466E-01
SD-6--443.5	Neutral	9.14	2.303	2.394E+00	5.302E-05	2.195E-01
SD-6--507.5	Neutral	9.05	2.572	1.862E+00	9.317E-05	3.625E-01
SD-6--1509.9	Neutral	11.16	3.374	3.518E-02	5.436E-01	2.953E-01
SD-7--370.3	Neutral	8.79	4.538	1.171E-02	3.693E-06	1.523E-03
SD-9--176.2	Neutral	9.56	3.187	5.409E-02	3.600E-04	1.059E+00
UZ-14--85.2	Neutral	8.54	3.766	7.896E-01	1.396E-05	2.259E-02
UZ-14--147.7	Neutral	9.01	3.568	7.481E-01	5.836E-05	2.238E-01
UZ-14--178.1	Neutral	8.36	4.043	5.005E-01	4.694E-06	3.667E-03
NRG-6--219.9	Alkaline	9.62	2.775	9.686E-01	2.096E-04	7.706E-01
NRG-7a--460.25	Alkaline	11.77	0.729	5.956E-02	2.911E+00	1.538E-01
SD-6--522.5	Alkaline	10.70	1.947	1.460E+00	4.158E-02	1.106E+00
SD-12--1495.5	Alkaline	11.44	2.226	1.809E-01	1.067E+00	6.560E-01
UZ-14--1,542	Alkaline	11.48	0.506	5.786E-02	3.216E+00	2.491E-01
UZ-14--1258.5	Alkaline	9.01	3.906	4.061E-01	4.261E-05	1.652E-01
UZ-14--1409.4	Alkaline	9.75	3.342	1.274E-01	2.208E-04	8.619E-01
UZ-14--1825.8	Alkaline	11.54	0.826	2.373E-01	2.790E+00	1.521E-01
UZ-14--2014.7	Alkaline	11.35	0.436	1.399E-02	3.496E+00	1.114E-01
UZ-16--1343.7	Alkaline	11.41	2.293	4.209E-01	1.229E+00	2.318E-01
WT-24--1937.0	Alkaline	11.52	2.307	1.843E-02	1.561E+00	1.427E-01

Temperature = 30 °C (P =0.038343 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	8.75	2.346	2.320E-01	1.715E-05	5.939E-03
NRG-6--160.8	Ca-Cl	8.74	2.260	3.056E-01	1.569E-05	6.378E-03
NRG-6--171.0	Ca-Cl	8.83	1.749	7.415E-01	2.099E-05	2.103E-02
NRG-6--175.6	Ca-Cl	8.89	1.629	8.522E-01	1.749E-05	2.147E-02
SD-6--471.3	Ca-Cl	8.89	1.567	9.029E-01	2.076E-05	2.744E-02
SD-9--94.2	Ca-Cl	8.82	2.408	8.909E-02	1.853E-06	1.028E-02
SD-9--114.1	Ca-Cl	8.89	2.312	1.044E-01	1.581E-05	1.919E-02
SD-9--135.1	Ca-Cl	8.93	2.272	1.082E-01	1.725E-05	2.631E-02
SD-12--296.1	Ca-Cl	8.48	2.143	3.676E-01	1.774E-05	9.647E-03
UZ-14--1,277	Ca-Cl	8.52	2.341	1.544E-01	1.287E-05	6.621E-03
UZ-16--1643.4	Ca-Cl	8.88	2.176	1.422E-01	5.555E-05	8.446E-02
NRG-6--244.6	Neutral	9.59	1.231	5.748E-01	8.762E-05	5.266E-01
NRG-6--255.9	Neutral	9.14	0.950	1.652E-01	1.472E-06	1.168E+00
SD-6--412.2	Neutral	9.19	1.180	1.118E+00	5.558E-05	1.715E-01
SD-6--443.5	Neutral	9.25	1.115	1.160E+00	5.576E-05	1.881E-01
SD-6--507.5	Neutral	9.37	0.826	5.981E-01	1.859E-04	9.110E-01
SD-6--1509.9	Neutral	11.14	1.694	1.766E-02	2.743E-01	1.773E-01
SD-7--370.3	Neutral	9.24	2.485	6.410E-03	9.674E-06	5.689E-03
SD-9--176.2	Neutral	9.44	1.325	2.250E-02	1.585E-04	8.951E-01
UZ-14--85.2	Neutral	9.06	1.868	3.916E-01	4.702E-05	1.157E-01
UZ-14--147.7	Neutral	9.17	1.751	3.671E-01	7.085E-05	2.263E-01
UZ-14--178.1	Neutral	8.96	2.135	2.643E-01	1.377E-05	2.157E-02
NRG-6--219.9	Alkaline	9.49	1.367	4.769E-01	8.944E-05	4.798E-01
NRG-7a--460.25	Alkaline	11.65	0.362	2.958E-02	1.420E+00	7.637E-02
SD-6--522.5	Alkaline	10.87	0.876	6.571E-01	6.508E-02	6.884E-01
SD-12--1495.5	Alkaline	11.36	1.080	8.778E-02	5.213E-01	3.847E-01
UZ-14--1,542	Alkaline	11.36	0.253	2.897E-02	1.601E+00	1.309E-01
UZ-14--1258.5	Alkaline	9.26	1.963	2.041E-01	6.614E-05	1.545E-01
UZ-14--1409.4	Alkaline	9.64	1.560	5.947E-02	9.297E-05	6.321E-01
UZ-14--1825.8	Alkaline	11.43	0.413	1.186E-01	1.384E+00	8.367E-02
UZ-14--2014.7	Alkaline	11.23	0.221	7.084E-03	1.761E+00	5.639E-02
UZ-16--1343.7	Alkaline	11.35	1.117	2.051E-01	6.047E-01	1.693E-01
WT-24--1937.0	Alkaline	11.46	1.168	9.328E-03	7.686E-01	7.225E-02

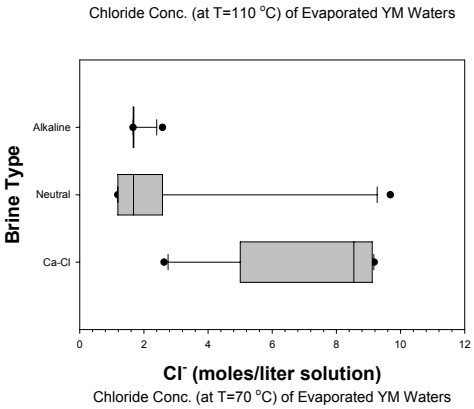
Temperature = 25 °C (P =0.030625 atm)						
			Concentration (moles per liter solution)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6--158.2	Ca-Cl	9.13	0.7239	7.159E-02	1.155E-05	1.082E-02
NRG-6--160.8	Ca-Cl	9.14	0.4956	2.101E-01	2.297E-05	2.876E-02
NRG-6--171.0	Ca-Cl	9.14	0.4956	2.101E-01	2.297E-05	2.876E-02
NRG-6--175.6	Ca-Cl	9.24	0.4479	2.343E-01	2.222E-05	3.311E-02
SD-6--471.3	Ca-Cl	9.21	0.4273	2.461E-01	2.520E-05	3.658E-02
SD-9--94.2	Ca-Cl	9.35	0.7227	2.674E-02	3.089E-06	1.727E-02
SD-9--114.1	Ca-Cl	9.28	0.6588	2.975E-02	1.872E-05	2.960E-02
SD-9--135.1	Ca-Cl	9.24	0.6381	3.040E-02	1.992E-05	3.073E-02
SD-12--296.1	Ca-Cl	8.84	0.6303	1.081E-01	2.079E-05	1.585E-02
UZ-14--1,277	Ca-Cl	8.90	0.6847	4.517E-02	1.253E-05	1.033E-02
UZ-16--1643.4	Ca-Cl	9.07	0.6034	3.942E-02	5.192E-05	6.403E-02
NRG-6--244.6	Neutral	9.67	0.3073	1.434E-01	5.342E-05	1.719E-01
NRG-6--255.9	Neutral	9.60	0.2506	4.361E-02	4.430E-06	3.147E-01
SD-6--412.2	Neutral	9.47	0.2835	2.686E-01	6.786E-05	1.139E-01
SD-6--443.5	Neutral	9.48	0.2648	2.753E-01	5.324E-05	1.235E-01
SD-6--507.5	Neutral	9.42	0.1796	1.300E-01	1.493E-04	3.466E-01
SD-6--1509.9	Neutral	10.96	0.4411	4.600E-03	5.556E-02	4.618E-02
SD-7--370.3	Neutral	9.57	0.7305	1.884E-03	5.805E-06	8.536E-03
SD-9--176.2	Neutral	9.77	0.3449	5.855E-03	3.007E-04	2.456E-01
UZ-14--85.2	Neutral	9.38	0.4589	9.621E-02	6.461E-05	1.298E-01
UZ-14--147.7	Neutral	9.36	0.4293	8.999E-02	7.157E-05	1.472E-01
UZ-14--178.1	Neutral	9.37	0.5908	7.313E-02	1.781E-05	3.255E-02
NRG-6--219.9	Alkaline	9.86	0.3570	1.246E-01	1.880E-04	1.309E-01
NRG-7a--460.25	Alkaline	11.49	0.0893	7.296E-03	3.414E-01	1.884E-02
SD-6--522.5	Alkaline	10.63	0.2226	1.669E-01	1.070E-02	1.749E-01
SD-12--1495.5	Alkaline	11.16	0.2709	2.201E-02	1.051E-01	9.646E-02
UZ-14--1,542	Alkaline	11.17	0.0609	6.962E-03	3.602E-01	3.145E-02
UZ-14--1258.5	Alkaline	9.75	0.5323	5.534E-02	1.925E-04	4.213E-02
UZ-14--1409.4	Alkaline	9.62	0.4113	1.568E-02	5.320E-05	1.742E-01
UZ-14--1825.8	Alkaline	11.24	0.0995	2.856E-02	3.029E-01	2.015E-02
UZ-14--2014.7	Alkaline	11.06	0.0548	1.757E-03	4.331E-01	1.398E-02
UZ-16--1343.7	Alkaline	11.16	0.2807	5.154E-02	1.259E-01	4.255E-02
WT-24--1937.0	Alkaline	11.27	0.2909	2.323E-03	1.566E-01	1.799E-02

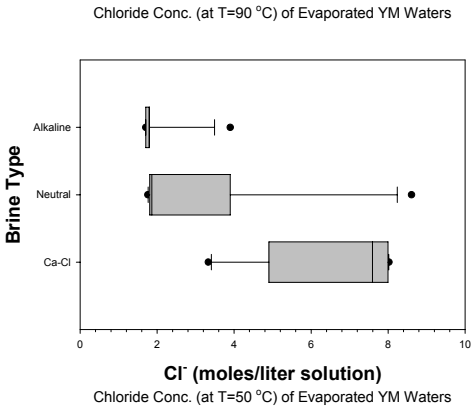
June 24, 2009

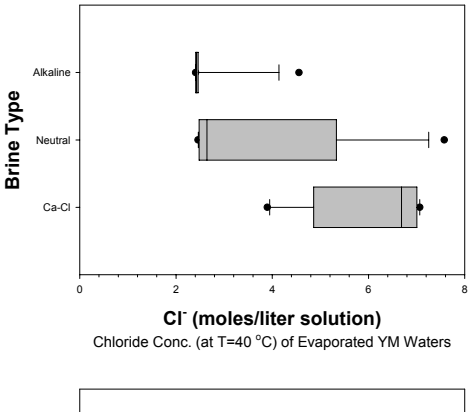
The following figures compare the calculated pH of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

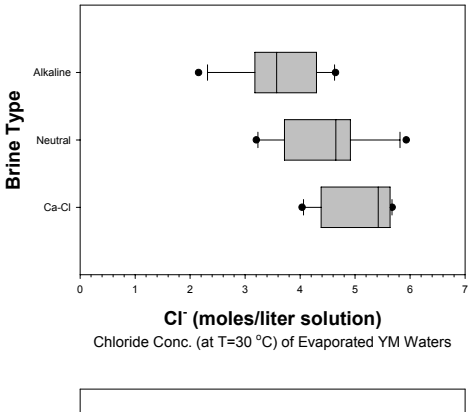


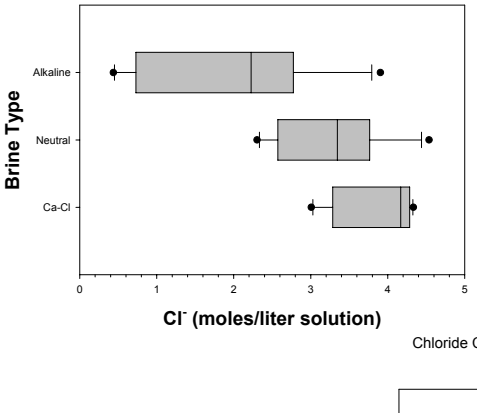
The following figures compare the calculated chloride concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

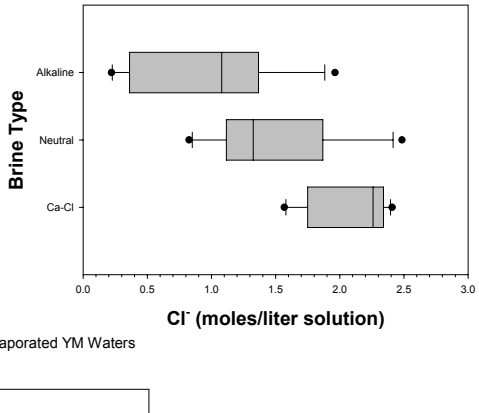


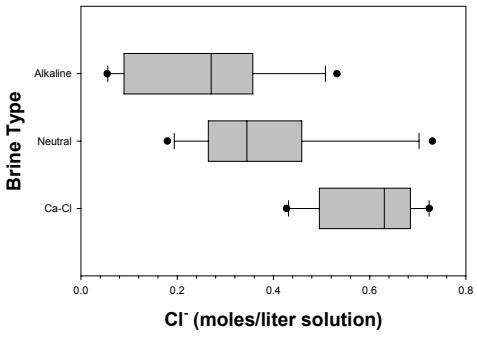






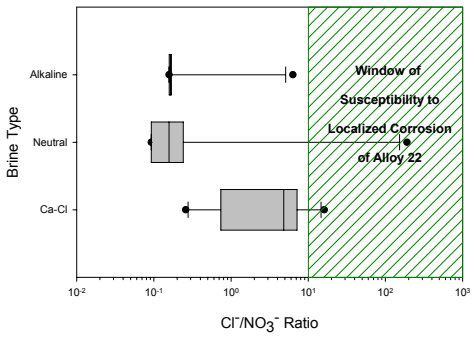




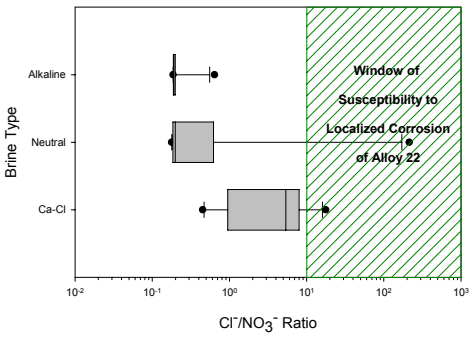


The following figures compare the calculated chloride to nitrate ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

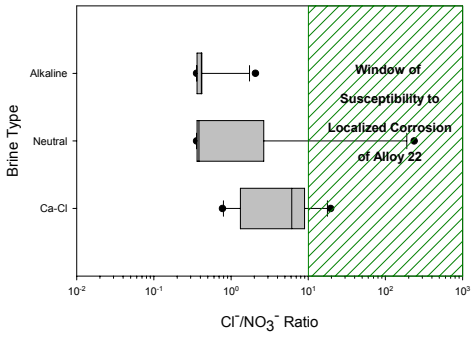
Cl^-/NO_3^- Ratio (at T=110 °C) of Evaporated YM Waters



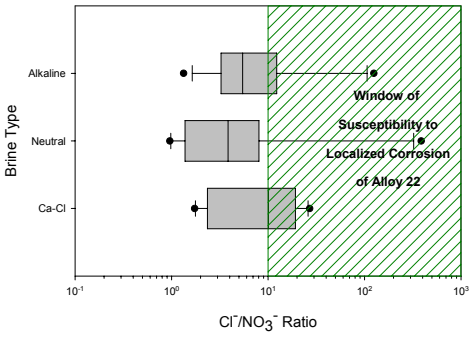
Cl^-/NO_3^- Ratio (at T=90 °C) of Evaporated YM Waters



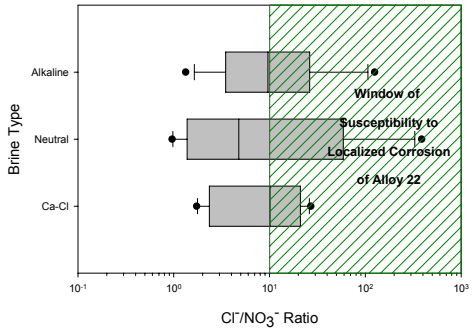
Cl^-/NO_3^- Ratio (at T=70 °C) of Evaporated YM Waters



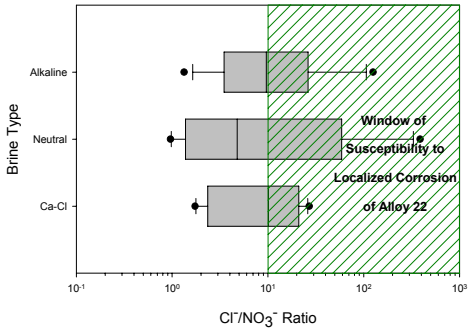
Cl^-/NO_3^- Ratio (at T=50 °C) of Evaporated YM Waters



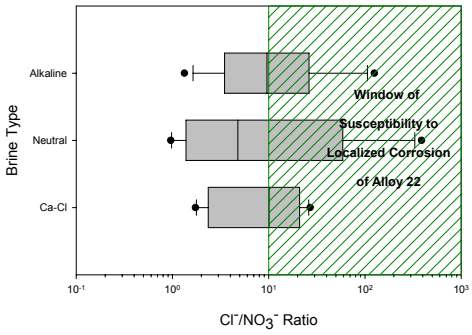
Cl^-/NO_3^- Ratio (at T=40 °C) of Evaporated YM Waters



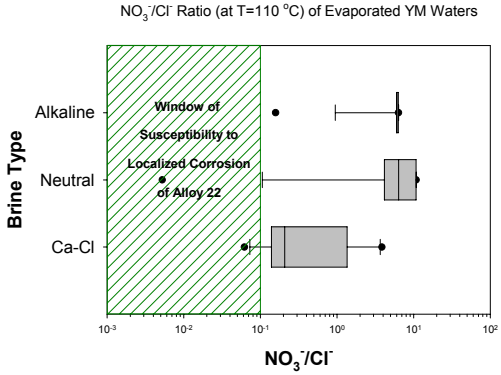
Cl^-/NO_3^- Ratio (at T=30 °C) of Evaporated YM Waters

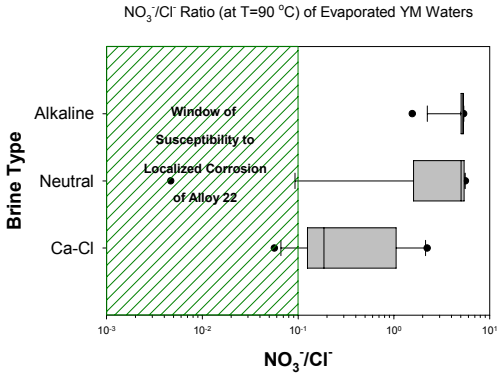


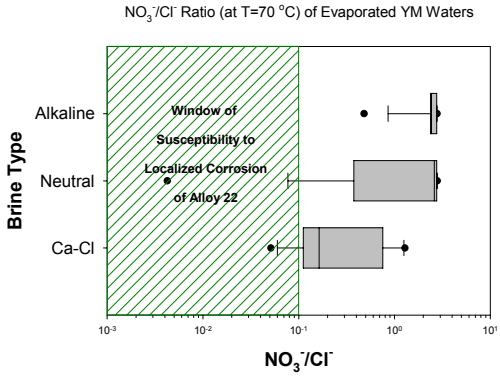
Cl^-/NO_3^- Ratio (at T=25 °C) of Evaporated YM Waters

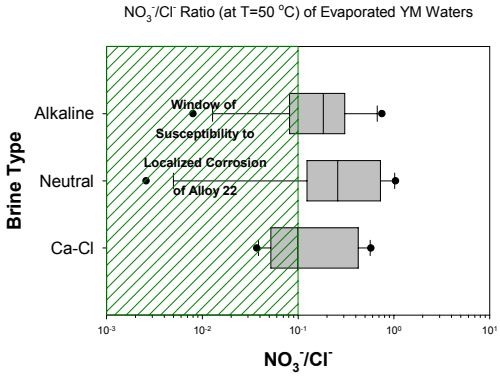


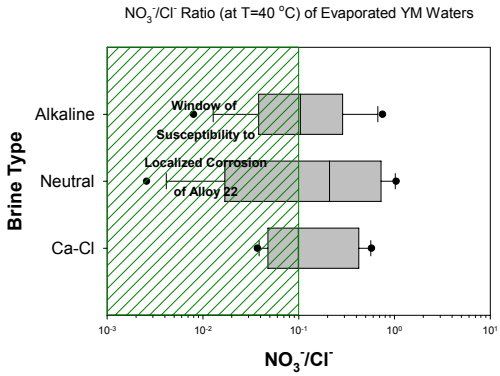
The following figures compare the calculated nitrate to chloride ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

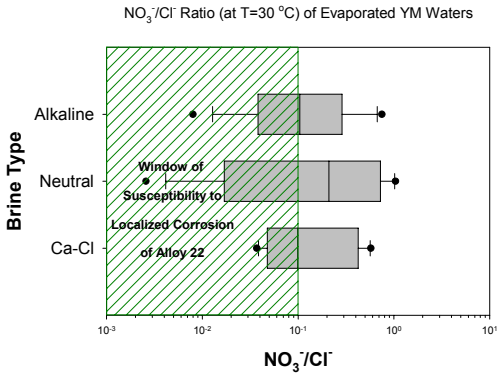


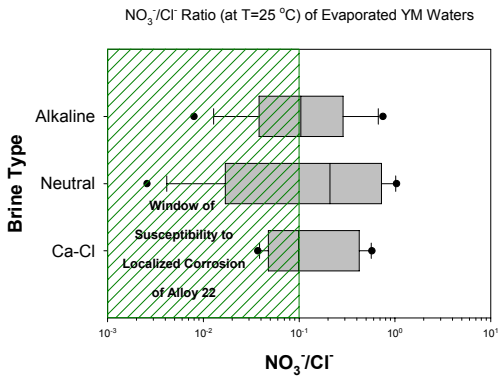




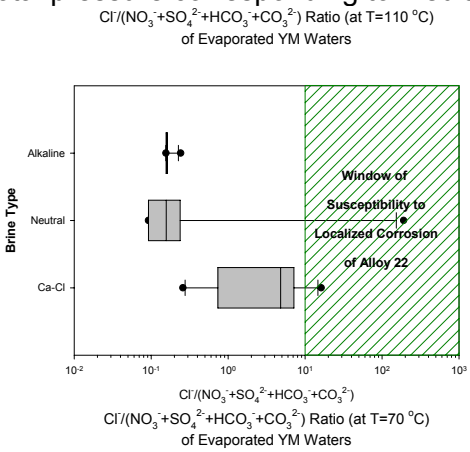


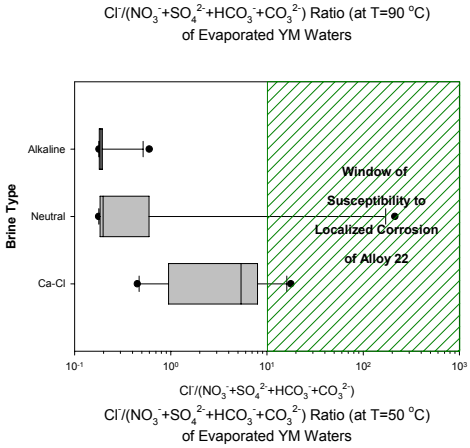


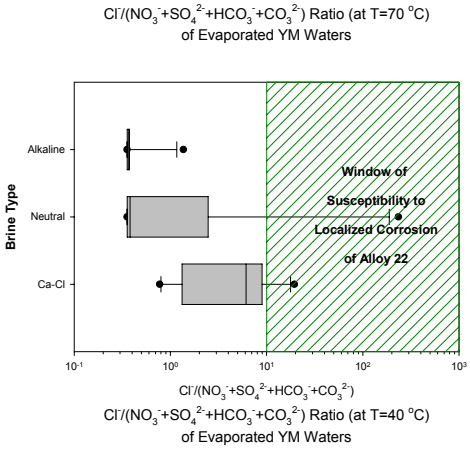


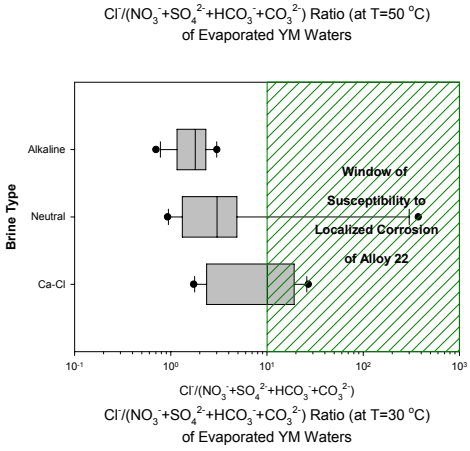


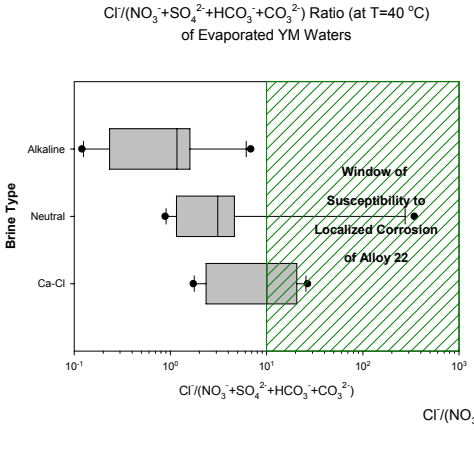
The following figures compare the calculated chloride to corrosion-inhibiting oxyanion ratio of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

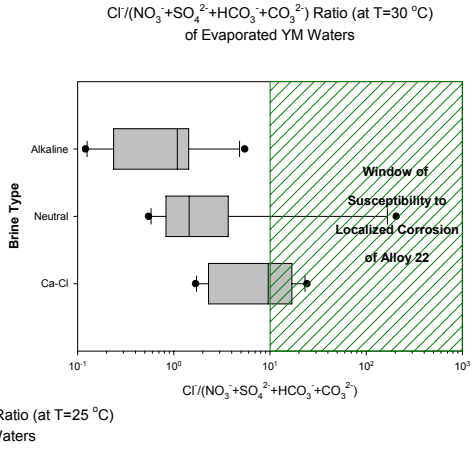


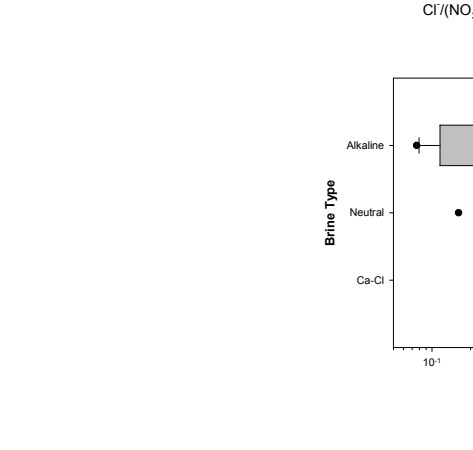


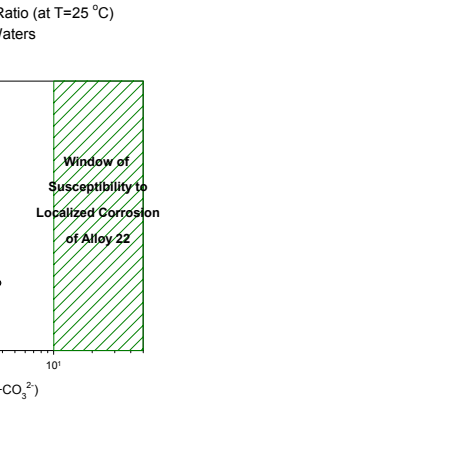




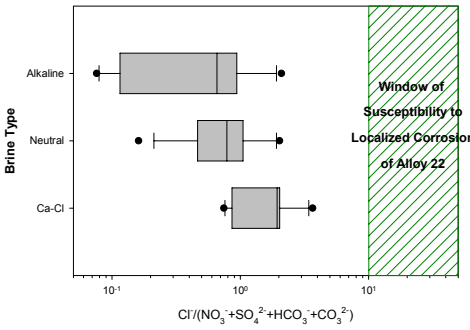




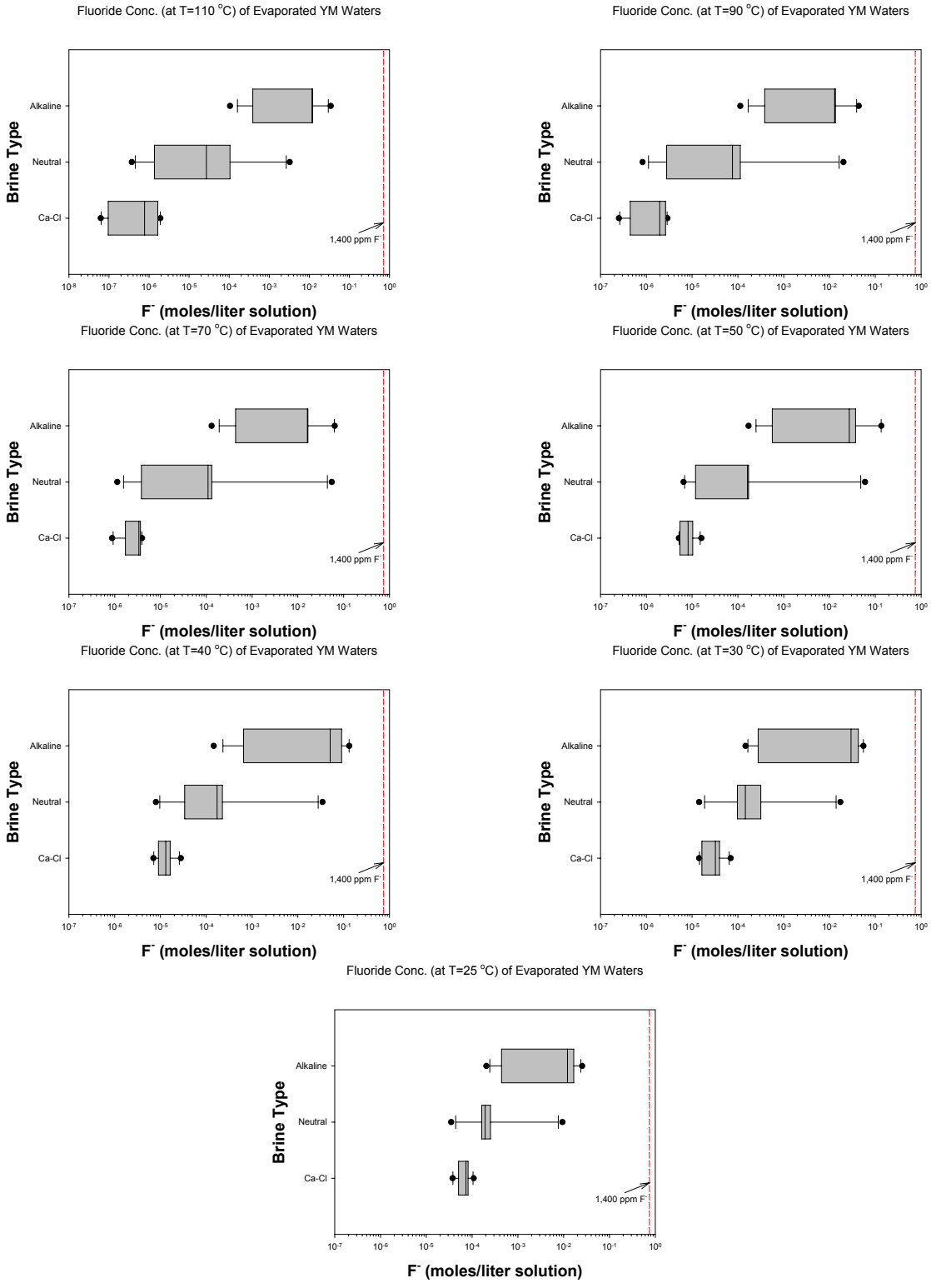




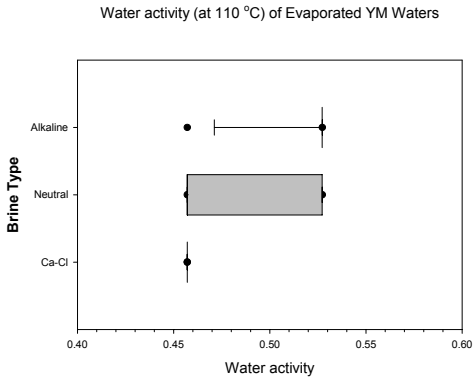
Cl⁻/(NO3⁻+SO4²⁻+HCO3⁻+CO3²⁻) Ratio (at T=25 °C)
of Evaporated YM Waters

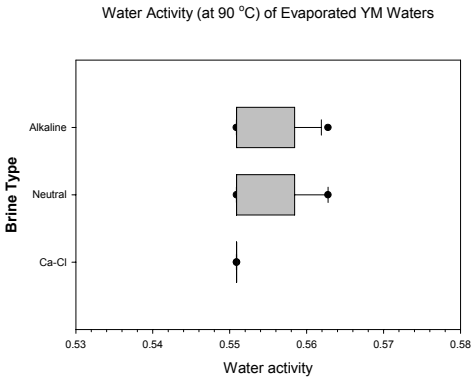


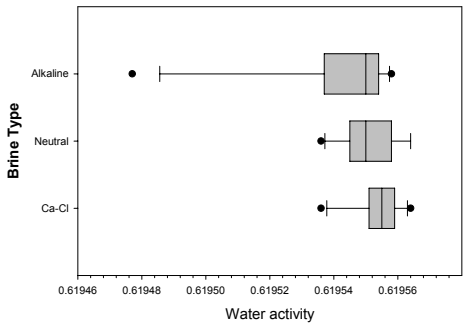
The following figures compare the calculated fluoride concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH). The 1,400 ppm F^- value is the maximum value in DOE titanium corrosion tests reported in the SER.

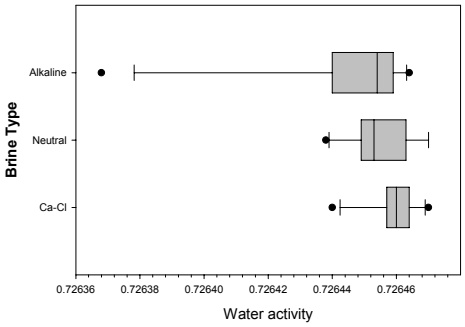


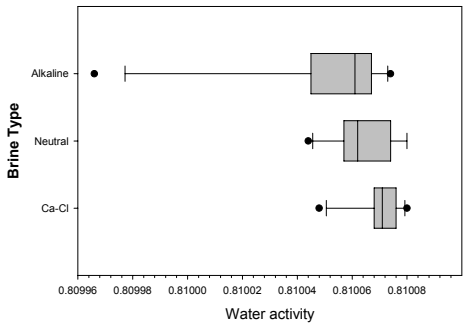
The following figures compare the calculated water activity of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

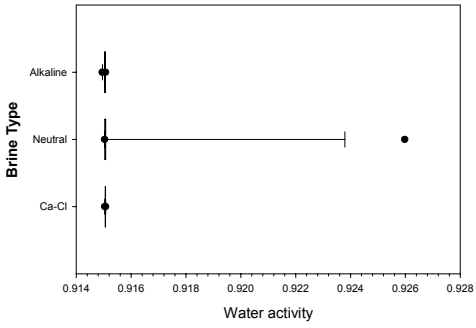


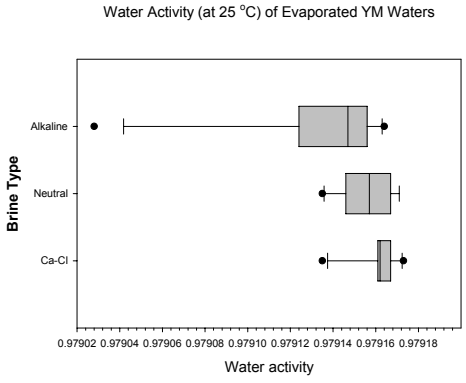




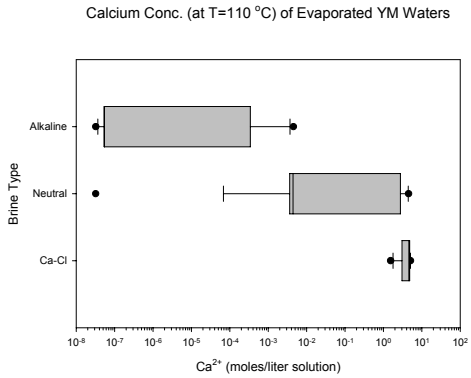


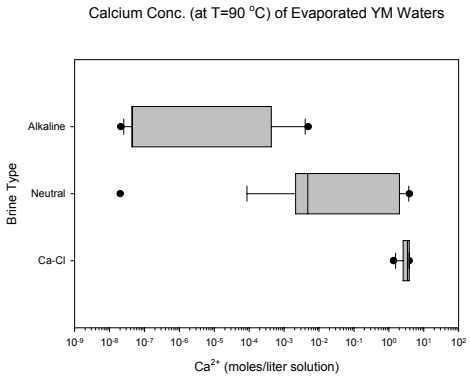


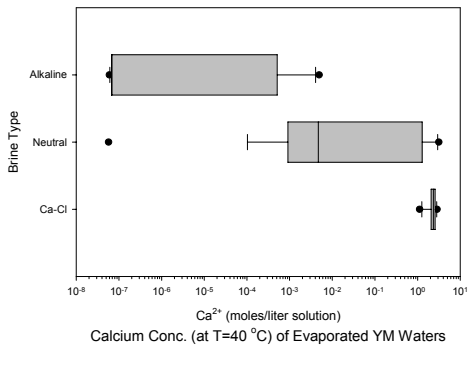


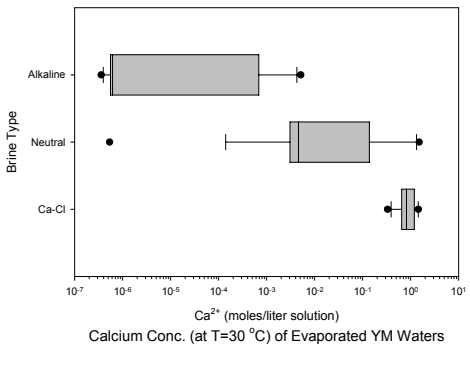


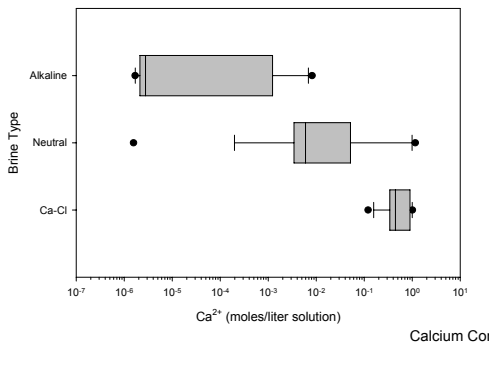
The following figures compare the calculated calcium concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

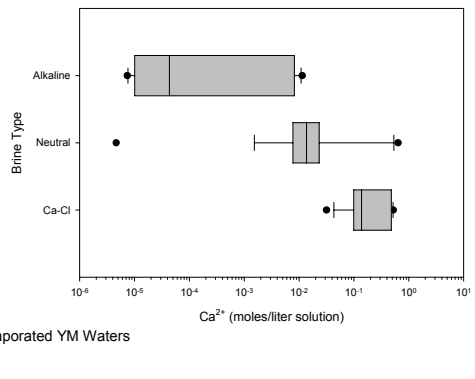


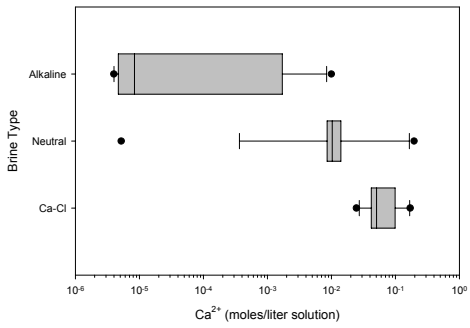




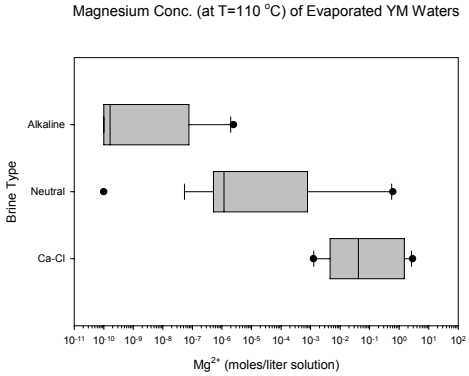


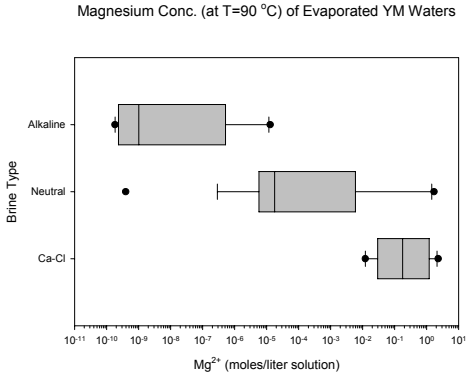


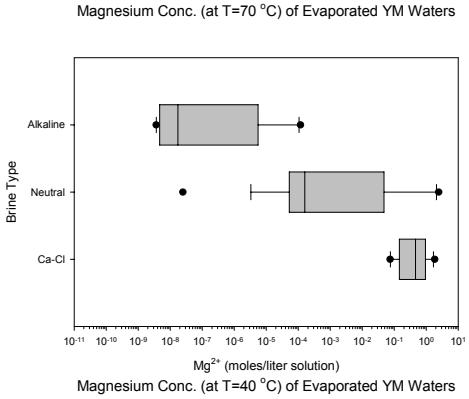


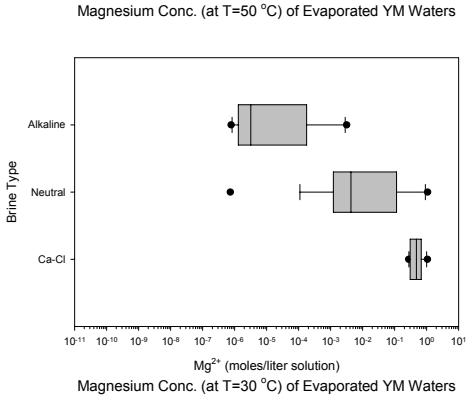


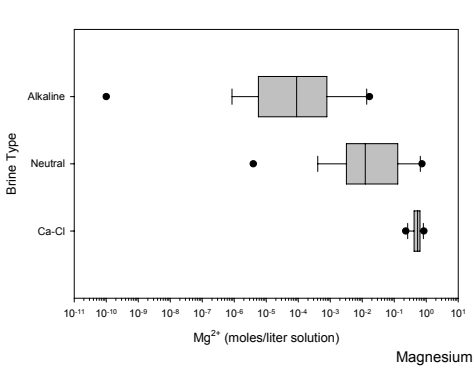
The following figures compare the calculated magnesium concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

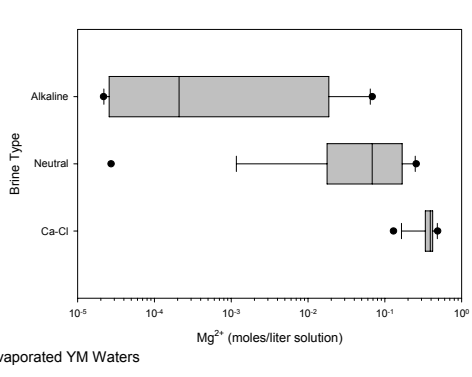


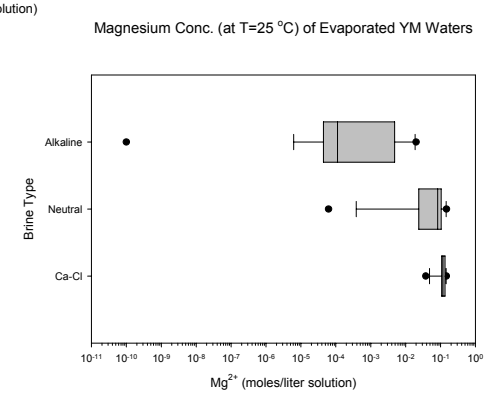




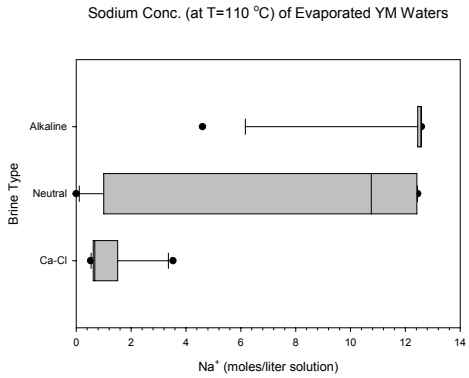


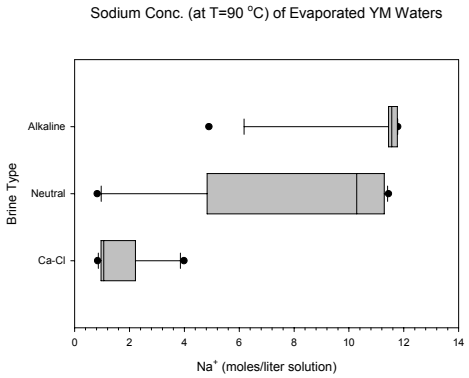


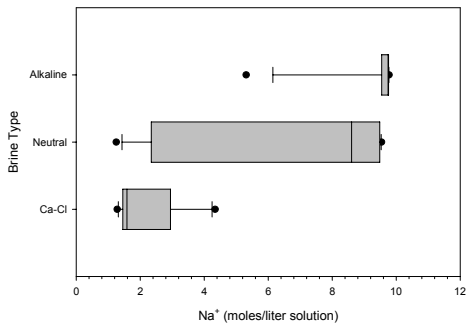


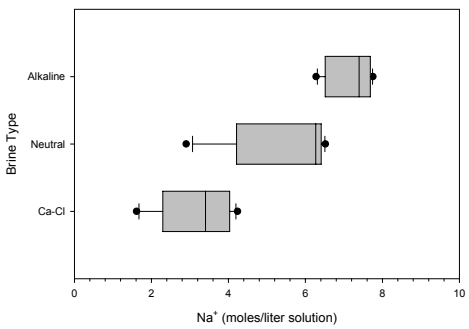


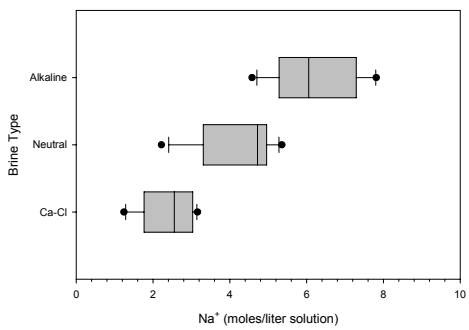
The following figures compare the calculated sodium concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

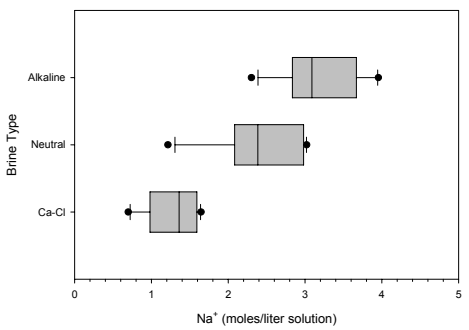


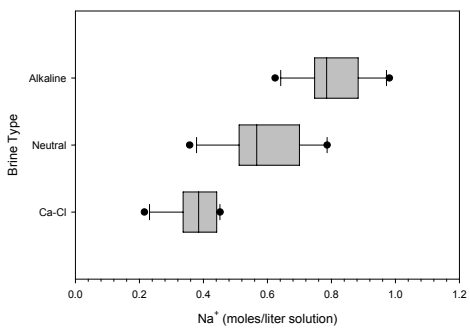




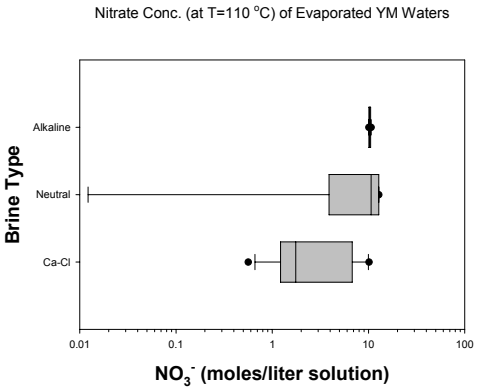


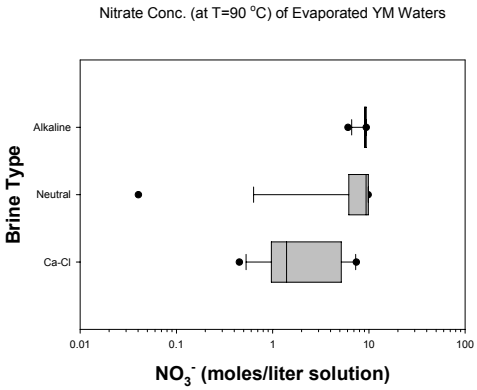


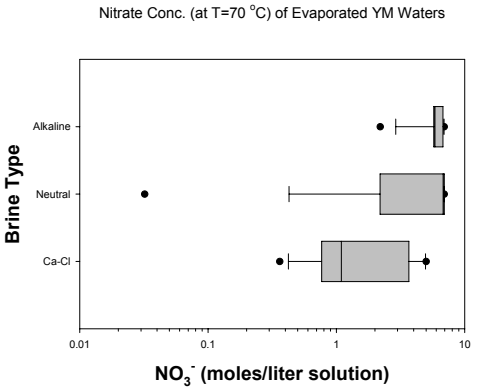


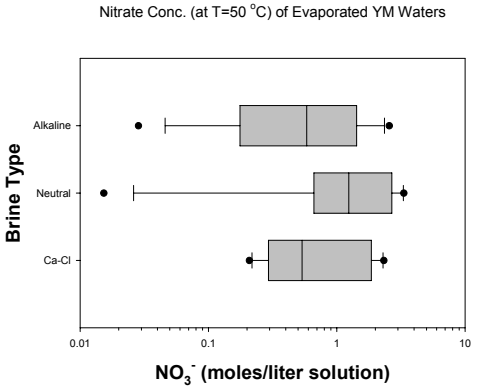


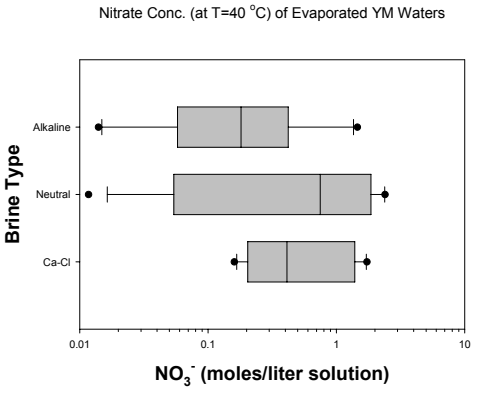
The following figures compare the calculated nitrate concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

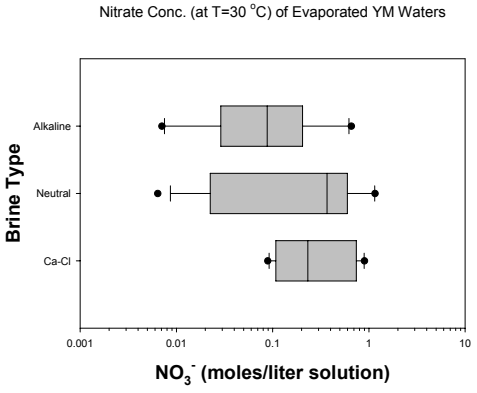


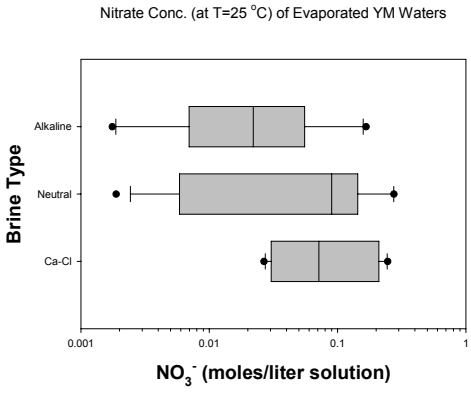






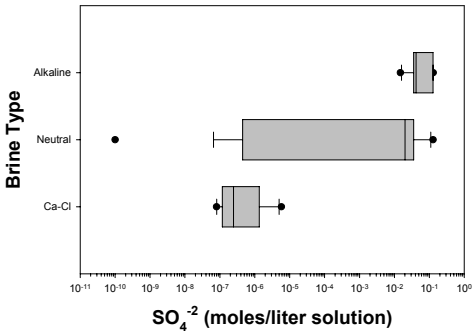




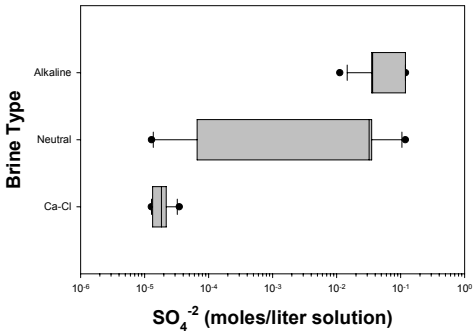


The following figures compare the calculated sulfate concentration (moles per liter solution) of brines formed by evaporation of Yucca Mountain pore waters at 110, 90, 70, 50, 40, 30, and 25 °C (total pressure corresponding to median RH).

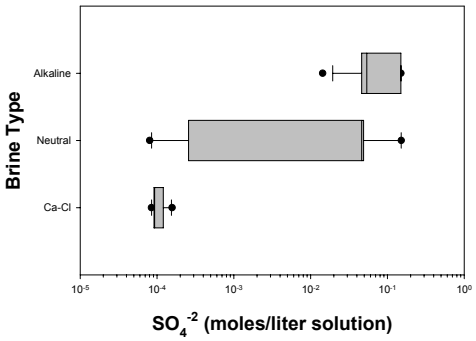
SO_4^{-2} Conc. (at T=110 °C) of Evap. YM Waters



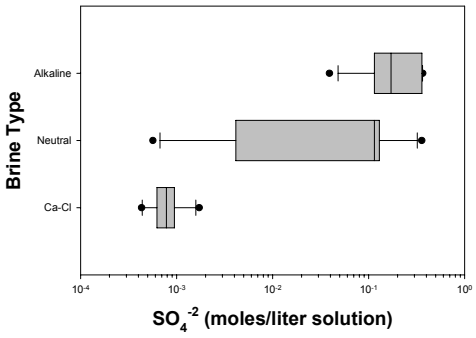
SO_4^{-2} Conc. (at T=90 °C) of Evap. YM Waters



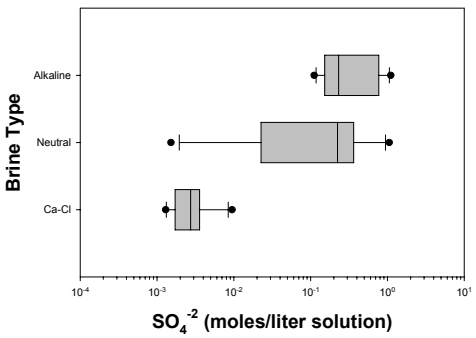
SO_4^{-2} Conc. (at T=70 °C) of Evap. YM Waters



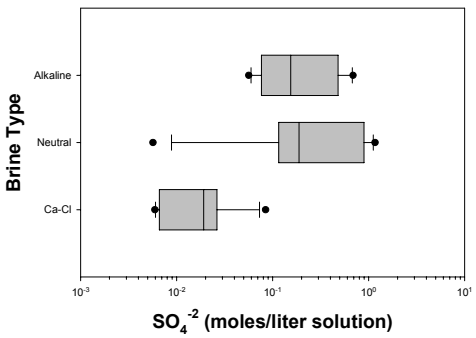
SO_4^{-2} Conc. (at T=50 °C) of Evap. YM Waters



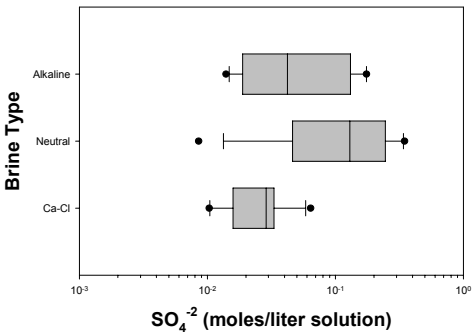
SO_4^{-2} Conc. (at T=40 °C) of Evap. YM Waters



SO_4^{-2} Conc. (at T=30 °C) of Evap. YM Waters



SO_4^{-2} Conc. (at T=25 °C) of Evap. YM Waters



June 30, 2009

In the DOE response to RAI:3.2.2.1.3.3-009, DOE compared the ranges of pH, Cl/NO3 ratio, Cl concentration, nitrate concentration, and ionic strength calculated by TSPA at 1,000,000 years with the values for the 34 pore water samples DOE considered for its near-field chemistry model. To allow comparison of the 33 U.S.G.S. pore water chemistry with TSPA calculated values, the following scripts were used with Geochemist's Workbench REACT version 7.0.6. The chemical compositions used for the 33 U.S.G.S. pore water samples are the same as those listed on pages 185 to 203 of this notebook. The waters were constrained by equilibrium with a log fCO2 of –3.0, log fO2 of 0.2, and equilibrium with low Albite. The thermodynamic database used is named thermo.com.v8.r6J.dat, which is the same as thermo.com.v8.r6.dat except that the mineral stellerite was added to the database by J. Myers.

NRG-6/158.2

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                    1.62100E-03     molal
Na+                                         1.54850E-03     molal
Mg++                                        9.58650E-04     molal
Ca++                                        3.04410E-03     molal
F-                                          1.14750E-04     molal
Cl-                                         5.21820E-03     molal
SO4--                                       1.65510E-03     molal
NO3-                                         5.16090E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  7.337             log fO2 =   -0.699
        Eh =   0.7847 volts      pe =  13.2651
        Ionic strength      =    0.013907
        Activity of water   =    0.999817
Reactants            remaining     reacted       reacted       reacted
 ------------------------------------------------------------------------------
  CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
 ------------------------------------------------------------------------------
  Stellerite          4.269e-010     -9.370     6.017e-007
```

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.71e-009	1.49e-014	4.03e-010			
Ca++	0.00304	0.00304	122.			
Cl-	0.00522	0.00522	185.			
F-	0.000115	0.000115	2.18			
H+	-0.000489	-0.000489	-0.493			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.000422	0.000422	25.7			
Mg++	0.000959	0.000959	23.3			
NH3(aq)	0.000516	0.000516	8.78			
Na+	0.00155	0.00155	35.6			
O2(aq)	0.00128	0.00128	41.1			
SO4--	0.00166	0.00166	159.			
SiO2(aq)	0.00162	0.00162	97.3			

NRG-6/160.8

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                  1.398030E-03          molal
Na+                                                       1.522400E-03          molal
Mg++                                                      7.405850E-04          molal
Ca++                                                      2.594930E-03          molal
F-                                                        1.147460E-04          molal
Cl-                                                       4.174520E-03          molal
SO4--                                                     1.446950E-03          molal
NO3-                                                      5.644690E-04          molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
      pH =  7.395            log fO2 =   -0.699
      Eh =   0.7813 volts      pe =  13.2070
      Ionic strength      =    0.011947
      Activity of water   =    0.999853
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	6.519e-010	-9.186	9.188e-007	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	2.61e-009	2.60e-014	7.01e-010			
Ca++	0.00259	0.00259	104.			
Cl-	0.00417	0.00417	148.			
F-	0.000115	0.000115	2.18			
H+	-0.000538	-0.000538	-0.542			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.000473	0.000473	28.8			
Mg++	0.000741	0.000741	18.0			
NH3(aq)	0.000564	0.000564	9.61			
Na+	0.00152	0.00152	35.0			
O2(aq)	0.00138	0.00138	44.2			
SO4--	0.00145	0.00145	139.			
SiO2(aq)	0.00140	0.00140	83.9			

NRG-6/171.0

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.321345E-03	molal
Na+	1.270111E-03	molal
Mg++	4.730543E-04	molal
Ca++	1.758974E-03	molal
F-	1.147500E-04	molal
Cl-	1.635962E-03	molal
SO4--	9.785914E-04	molal
NO3-	6.934334E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite
precip = on
go

OUTPUT SUMMARY:

pH = 7.803 log fO2 = -0.699
Eh = 0.7571 volts pe = 12.7984
Ionic strength = 0.008066
Activity of water = 0.999942

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	2.047e-005	-4.689	0.002049	0.0007562
Sepiolite	2.088e-005	-4.680	0.01352	0.005962
Stellerite	8.413e-010	-9.075	1.186e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Kd mg/kg	Kd L/kg
Al+++	3.37e-009	4.91e-014	1.33e-009			
Ca++	0.00176	0.00174	69.6			
Cl-	0.00164	0.00164	58.0			
F-	0.000115	0.000115	2.18			
H+	-0.000869	-0.000682	-0.687			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00116	0.00114	69.3			
Mg++	0.000473	0.000390	9.46			
NH3(aq)	0.000693	0.000693	11.8			
Na+	0.00127	0.00127	29.2			
O2(aq)	0.00164	0.00164	52.4			
SO4--	0.000979	0.000979	94.0			
SiO2(aq)	0.00132	0.00120	71.8			

NRG-6/175.6

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                  1.30E-03          molal
Na+                                                       1.28E-03          molal
Mg++                                                      3.54E-04          molal
Ca++                                                      1.23E-03          molal
F-                                                        1.15E-04          molal
Cl-                                                       1.33E-03          molal
SO4--                                                     6.66E-04          molal
NO3-                                                      6.934334E-04      molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

pH = 7.750 log fO2 = -0.699
Eh = 0.7603 volts pe = 12.8518
Ionic strength = 0.006360
Activity of water = 0.999953

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	8.607e-010	-9.065	1.213e-006	

Original basis	In fluid total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	3.44e-009	4.23e-014	1.14e-009			
Ca++	0.00123	0.00123	49.3			
Cl-	0.00133	0.00133	47.1			
F-	0.000115	0.000115	2.18			
H+	-0.000677	-0.000677	-0.682			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.000994	0.000994	60.6			
Mg++	0.000354	0.000354	8.60			
NH3(aq)	0.000693	0.000693	11.8			
Na+	0.00128	0.00128	29.4			
O2(aq)	0.00164	0.00164	52.4			
SO4--	0.000666	0.000666	64.0			
SiO2(aq)	0.00130	0.00130	78.1			

SD-12/296.1

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                1.201600E-03    molal
Na+                                                     9.134400E-04    molal
Mg++                                                    3.291500E-04    molal
Ca++                                                    1.871300E-03    molal
F-                                                      1.147500E-04    molal
Cl-                                                     1.692400E-03    molal
SO4--                                                   2.186000E-04    molal
NO3-                                                    2.903000E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
```

suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite

precip = on
go

OUTPUT SUMMARY:

pH = 7.869 log fO2 = -0.699
Eh = 0.7532 volts pe = 12.7329
Ionic strength = 0.005337
Activity of water = 0.999940

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0006995	-3.155	0.07002	0.02584
Sepiolite	1.254e-005	-4.902	0.008123	0.003581
Stellerite	1.556e-009	-8.808	2.193e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Kd mg/kg	Kd L/kg
Al+++	6.22e-009	6.93e-014		1.87e-009		
Ca++	0.00187	0.00117	46.9			
Cl-	0.00169	0.00169	60.0			
F-	0.000115	0.000115	2.18			
H+	-0.00108	-0.000281	-0.283			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00199	0.00129	78.7			
Mg++	0.000329	0.000279	6.78			
NH3(aq)	0.000290	0.000290	4.94			
Na+	0.000913	0.000913	21.0			
O2(aq)	0.000833	0.000833	26.7			
SO4--	0.000219	0.000219	21.0			
SiO2(aq)	0.00120	0.00113	67.7			

SD-6/471.3

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	9.736300E-04	molal
Na+	1.953000E-03	molal
K+	6.649900E-05	molal
Mg++	5.060700E-04	molal
Ca++	1.532000E-03	molal
F-	4.526700E-04	molal
Cl-	1.884200E-03	molal
SO4--	7.078600E-04	molal
NO3-	1.085400E-03	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.834 log fO2 = -0.699
Eh = 0.7553 volts pe = 12.7677
Ionic strength = 0.008163
Activity of water = 0.999933

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Fluorite	5.542e-005	-4.256	0.004327	0.001360
Sepiolite	6.521e-006	-5.186	0.004224	0.001862
Stellerite	1.384e-009	-8.859	1.951e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	5.54e-009	1.27e-013	3.42e-009			
Ca++	0.00153	0.00148	59.2			
Cl-	0.00188	0.00188	66.8			
F-	0.000453	0.000342	6.49			
H+	-0.00113	-0.00107	-1.08			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00122	0.00122	74.3			
K+	6.65e-005	6.65e-005	2.60			
Mg++	0.000506	0.000480	11.7			
NH3(aq)	0.00109	0.00109	18.5			
Na+	0.00195	0.00195	44.9			
O2(aq)	0.00242	0.00242	77.5			
SO4--	0.000708	0.000708	68.0			
SiO2(aq)	0.000974	0.000934	56.1			

SD-9/114.1

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.035210E-03	molal
Na+	2.392340E-03	molal
Mg++	7.405850E-04	molal
Ca++	2.370370E-03	molal
F-	1.147460E-04	molal
Cl-	3.892460E-03	molal
SO4--	1.884160E-03	molal
NO3-	1.757920E-04	molal

```
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  7.566             log fO2 =   -0.699
        Eh =   0.7711 volts      pe =  13.0356
        Ionic strength      =    0.012367
        Activity of water   =    0.999863

                      moles       moles        grams         cm3
 Reactants            remaining   reacted      reacted       reacted
-------------------------------------------------------------------------------
  CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
  Stellerite          9.871e-010     -9.006     1.391e-006

                              In fluid             Sorbed           Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
  Al+++          3.95e-009  7.59e-014 2.05e-009
  Ca++             0.00237    0.00237      94.9
  Cl-              0.00389    0.00389      138.
  F-              0.000115   0.000115      2.18
  H+              -0.000152  -0.000152    -0.153
  H2O                55.5       55.5 9.99e+005
  HCO3-           0.000687   0.000687      41.9
  Mg++            0.000741   0.000741      18.0
  NH3(aq)         0.000176   0.000176      2.99
  Na+              0.00239    0.00239      55.0
  O2(aq)          0.000604   0.000604      19.3
  SO4--            0.00188    0.00188      181.
  SiO2(aq)         0.00104    0.00104      62.2
```

SD-9/135.1

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
```

```
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                          9.985900E-04          molal
Na+                                               2.870800E-03          molal
Mg++                                              6.171500E-04          molal
Ca++                                              2.270600E-03          molal
F-                                                1.147500E-04          molal
Cl-                                               4.061700E-03          molal
SO4--                                             1.686400E-03          molal
NO3-                                              1.935300E-04          molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  7.699             log fO2 =   -0.699
        Eh =   0.7632 volts      pe =  12.9024
        Ionic strength      =    0.012152
        Activity of water   =    0.999857

                      moles        moles        grams         cm3
 Reactants             remaining     reacted       reacted       reacted
-------------------------------------------------------------------------------
  CO2(g)              -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
  Stellerite          9.016e-010     -9.045     1.271e-006

                              In fluid              Sorbed           Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
  Al+++          3.61e-009  8.65e-014 2.33e-009
  Ca++             0.00227    0.00227      90.9
  Cl-              0.00406    0.00406      144.
  F-              0.000115   0.000115      2.18
  H+              -0.000176  -0.000176    -0.177
  H2O                55.5       55.5 9.99e+005
  HCO3-           0.000921   0.000921      56.2
  Mg++            0.000617   0.000617      15.0
  NH3(aq)         0.000194   0.000194      3.29
  Na+              0.00287    0.00287      66.0
  O2(aq)          0.000640   0.000640      20.5
  SO4--            0.00169    0.00169      162.
  SiO2(aq)        0.000999   0.000999      60.0
```

SD-9/94.2

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
```

-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.231600E-03	molal
Na+	1.870400E-03	molal
Mg++	9.874500E-04	molal
Ca++	3.118900E-03	molal
F-	1.147500E-04	molal
Cl-	4.795100E-03	molal
SO4--	2.706500E-03	molal
NO3-	1.774000E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip = on
go

OUTPUT SUMMARY:

pH = 3.826 log fO2 = -0.699
Eh = 0.9924 volts pe = 16.7757
Ionic strength = 0.015235
Activity of water = 0.999831

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	1.146e-005	-4.941	0.01615	

Original basis total	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	0.000138	9.19e-005		2.48	
Ca++	0.00312	0.00310		124.	
Cl-	0.00480	0.00480		170.	
F-	0.000115	0.000115		2.18	
H+	-0.000139	4.41e-005		0.0444	
H2O	55.5	55.5	9.99e+005		
HCO3-	3.41e-005	3.41e-005		2.08	
Mg++	0.000987	0.000987		24.0	
NH3(aq)	0.000177	0.000177		3.02	
Na+	0.00187	0.00187		43.0	
O2(aq)	0.000608	0.000608		19.4	
SO4--	0.00271	0.00271		260.	
SiO2(aq)	0.00123	0.00107		64.3	

UZ-16/1643.4

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0

fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.164914E-03	molal
Na+	1.478897E-03	molal
Mg++	4.936220E-04	molal
Ca++	2.270449E-03	molal
F-	1.147500E-04	molal
Cl-	1.974436E-03	molal
SO4--	2.914953E-04	molal
NO3-	1.290108E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.901 log fO2 = -0.699
Eh = 0.7513 volts pe = 12.7003
Ionic strength = 0.005652
Activity of water = 0.999930

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.001249	-2.903	0.1250	0.04615
Sepiolite	4.072e-005	-4.390	0.02638	0.01163
Stellerite	1.103e-009	-8.957	1.555e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	4.41e-009	1.52e-013	4.09e-009			
Ca++	0.00227	0.00102	40.9			
Cl-	0.00197	0.00197	70.0			
F-	0.000115	0.000115	2.18			
H+	-0.00169	-0.000120	-0.120			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00264	0.00139	84.8			
Mg++	0.000494	0.000331	8.04			
NH3(aq)	0.000129	0.000129	2.20			
Na+	0.00148	0.00148	34.0			
O2(aq)	0.000511	0.000511	16.3			
SO4--	0.000291	0.000291	28.0			
SiO2(aq)	0.00116	0.000921	55.3			

UZ-14/1,277

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                    6.324400E-04    molal
Na+                                         1.957400E-03    molal
Mg++                                        2.098300E-04    molal
Ca++                                        1.846400E-03    molal
F-                                          1.147500E-04    molal
Cl-                                         3.666800E-03    molal
SO4--                                       3.955700E-04    molal
NO3-                                        2.419200E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
      pH =  7.793           log fO2 =   -0.699
      Eh =   0.7577 volts     pe =  12.8087
      Ionic strength     =    0.008032
      Activity of water  =    0.999871
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	8.069e-005	-4.093	0.008076	0.002980
Stellerite	4.969e-009	-8.304	7.004e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.99e-008	4.47e-013	1.21e-008			
Ca++	0.00185	0.00177	70.7			
Cl-	0.00367	0.00367	130.			
F-	0.000115	0.000115	2.18			
H+	-0.000306	-0.000225	-0.227			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00119	0.00111	67.7			
Mg++	0.000210	0.000210	5.10			
NH3(aq)	0.000242	0.000242	4.12			
Na+	0.00196	0.00196	45.0			
O2(aq)	0.000737	0.000737	23.6			

SO4--	0.000396	0.000396	38.0
SiO2(aq)	0.000632	0.000632	38.0

SD-6/412.2

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                    6.923600E-04        molal
Na+                                                         2.553300E-03        molal
K+                                                          1.662500E-04        molal
Mg++                                                        4.649200E-04        molal
Ca++                                                        1.142800E-03        molal
F-                                                          5.947800E-04        molal
Cl-                                                         1.331300E-03        molal
SO4--                                                       5.517200E-04        molal
NO3-                                                        1.261200E-03        molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go
```

OUTPUT SUMMARY:

```
       pH =  7.925            log fO2 =   -0.699
       Eh =   0.7499 volts      pe =  12.6769
       Ionic strength     =    0.007261
       Activity of water  =    0.999953
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	8.609e-005	-4.065	0.008617	0.003180
Fluorite	8.948e-005	-4.048	0.006986	0.002196
Stellerite	2.919e-009	-8.535	4.115e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.17e-008	4.41e-013	1.19e-008			
Ca++	0.00114	0.000967	38.7			
Cl-	0.00133	0.00133	47.2			

F-	0.000595	0.000416	7.90
H+	-0.00134	-0.00125	-1.26
H2O	55.5	55.5	1.00e+006
HCO3-	0.00157	0.00148	90.4
K+	0.000166	0.000166	6.50
Mg++	0.000465	0.000465	11.3
NH3(aq)	0.00126	0.00126	21.5
Na+	0.00255	0.00255	58.7
O2(aq)	0.00278	0.00278	88.8
SO4--	0.000552	0.000552	53.0
SiO2(aq)	0.000692	0.000692	41.6

SD-6/443.5

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.404700E-03	molal
Na+	2.849100E-03	molal
K+	1.023100E-04	molal
Mg++	4.813800E-04	molal
Ca++	1.202600E-03	molal
F-	3.316100E-04	molal
Cl-	1.334200E-03	molal
SO4--	1.020200E-03	molal
NO3-	1.387000E-03	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.779 log fO2 = -0.699
Eh = 0.7585 volts pe = 12.8225
Ionic strength = 0.008284
Activity of water = 0.999953

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Sepiolite	2.087e-005	-4.681	0.01352	0.005960
Stellerite	3.150e-010	-9.502	4.440e-007	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.26e-009	4.75e-014	1.28e-009			
Ca++	0.00120	0.00120	48.2			
Cl-	0.00133	0.00133	47.3			
F-	0.000332	0.000332	6.30			
H+	-0.00154	-0.00137	-1.38			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00107	0.00107	65.5			
K+	0.000102	0.000102	4.00			
Mg++	0.000481	0.000398	9.67			
NH3(aq)	0.00139	0.00139	23.6			
Na+	0.00285	0.00285	65.5			
O2(aq)	0.00303	0.00303	96.8			
SO4--	0.00102	0.00102	98.0			
SiO2(aq)	0.00140	0.00128	76.8			

SD-6/507.5

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.065200E-03	molal
Na+	2.100900E-03	molal
K+	6.138300E-05	molal
Mg++	1.012100E-03	molal
Ca++	3.118900E-03	molal
F-	1.631700E-04	molal
Cl-	5.725900E-04	molal
SO4--	3.112500E-03	molal
NO3-	4.144800E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.778 log fO2 = -0.699
Eh = 0.7586 volts pe = 12.8238
Ionic strength = 0.012742
Activity of water = 0.999980

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted

```
-------------------------------------------------------------------------------
 CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
 Calcite             0.0008482     -3.071        0.08490         0.03133
 Sepiolite           3.320e-005    -4.479        0.02151         0.009481
 Stellerite          1.052e-009    -8.978     1.483e-006

                              In fluid             Sorbed          Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
 Al+++          4.21e-009  1.47e-013 3.96e-009
 Ca++             0.00312    0.00227      90.9
 Cl-             0.000573   0.000573      20.3
 F-              0.000163   0.000163      3.10
 H+               -0.00151  -0.000400    -0.403
 H2O                 55.5       55.5 9.99e+005
 HCO3-            0.00195    0.00110      67.1
 K+              6.14e-005  6.14e-005      2.40
 Mg++             0.00101   0.000879      21.4
 NH3(aq)          0.000414   0.000414      7.05
 Na+              0.00210    0.00210      48.3
 O2(aq)           0.00108    0.00108      34.6
 SO4--            0.00311    0.00311      299.
 SiO2(aq)         0.00107    0.000866     52.0
```

SD-6/1509.9

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                  9.070500E-04        molal
Na+                                                       4.301900E-03        molal
K+                                                        2.122800E-04        molal
Mg++                                                      1.069700E-04        molal
Ca++                                                      1.641800E-03        molal
F-                                                        7.737500E-04        molal
Cl-                                                       2.784000E-03        molal
SO4--                                                     2.914700E-04        molal
NO3-                                                      2.903000E-05        molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY

pH = 8.040 log fO2 = -0.699
Eh = 0.7431 volts pe = 12.5615
Ionic strength = 0.006688
Activity of water = 0.999902

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0009659	-3.015	0.09668	0.03568
Fluorite	0.0001183	-3.927	0.009237	0.002904
Stellerite	8.082e-010	-9.092	1.139e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	3.23e-009	2.24e-013	6.05e-009			
Ca++	0.00164	0.000558	22.3			
Cl-	0.00278	0.00278	98.7			
F-	0.000774	0.000537	10.2			
H+	-0.000996	-3.01e-005	-0.0303			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00288	0.00191	116.			
K+	0.000212	0.000212	8.30			
Mg++	0.000107	0.000107	2.60			
NH3(aq)	2.90e-005	2.90e-005	0.494			
Na+	0.00430	0.00430	98.9			
O2(aq)	0.000311	0.000311	9.94			
SO4--	0.000291	0.000291	28.0			
SiO2(aq)	0.000907	0.000907	54.5			

SD-7/370.3

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 gram Albite_low  [Note:  All other scripts specified 1 “free” gram.  For SD-7/370.3, specifying 1 free gram caused nonconvergence.  The program converged if the amount of Albite_low was specified as “1 gram” instead of “1 free gram”]
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                4.310590E-04        molal
Na+                                                     1.696380E-03        molal
Mg++                                                    8.228720E-06        molal
Ca++                                                    7.210910E-03        molal
F-                                                      1.147460E-04        molal
Cl-                                                     3.751430E-03        molal
SO4--                                                   6.766320E-03        molal
NO3-                                                    9.676610E-06        molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
```

```
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  3.572             log fO2 =   -0.699
        Eh =   1.0074 volts      pe =  17.0301
        Ionic strength      =
        Activity of water   =    0.999868


                      moles       moles        grams         cm3
 Reactants             remaining    reacted      reacted       reacted
-------------------------------------------------------------------------------
 CO2(g)              -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
 Stellerite          2.606e-005     -4.584        0.03673
                                                 _____________  _____________
       (total)                                     0.03673        0.0000*


                              In fluid              Sorbed           Kd
 Original basis total moles   moles     mg/kg       moles     mg/kg      L/kg
-------------------------------------------------------------------------------
 Al+++          0.000326   0.000221      5.96
 Ca++            0.00721    0.00716      287.
 Cl-             0.00375    0.00375      133.
 F-             0.000115   0.000115      2.18
 H+            -4.12e-006   0.000413     0.416
 H2O                55.5       55.5 9.99e+005
 HCO3-          3.40e-005  3.40e-005      2.07
 Mg++           8.23e-006  8.23e-006     0.200
 NH3(aq)        9.68e-006  9.68e-006     0.165
 Na+              0.00202    0.00202      46.4
 O2(aq)          0.000272   0.000272      8.70
 SO4--            0.00677    0.00677      649.
 SiO2(aq)         0.00141    0.00104      62.6
```

SD-9/176.2

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                          9.736300E-04        molal
Na+                                               4.132200E-03        molal
Mg++                                              3.908600E-04        molal
Ca++                                              1.072900E-03        molal
F-                                                1.147500E-04        molal
Cl-                                               1.805200E-03        molal
SO4--                                             1.290800E-03        molal
NO3-                                              3.064300E-05        molal
go
```

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.989 log fO2 = -0.699
Eh = 0.7461 volts pe = 12.6124
Ionic strength = 0.008147
Activity of water = 0.999936

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0003138	-3.503	0.03141	0.01159
Sepiolite	2.306e-005	-4.637	0.01494	0.006586
Stellerite	6.633e-010	-9.178	9.350e-007	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Kd mg/kg	Kd L/kg
Al+++	2.65e-009	2.67e-013	7.19e-009			
Ca++	0.00107	0.000759	30.4			
Cl-	0.00181	0.00181	64.0			
F-	0.000115	0.000115	2.18			
H+	-0.000526	-2.74e-005	-0.0276			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00203	0.00172	105.			
Mg++	0.000391	0.000299	7.25			
NH3(aq)	3.06e-005	3.06e-005	0.522			
Na+	0.00413	0.00413	95.0			
O2(aq)	0.000314	0.000314	10.0			
SO4--	0.00129	0.00129	124.			
SiO2(aq)	0.000974	0.000835	50.2			

UZ-14/85.2

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.494600E-03	molal
Na+	1.892100E-03	molal

Mg++	5.431000E-04	molal
Ca++	1.245100E-03	molal
F-	1.147500E-04	molal
Cl-	1.692400E-03	molal
SO4--	6.870400E-04	molal
NO3-	3.548100E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.878 log fO2 = -0.699
Eh = 0.7527 volts pe = 12.7239
Ionic strength = 0.006690
Activity of water = 0.999940

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	5.599e-005	-4.252	0.005604	0.002068
Sepiolite	6.261e-005	-4.203	0.04056	0.01788
Stellerite	3.880e-010	-9.411	5.469e-007	

Original basis total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.55e-009	7.31e-014	1.97e-009		
Ca++	0.00125	0.00119	47.6		
Cl-	0.00169	0.00169	60.0		
F-	0.000115	0.000115	2.18		
H+	-0.000903	-0.000346	-0.349		
H2O	55.5	55.5	1.00e+006		
HCO3-	0.00138	0.00133	81.0		
Mg++	0.000543	0.000293	7.11		
NH3(aq)	0.000355	0.000355	6.04		
Na+	0.00189	0.00189	43.5		
O2(aq)	0.000962	0.000962	30.8		
SO4--	0.000687	0.000687	66.0		
SiO2(aq)	0.00149	0.00112	67.2		

UZ-14/147.7

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+

suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.286520E-03	molal
Na+	2.244450E-03	molal
Mg++	4.731520E-04	molal
Ca++	1.367330E-03	molal
F-	1.147460E-04	molal
Cl-	1.692370E-03	molal
SO4--	6.870420E-04	molal
NO3-	3.548090E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.905 log fO2 = -0.699
Eh = 0.7511 volts pe = 12.6967
Ionic strength = 0.006656
Activity of water = 0.999940

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0003168	-3.499	0.03171	0.01170
Sepiolite	4.414e-005	-4.355	0.02859	0.01261
Stellerite	5.187e-010	-9.285	7.311e-007	

Original basis total	moles	In fluid mg/kg	moles	Sorbed mg/kg	Kd L/kg
Al+++	2.07e-009	1.07e-013	2.89e-009		
Ca++	0.00137	0.00105	42.1		
Cl-	0.00169	0.00169	60.0		
F-	0.000115	0.000115	2.18		
H+	-0.00102	-0.000347	-0.349		
H2O	55.5	55.5	1.00e+006		
HCO3-	0.00173	0.00141	86.0		
Mg++	0.000473	0.000297	7.21		
NH3(aq)	0.000355	0.000355	6.04		
Na+	0.00224	0.00224	51.6		
O2(aq)	0.000962	0.000962	30.8		
SO4--	0.000687	0.000687	66.0		
SiO2(aq)	0.00129	0.00102	61.4		

NRG-6/244.6

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0

```
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                    8.488100E-04    molal
Na+                                         3.131800E-03    molal
Mg++                                        2.016000E-04    molal
Ca++                                        8.233900E-04    molal
F-                                          1.147500E-04    molal
Cl-                                         1.382100E-03    molal
SO4--                                       1.197100E-03    molal
NO3-                                        6.451100E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
      pH =  7.574           log fO2 =  -0.699
      Eh =  0.7707 volts    pe =  13.0281
      Ionic strength     =   0.007034
      Activity of water  =   0.999951

                  moles       moles       grams       cm3
 Reactants        remaining   reacted     reacted     reacted
-------------------------------------------------------------------------------
 CO2(g)           -- fixed fugacity buffer --

 Minerals in system    moles     log moles     grams       volume (cm3)
-------------------------------------------------------------------------------
 Stellerite         1.301e-009    -8.886    1.833e-006
                        In fluid          Sorbed          Kd
 Original basis total moles   moles   mg/kg    moles   mg/kg    L/kg
-------------------------------------------------------------------------------
 Al+++        5.20e-009  2.40e-013 6.46e-009
 Ca++          0.000823   0.000823     33.0
 Cl-           0.00138    0.00138     49.0
 F-           0.000115   0.000115     2.18
 H+           -0.000619  -0.000619   -0.623
 H2O             55.5       55.5 1.00e+006
 HCO3-         0.000672   0.000672     41.0
 Mg++          0.000202   0.000202     4.90
 NH3(aq)       0.000645   0.000645     11.0
 Na+           0.00313    0.00313     72.0
 O2(aq)        0.00154    0.00154     49.4
 SO4--         0.00120    0.00120     115.
 SiO2(aq)      0.000849   0.000849    51.0
```

NRG-6/255.9

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
```

```
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                    1.131700E-03    molal
Na+                                         9.351900E-03    molal
Mg++                                        7.817300E-04    molal
Ca++                                        4.391400E-03    molal
F-                                          1.147460E-04    molal
Cl-                                         3.243700E-03    molal
SO4--                                       8.744200E-03    molal
NO3-                                        5.644700E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
       pH =  3.599             log fO2 =   -0.699
        Eh =   1.0058 volts      pe =  17.0028
        Ionic strength      =    0.029621
        Activity of water   =    0.999886

                    moles       moles        grams         cm3
 Reactants          remaining   reacted      reacted       reacted
-------------------------------------------------------------------------------
 CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
 Stellerite          2.354e-005     -4.628        0.03318

                              In fluid             Sorbed          Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
 Al+++          0.000568   0.000474      12.8
 Ca++            0.00439    0.00434      174.
 Cl-             0.00324    0.00324      115.
 F-             0.000115   0.000115      2.18
 H+             -0.000521  -0.000144    -0.145
 H2O                 55.5       55.5 9.99e+005
 HCO3-          3.40e-005  3.40e-005      2.07
 Mg++           0.000782   0.000782      19.0
 NH3(aq)        0.000564   0.000564      9.60
 Na+             0.00935    0.00935      215.
 O2(aq)          0.00138    0.00138      44.1
 SO4--           0.00874    0.00874      839.
 SiO2(aq)        0.00113   0.000802      48.1
```

UZ-14/178.1

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                    1.549500E-03    molal
Na+                                         2.135700E-03    molal
Mg++                                        4.361200E-04    molal
Ca++                                        1.596900E-03    molal
F-                                          1.147500E-04    molal
Cl-                                         2.736000E-03    molal
SO4--                                       1.249200E-03    molal
NO3-                                        3.386800E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
       pH =  7.465            log fO2 =   -0.699
       Eh =   0.7771 volts     pe =  13.1363
       Ionic strength     =    0.008841
       Activity of water  =    0.999903

                    moles       moles        grams         cm3
 Reactants          remaining   reacted      reacted       reacted
-------------------------------------------------------------------------------
  CO2(g)            -- fixed fugacity buffer --

 Minerals in system    moles      log moles     grams        volume (cm3)
-------------------------------------------------------------------------------
  Stellerite        3.258e-010     -9.487     4.592e-007


                              In fluid            Sorbed          Kd
 Original basis total moles   moles     mg/kg     moles     mg/kg     L/kg
-------------------------------------------------------------------------------
  Al+++          1.30e-009  2.18e-014 5.89e-010
  Ca++             0.00160    0.00160      64.0
  Cl-              0.00274    0.00274      96.9
  F-              0.000115   0.000115      2.18
  H+             -0.000313  -0.000313    -0.316
  H2O                55.5       55.5 9.99e+005
  HCO3-           0.000539   0.000539      32.9
  Mg++            0.000436   0.000436      10.6
  NH3(aq)         0.000339   0.000339      5.77
  Na+              0.00214    0.00214      49.1
  O2(aq)          0.000930   0.000930      29.7
```

SO4--	0.00125	0.00125	120.
SiO2(aq)	0.00155	0.00155	93.1

UZ-14/1258.5

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
```

SiO2(aq)	5.825120E-04	molal
Na+	2.914300E-03	molal
Mg++	1.522310E-04	molal
Ca++	1.072900E-03	molal
F-	1.147460E-04	molal
Cl-	2.482150E-03	molal
SO4--	1.977850E-04	molal
NO3-	2.580430E-04	molal

```
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
       pH =  7.956             log fO2 =   -0.699
       Eh =   0.7481 volts      pe =  12.6457
       Ionic strength      =    0.005853
       Activity of water   =    0.999912
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0002763	-3.559	0.02765	0.01020
Stellerite	4.222e-009	-8.374	5.951e-006	

Original basis total	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.69e-008	8.58e-013	2.31e-008		
Ca++	0.00107	0.000797	31.9		
Cl-	0.00248	0.00248	88.0		
F-	0.000115	0.000115	2.18		
H+	-0.000524	-0.000248	-0.250		
H2O	55.5	55.5	1.00e+006		

HCO3-	0.00185	0.00157	95.9
Mg++	0.000152	0.000152	3.70
NH3(aq)	0.000258	0.000258	4.39
Na+	0.00291	0.00291	67.0
O2(aq)	0.000769	0.000769	24.6
SO4--	0.000198	0.000198	19.0
SiO2(aq)	0.000583	0.000582	35.0

UZ-14/1409.4

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                        9.486630E-04    molal
Na+                                             3.827740E-03    molal
Mg++                                            2.880050E-05    molal
Ca++                                            7.485370E-04    molal
F-                                              1.147460E-04    molal
Cl-                                             2.115470E-03    molal
SO4--                                           1.103430E-03    molal
NO3-                                            8.063840E-05    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
       pH =  7.700            log fO2 =   -0.699
       Eh =   0.7632 volts      pe =  12.9021
       Ionic strength      =    0.007007
       Activity of water   =    0.999925
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	7.518e-010	-9.124	1.060e-006	

Original basis total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	3.01e-009	1.68e-013	4.53e-009		
Ca++	0.000749	0.000749	30.0		

Cl-	0.00212	0.00212	75.0
F-	0.000115	0.000115	2.18
H+	-5.83e-005	-5.83e-005	-0.0587
H2O	55.5	55.5	1.00e+006
HCO3-	0.000887	0.000887	54.1
Mg++	2.88e-005	2.88e-005	0.700
NH3(aq)	8.06e-005	8.06e-005	1.37
Na+	0.00383	0.00383	88.0
O2(aq)	0.000414	0.000414	13.2
SO4--	0.00110	0.00110	106.
SiO2(aq)	0.000949	0.000949	57.0

UZ-14/1,542

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                2.380000E-03        molal
Na+                                                     9.003900E-03        molal
Mg++                                                    2.057200E-05        molal
Ca++                                                    8.982400E-05        molal
F-                                                      1.147500E-04        molal
Cl-                                                     5.641200E-04        molal
SO4--                                                   2.914700E-04        molal
NO3-                                                    6.451100E-05        molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  8.625             log fO2 =   -0.699
        Eh =   0.7085 volts      pe =  11.9767
        Ionic strength      =    0.009481
        Activity of water   =    0.999980
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	4.214e-005	-4.375	0.004218	0.001557
Sepiolite	4.002e-006	-5.398	0.002592	0.001143
SiO2(am)	0.0002888	-3.539	0.01735	0.008374

Stellerite 2.399e-011 -10.620 3.381e-008

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	9.60e-011	5.74e-014	1.55e-009			
Ca++	8.98e-005	4.77e-005	1.91			
Cl-	0.000564	0.000564	20.0			
F-	0.000115	0.000115	2.18			
H+	-0.000445	-0.000371	-0.373			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00752	0.00748	456.			
Mg++	2.06e-005	4.56e-006	0.111			
NH3(aq)	6.45e-005	6.45e-005	1.10			
Na+	0.00900	0.00900	207.			
O2(aq)	0.000382	0.000382	12.2			
SO4--	0.000291	0.000291	28.0			
SiO2(aq)	0.00238	0.00207	124.			

UZ-14/1825.8

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                7.972100E-04    molal
Na+                                                     5.959100E-03    molal
Mg++                                                    4.114400E-06    molal
Ca++                                                    1.497100E-05    molal
F-                                                      1.147500E-04    molal
Cl-                                                     6.628500E-04    molal
SO4--                                                   1.342900E-04    molal
NO3-                                                    1.903100E-04    molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  8.435             log fO2 =   -0.699
        Eh =   0.7197 volts      pe =  12.1671
        Ionic strength      =    0.006172
        Activity of water   =    0.999976
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted

CO2(g) -- fixed fugacity buffer --

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	8.521e-010	-9.070	1.201e-006	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	3.41e-009	2.37e-012	6.38e-008			
Ca++	1.50e-005	1.50e-005	0.600			
Cl-	0.000663	0.000663	23.5			
F-	0.000115	0.000115	2.18			
H+	-0.000267	-0.000267	-0.269			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00468	0.00468	286.			
Mg++	4.11e-006	4.11e-006	0.0999			
NH3(aq)	0.000190	0.000190	3.24			
Na+	0.00596	0.00596	137.			
O2(aq)	0.000633	0.000633	20.3			
SO4--	0.000134	0.000134	12.9			
SiO2(aq)	0.000797	0.000797	47.9			

UZ-14/2014.7

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	6.274490E-04	molal
Na+	1.705080E-02	molal
Mg++	8.228720E-06	molal
Ca++	7.984400E-05	molal
F-	1.147460E-04	molal
Cl-	9.054200E-04	molal
SO4--	2.310960E-04	molal
NO3-	2.902980E-05	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 8.893 log fO2 = -0.699
Eh = 0.6926 volts pe = 11.7086
Ionic strength = 0.017744

```
       Activity of water   =    0.999968
                        moles       moles        grams         cm3
 Reactants            remaining     reacted      reacted      reacted
--------------------------------------------------------------------------------
 CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams       volume (cm3)
--------------------------------------------------------------------------------
 Calcite            5.920e-005     -4.228       0.005925       0.002186
 Stellerite         9.314e-010     -9.031      1.313e-006
                          In fluid             Sorbed           Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
--------------------------------------------------------------------------------
 Al+++          3.73e-009  9.37e-012 2.52e-007
 Ca++           7.98e-005  2.06e-005     0.826
 Cl-            0.000905   0.000905      32.1
 F-             0.000115   0.000115      2.18
 H+            -0.000923  -0.000864    -0.870
 H2O                55.5       55.5 9.99e+005
 HCO3-            0.0148     0.0148      899.
 Mg++           8.23e-006  8.23e-006     0.200
 NH3(aq)        2.90e-005  2.90e-005     0.494
 Na+              0.0171     0.0171      391.
 O2(aq)         0.000311   0.000311      9.93
 SO4--          0.000231   0.000231      22.2
 SiO2(aq)       0.000627   0.000627      37.6
```

UZ-16/1343.7

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                          1.033500E-03        molal
Na+                                               4.306200E-03        molal
Mg++                                              9.874500E-05        molal
Ca++                                              4.241700E-04        molal
F-                                                1.147500E-04        molal
Cl-                                               1.579500E-03        molal
SO4--                                             2.394200E-04        molal
NO3-                                              2.90E-04            molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go
```

OUTPUT SUMMARY:

pH = 8.176 log fO2 = -0.699
Eh = 0.7350 volts pe = 12.4254
Ionic strength = 0.005609
Activity of water = 0.999944

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0001292	-3.889	0.01294	0.004773
Sepiolite	3.844e-006	-5.415	0.002490	0.001098
Stellerite	5.164e-010	-9.287	7.278e-007	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	2.07e-009	2.11e-013	5.69e-009			
Ca++	0.000424	0.000295	11.8			
Cl-	0.00158	0.00158	56.0			
F-	0.000115	0.000115	2.18			
H+	-0.000469	-0.000309	-0.311			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00271	0.00258	157.			
Mg++	9.87e-005	8.34e-005	2.03			
NH3(aq)	0.000290	0.000290	4.94			
Na+	0.00431	0.00431	99.0			
O2(aq)	0.000833	0.000833	26.6			
SO4--	0.000239	0.000239	23.0			
SiO2(aq)	0.00103	0.00101	60.7			

WT-24/1937.0

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                                7.556000E-04        molal
Na+                                                     2.522800E-03        molal
K+                                                      1.713600E-04        molal
Mg++                                                    2.468600E-05        molal
Ca++                                                    3.967200E-04        molal
F-                                                      2.210700E-04        molal
Cl-                                                     1.009800E-03        molal
SO4--                                                   6.245800E-05        molal
NO3-                                                    8.063800E-06        molal
go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
```

```
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  8.103             log fO2 =   -0.699
        Eh =   0.7394 volts      pe =  12.4988
        Ionic strength      =    0.003956
        Activity of water   =    0.999964

                        moles        moles        grams         cm3
 Reactants               remaining     reacted       reacted       reacted
-------------------------------------------------------------------------------
 CO2(g)              -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
 Calcite             8.685e-006     -5.061      0.0008693       0.0003208
 Stellerite          2.158e-009     -8.666     3.041e-006
                              In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
 Al+++          8.63e-009  4.81e-013 1.30e-008
 Ca++            0.000397   0.000388      15.5
 Cl-             0.00101    0.00101      35.8
 F-             0.000221   0.000221      4.20
 H+            -1.90e-005 -1.03e-005   -0.0104
 H2O                 55.5       55.5 1.00e+006
 HCO3-            0.00216    0.00215      131.
 K+              0.000171   0.000171      6.70
 Mg++             2.47e-005  2.47e-005     0.600
 NH3(aq)          8.06e-006  8.06e-006     0.137
 Na+              0.00252    0.00252      58.0
 O2(aq)           0.000269   0.000269      8.60
 SO4--            6.25e-005  6.25e-005     6.00
 SiO2(aq)         0.000756   0.000756      45.4
```

NRG-6/219.9

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                          1.021900E-03        molal
Na+                                               4.319300E-03        molal
Mg++                                              1.728000E-04        molal
Ca++                                              6.063100E-04        molal
F-                                                1.147500E-04        molal
Cl-                                               2.171900E-03        molal
SO4--                                             8.015500E-04        molal
NO3-                                              7.580000E-04        molal
go

pickup fluid
```

```
fix fugacity of CO2(g)
remove H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip = on
go
```

OUTPUT SUMMARY:

```
        pH =  7.850             log fO2 =   -0.699
        Eh =   0.7543 volts      pe =  12.7518
        Ionic strength      =    0.007227
        Activity of water   =    0.999923

                        moles       moles        grams         cm3
 Reactants               remaining    reacted      reacted      reacted
-------------------------------------------------------------------------------
  CO2(g)             -- fixed fugacity buffer --

 Minerals in system     moles      log moles      grams        volume (cm3)
-------------------------------------------------------------------------------
  Stellerite          5.304e-010     -9.275     7.475e-007
                            In fluid              Sorbed             Kd
 Original basis total moles   moles      mg/kg      moles      mg/kg      L/kg
-------------------------------------------------------------------------------
  Al+++          2.12e-009  1.43e-013 3.85e-009
  Ca++            0.000606   0.000606      24.3
  Cl-             0.00217    0.00217       77.0
  F-             0.000115   0.000115       2.18
  H+             -0.000744  -0.000744     -0.749
  H2O                55.5       55.5  1.00e+006
  HCO3-           0.00124    0.00124       75.9
  Mg++            0.000173   0.000173      4.20
  NH3(aq)         0.000758   0.000758      12.9
  Na+             0.00432    0.00432       99.3
  O2(aq)          0.00177    0.00177       56.6
  SO4--           0.000802   0.000802      77.0
  SiO2(aq)        0.00102    0.00102       61.4
```

NRG-7a/460.25

```
swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress  Dolomite Dolomite-dis Dolomite-ord Quartz
suppress  Tridymite Chalcedony Talc Coesite
suppress  Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress  Saponite-K Saponite-Na Saponite-H
precip off
SiO2(aq)                                          1.497900E-04        molal
Na+                                               1.826900E-03        molal
K+                                                1.739200E-04        molal
Ca++                                              7.485400E-05        molal
F-                                                1.147500E-04        molal
Cl-                                               1.974400E-04        molal
SO4--                                             4.163900E-05        molal
NO3-                                              1.612800E-05        molal
```

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip = on
go

OUTPUT SUMMARY:

pH = 8.023 log fO2 = -0.699
Eh = 0.7441 volts pe = 12.5785
Ionic strength = 0.002263
Activity of water = 0.999993

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Stellerite	3.681e-007	-6.434	0.0005188	

Original basis total	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	1.47e-006	3.39e-010	9.15e-006		
Ca++	7.49e-005	7.41e-005	2.97		
Cl-	0.000197	0.000197	7.00		
F-	0.000115	0.000115	2.18		
H+	-1.98e-006	3.90e-006	0.00393		
H2O	55.5	55.5	1.00e+006		
HCO3-	0.00176	0.00176	107.		
K+	0.000174	0.000174	6.80		
NH3(aq)	1.61e-005	1.61e-005	0.275		
Na+	0.00183	0.00183	42.0		
O2(aq)	0.000285	0.000285	9.12		
SO4--	4.16e-005	4.16e-005	4.00		
SiO2(aq)	0.000150	0.000145	8.69		

SD-12/1495.5

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip off

SiO2(aq)	1.453000E-03	molal
Na+	4.697700E-03	molal
Mg++	8.228700E-06	molal
Ca++	3.992200E-04	molal

F-	1.147500E-04	molal
Cl-	1.607800E-03	molal
SO4--	5.725300E-04	molal
NO3-	1.306300E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
precip = on
go

OUTPUT SUMMARY:

pH = 8.143 log fO2 = -0.699
Eh = 0.7370 volts pe = 12.4588
Ionic strength = 0.006248
Activity of water = 0.999943

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	4.546e-005	-4.342	0.004550	0.001679
Stellerite	1.703e-010	-9.769	2.401e-007	

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	6.81e-010	5.48e-014	1.48e-009			
Ca++	0.000399	0.000354	14.2			
Cl-	0.00161	0.00161	57.0			
F-	0.000115	0.000115	2.18			
H+	-0.000199	-0.000153	-0.154			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00245	0.00240	146.			
Mg++	8.23e-006	8.23e-006	0.200			
NH3(aq)	0.000131	0.000131	2.22			
Na+	0.00470	0.00470	108.			
O2(aq)	0.000514	0.000514	16.4			
SO4--	0.000573	0.000573	55.0			
SiO2(aq)	0.00145	0.00145	87.3			

SD-6/522.5

swap NO3- for NH3(aq)
swap O2(g) for O2(aq)
swap CO2(g) for HCO3-
f O2(g) = .2
log f CO2(g) = -3.0
fix f CO2(g)
swap Albite_low for Al+++
1 free gram Albite_low
-7.7 log molarity H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H

precip off

SiO2(aq)	1.060170E-03	molal
Na+	2.566330E-03	molal
K+	1.534590E-04	molal
Mg++	4.073220E-04	molal
Ca++	1.090370E-03	molal
F-	4.052950E-04	molal
Cl-	7.418240E-04	molal
SO4--	5.829450E-04	molal
NO3-	5.564050E-04	molal

go

pickup fluid

fix fugacity of CO2(g)
remove H+
balance on H+
suppress Dolomite Dolomite-dis Dolomite-ord Quartz
suppress Tridymite Chalcedony Talc Coesite
suppress Cristobalite(beta) Cristobalite(alpha) Saponite-Ca Saponite-Mg
suppress Saponite-K Saponite-Na Saponite-H
suppress Tremolite Antigorite
precip = on
go

OUTPUT SUMMARY:

pH = 7.997 log fO2 = -0.699
Eh = 0.7456 volts pe = 12.6043
Ionic strength = 0.005881
Activity of water = 0.999974

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			

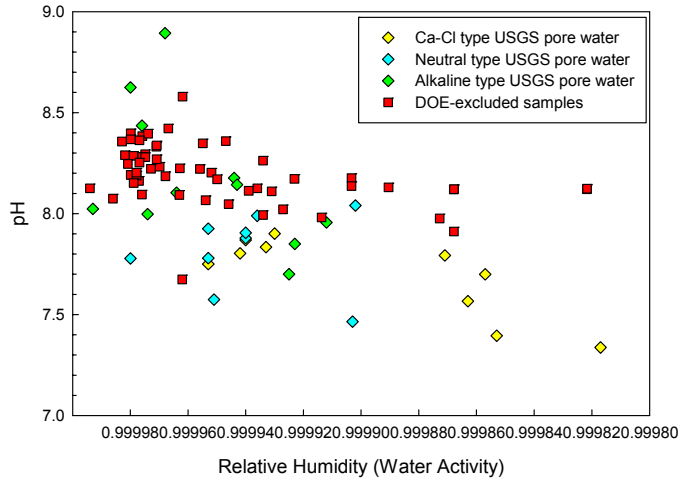
Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.0004132	-3.384	0.04136	0.01526
Sepiolite	3.724e-005	-4.429	0.02412	0.01063
Stellerite	8.121e-010	-9.090	1.145e-006	

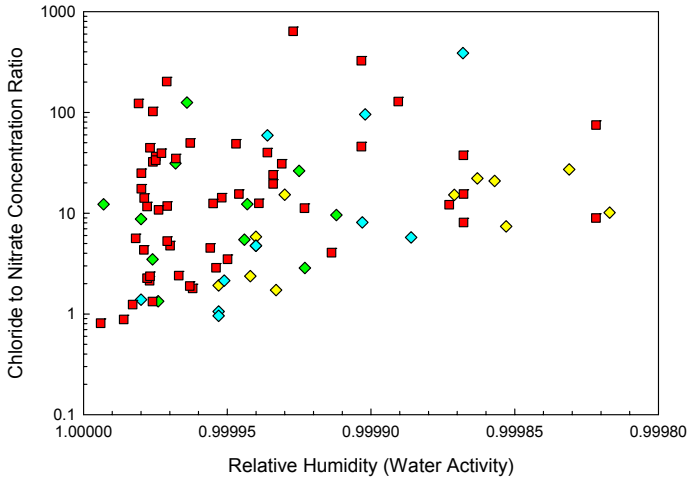
Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Al+++	3.25e-009	2.66e-013	7.19e-009			
Ca++	0.00109	0.000677	27.1			
Cl-	0.000742	0.000742	26.3			
F-	0.000405	0.000405	7.70			
H+	-0.00126	-0.000553	-0.557			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00214	0.00173	105.			
K+	0.000153	0.000153	6.00			
Mg++	0.000407	0.000258	6.28			
NH3(aq)	0.000556	0.000556	9.47			
Na+	0.00257	0.00257	59.0			
O2(aq)	0.00137	0.00137	43.7			
SO4--	0.000583	0.000583	56.0			
SiO2(aq)	0.00106	0.000837	50.3			

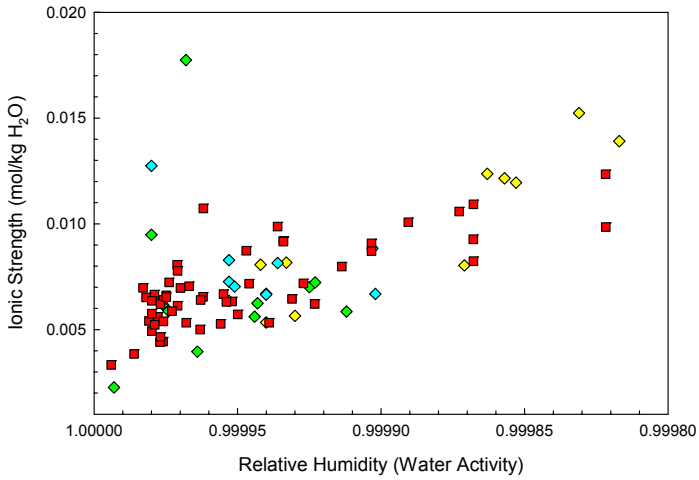
The following table summarizes the results of the REACT calculations:

Sample Name	Brine type	pH	ionic strength	aH2O	Cl- molal	NH3(aq) = NO3- molal	Cl/NO3 ratio
NRG-6/158.2	Ca-Cl	7.34	0.013907	0.999817	0.00522	0.000516	10.12
NRG-6/160.8	Ca-Cl	7.40	0.011947	0.999853	0.00417	0.000564	7.39
NRG-6/171.0	Ca-Cl	7.80	0.008066	0.999942	0.00164	0.000693	2.37
NRG-6/175.6	Ca-Cl	7.75	0.00636	0.999953	0.00133	0.000693	1.92
SD-12/296.1	Ca-Cl	7.87	0.005337	0.99994	0.00169	0.00029	5.83
SD-6/471.3	Ca-Cl	7.83	0.008163	0.999933	0.00188	0.00109	1.72
SD-9/114.1	Ca-Cl	7.57	0.012367	0.999863	0.00389	0.000176	22.10
SD-9/135.1	Ca-Cl	7.70	0.012152	0.999857	0.00406	0.000194	20.93
SD-9/94.2	Ca-Cl	**3.83**	0.015235	0.999831	0.0048	0.000177	27.12
UZ-16/1643.4	Ca-Cl	7.90	0.005652	0.99993	0.00197	0.000129	15.27
UZ-14/1,277	Ca-Cl	7.79	0.008032	0.999871	0.00367	0.000242	15.17
SD-6/412.2	Neutral	7.93	0.007261	0.999953	0.00133	0.00126	1.06
SD-6/443.5	Neutral	7.78	0.008284	0.999953	0.00133	0.00139	0.96
SD-6/507.5	Neutral	7.78	0.012742	0.99998	0.000573	0.000414	1.38
SD-6/1509.9	Neutral	8.04	0.006688	0.999902	0.00278	0.000029	95.86
SD-7/370.3	Neutral	**3.57**	0.026073	0.999868	0.00375	9.68E-06	387.40
SD-9/176.2	Neutral	7.99	0.008147	0.999936	0.00181	0.0000306	59.15
UZ-14/85.2	Neutral	7.88	0.00669	0.99994	0.00169	0.000355	4.76
UZ-14/147.7	Neutral	7.91	0.006656	0.99994	0.00169	0.000355	4.76
NRG-6/244.6	Neutral	7.57	0.007034	0.999951	0.00138	0.000645	2.14
NRG-6/255.9	Neutral	**3.60**	0.029621	0.999886	0.00324	0.000564	5.74
UZ-14/178.1	Neutral	7.47	0.008841	0.999903	0.00274	0.000339	8.08
UZ-14/1258.5	Alkaline	7.96	0.005853	0.999912	0.00248	0.000258	9.61
UZ-14/1409.4	Alkaline	7.70	0.007007	0.999925	0.00212	0.0000806	26.30
UZ-14/1,542	Alkaline	8.63	0.009481	0.99998	0.000564	0.0000645	8.74
UZ-14/1825.8	Alkaline	8.44	0.006172	0.999976	0.000663	0.00019	3.49
UZ-14/2014.7	Alkaline	8.89	0.017744	0.999968	0.000905	0.000029	31.21
UZ-16/1343.7	Alkaline	8.18	0.005609	0.999944	0.00158	0.00029	5.45
WT-24/1937.0	Alkaline	8.10	0.003956	0.999964	0.00101	0.00000806	125.31
NRG-6/219.9	Alkaline	7.85	0.007227	0.999923	0.00217	0.000758	2.86
NRG-7a/460.25	Alkaline	8.02	0.002263	0.999993	0.000197	0.0000161	12.24
SD-12/1495.5	Alkaline	8.14	0.006248	0.999943	0.00161	0.000131	12.29
SD-6/522.5	Alkaline	8.00	0.005881	0.999974	0.000742	0.000556	1.33

The following plot compares the calculated results for the 33 U.S.G.S. pore waters with the 56 samples DOE excluded from consideration for its near-field chemistry model.







July 6, 2009

The following text is from the DOE Safety Evaluation Report:

2.3.5.5.4.2.1 Seepage Evaporation Abstraction Description

The seepage evaporation abstraction includes multiple sets of lookup tables representing possible in-drift crown and invert water compositions due to evaporation or dilution of seepage or imbibed water and the associated model uncertainties (SNL 2007b, Section 6.9). TSPA implementation of the lookup tables is discussed in Section 2.3.5.5.4.3.

As described in Section 2.3.5.5.3.2, the near-field chemistry model provides the potential seepage water compositions that are the inputs to the seepage evaporation analyses. The near-field chemistry model inputs consist of the four representative group waters, modified by the addition of 11 discrete amounts of alkali feldspar (water–rock interaction parameter values) to generate 44 water compositions, and brought to equilibrium at three discrete temperatures at the evaporation front (30°C, 70°C, and 96°C). The 44 waters at each temperature provide feeds to in-drift seepage evaporation simulations at corresponding temperatures of 30°C, 70°C, and 100°C (the near-field chemistry model does not predict water compositions at temperatures above the boiling point of water, so 96°C near-field chemistry water compositions are used as the feed for the 100°C seepage evaporation simulations). At each temperature, the waters are evaporated at three different pCO_2 values (10^{-2}, 10^{-3}, and 10^{-4}) bars; in a second set of EQ3/6 simulations, the waters were diluted by a factor of 100. The results of the evaporation and dilution simulations for each water, at each combination of temperature and pCO_2, were combined), resulting in 396 lookup tables (4 pore waters × 11 water–rock interaction parameter values × 3 temperatures × 3 pCO_2 values). These lookup tables represent the range of chemical compositions potentially generated by evaporation or dilution of crown seepage or condensation, or waters imbibed into the invert. Dilution is implemented when the in-drift relative humidity at the waste package surface exceeds the equilibrium relative humidity of the seepage input water from the near-field chemistry model (SNL 2007b, Section 6.9.1).

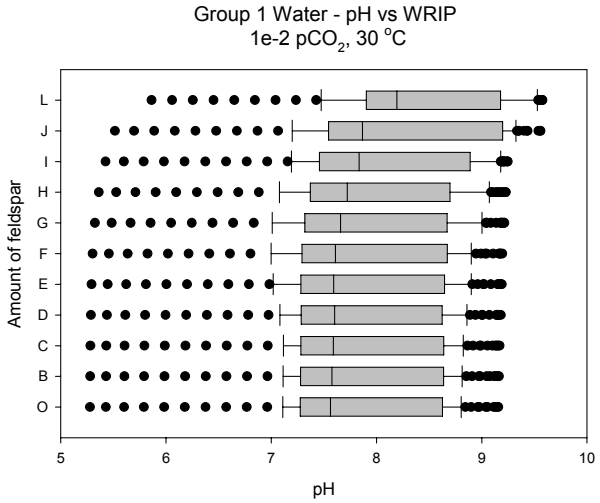
In order to be able to compare the water chemistry of evaporated pore waters calculated using OLIAnalyzer with the water chemistry used in the DOE TSPA, the chemistry information DOE abstracted in the form of 396 lookup tables were extracted from the TSPA GoldSim. The following procedure was used to extract the GoldSim information into Excel files:

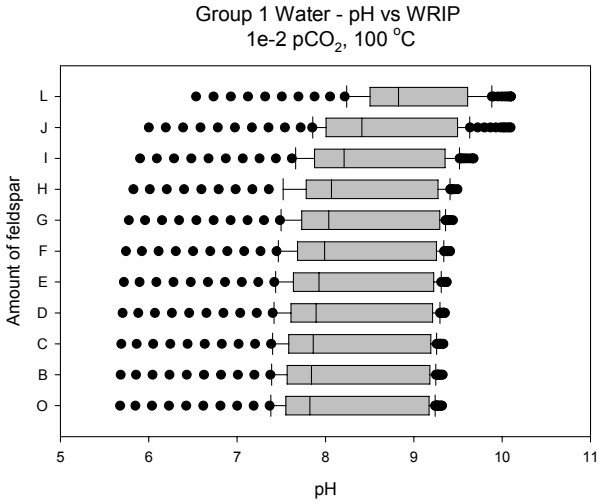
1. Run GoldSim player. Open la_v5.005_sm_009000_003.gsp.
2. Type this into search box (upper left hand corner of screen): Chemical_Comp_LUTs
3. Click on search symbol.
4. Expand the box “Chemical composition lookup tables for PCE model” by left-clicking on the (+) sign.
5. There are four boxes for “Chemical Composition Look-Up Tables”: Starting Waters 1, 2, 3, and 4
6. Expand box for Starting Water 1
7. There are 11 boxes for each value of Water-Rock Interaction Parameter (WRIP)
8. Expand box for “Chemical Composition Look-Up Tables for Starting Water 1, WRIP Parameter 0”
9. There are 9 boxes representing three temperatures (30, 70, and 100 °C) and three pCO2 values (1E-2, 1E-3, and 1E-4 atm)

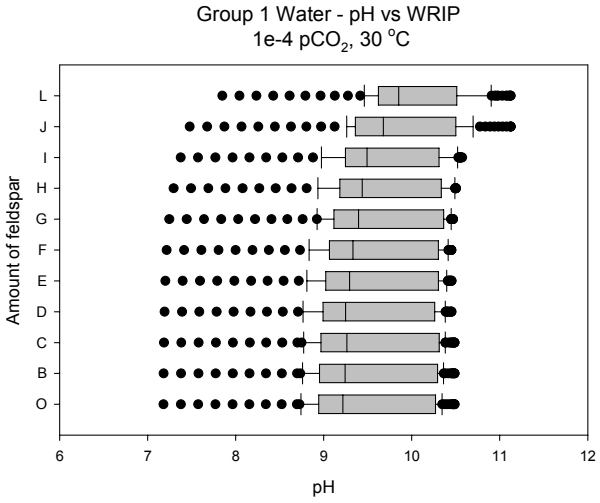
10. Right click on one box and click on Properties. This will open a window.
11. Click on "View Data" button, which will open a table with 7 columns.
12. Drag the cursor from the top leftmost corner to the bottom rightmost corner to highlight all data in the table. On the keyboard, press ctrl-C (to copy the highlighted data).
13. Open an Excel file, then paste the data into a worksheet (ctrl-V on keyboard).
14. Add a row at the top of the worksheet.
15. Label the columns as follows:
    A: Relative Humidity
    B: pH
    C: Ionic Strength
    D: Chloride concentration
    E: Nitrate concentration
    F: Concentration Factor
    G. Dilution Factor
16. In column H, add the label Chloride/Nitrate Ratio
17. Calculate values in Column H by dividing Column D by Column E (e.g., type in "=D2/E2" in Column H, Row 2)
18. Close the GoldSim data window. In the Lookup Table Properties window, copy the Description (e.g., "P&CE: In-drift Chemistry Table, Group 1, Amt Feldspar = 0, pCO2 = 1e-2, T=30°C"). Switch to Excel then paste the Description onto Column I, Row 1.
19. Label the worksheet "pCO2 = 1e-2, T=30°C".
20. Save the Excel file with filename "Group 1, Amt Feldspar = 0"
21. Close the Lookup Table Properties window, then go to the next one (do all nine; copy the results into separate worksheets).
22. After completing all nine tables for WRIP Parameter 0, save the Excel file (filename "Group 1, Amt Feldspar = 0"). Then do the same for the following (save in separate Excel files, each having nine worksheets)
    a. WRIP Parameter B
    b. WRIP Parameter C
    c. WRIP Parameter D
    d. WRIP Parameter E
    e. WRIP Parameter F
    f. WRIP Parameter G
    g. WRIP Parameter H
    h. WRIP Parameter I
    i. WRIP Parameter J
    j. WRIP Parameter L
23. After completing the eleven WRIP Parameter tables for Starting Water 1, do the same for Starting Waters 2, 3, and 4.
    There are a total of 396 tables that need to be exported into forty-four Excel files (each having nine worksheets).
24. Horizontal box plots will be generated using Sigmaplot.

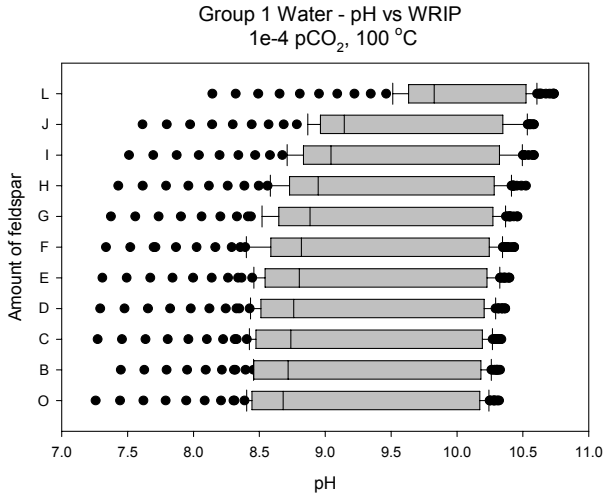
July 13, 2009

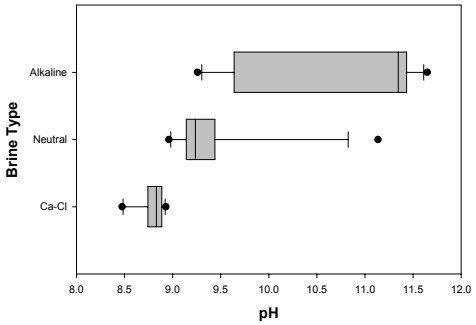
The following compares the pH range of Group 1 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in pH at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 234 of this notebook also are shown.

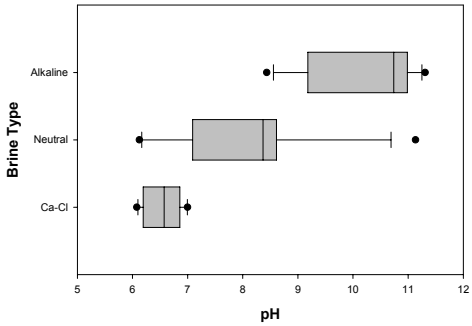






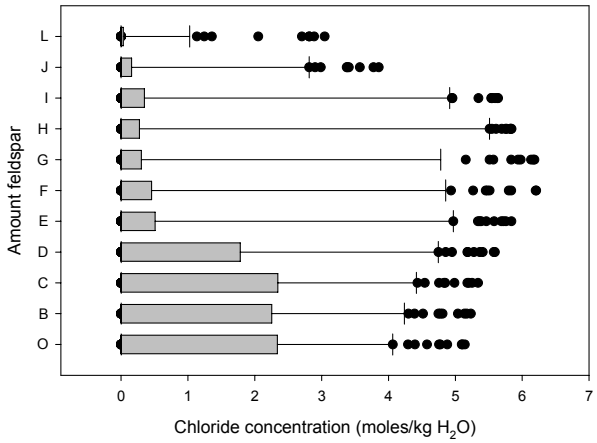




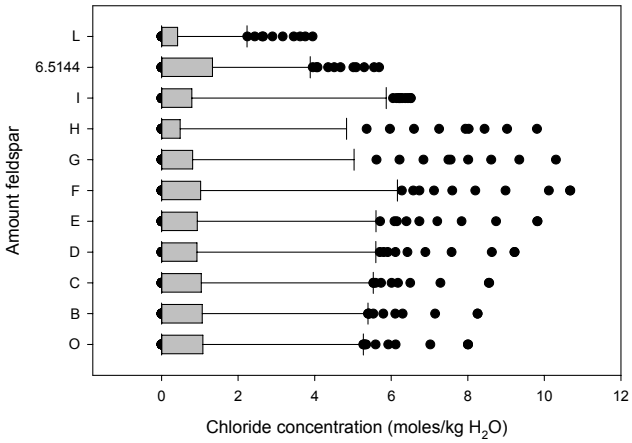


The following compares the chloride concentration range of Group 1 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in chloride concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 235 of this notebook also are shown.

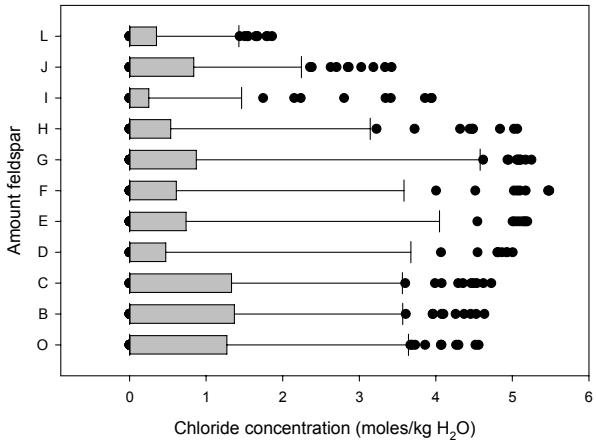
Group 1 Water - Chloride vs WRIP
1e-2 pCO_2, 30 °C



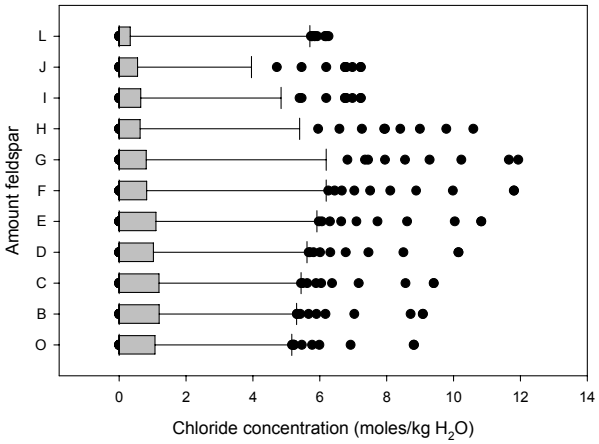
Group 1 Water - Chloride vs WRIP
1e-2 pCO_2, 100 °C



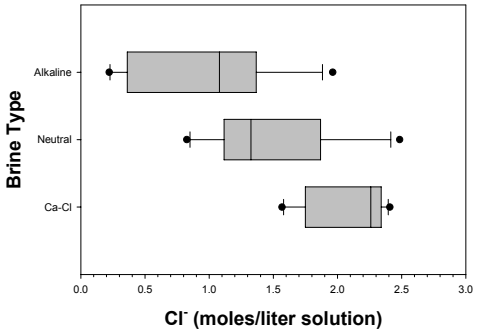
Group 1 Water - Chloride Concentration vs WRIP
1e-4 pCO_2, 30 °C



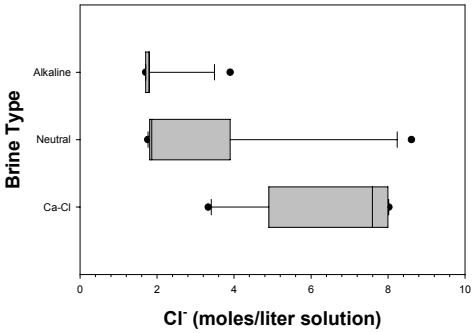
Group 1 Water - Chloride vs WRIP
1e-4 pCO_2, 100 °C



Chloride Conc. (at T=30 °C) of Evaporated YM Waters

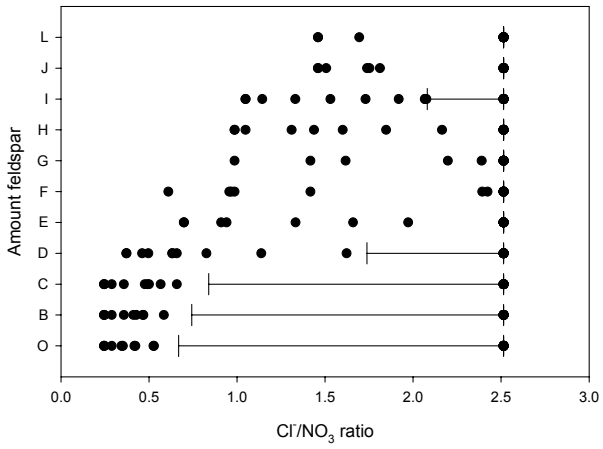


Chloride Conc. (at T=90 °C) of Evaporated YM Waters

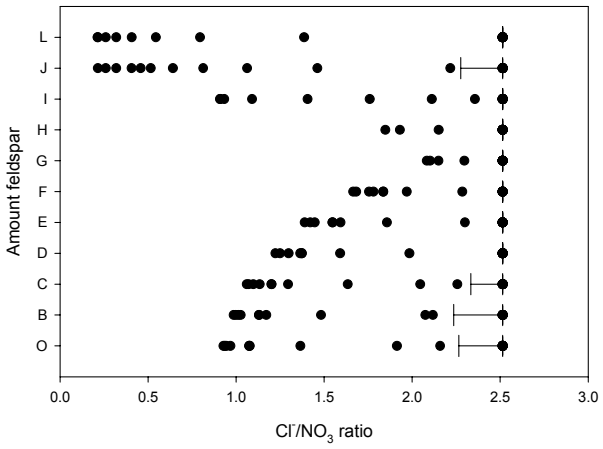


The following compares the range in Cl^-/NO_3^- ratio of Group 1 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 236 of this notebook also are shown.

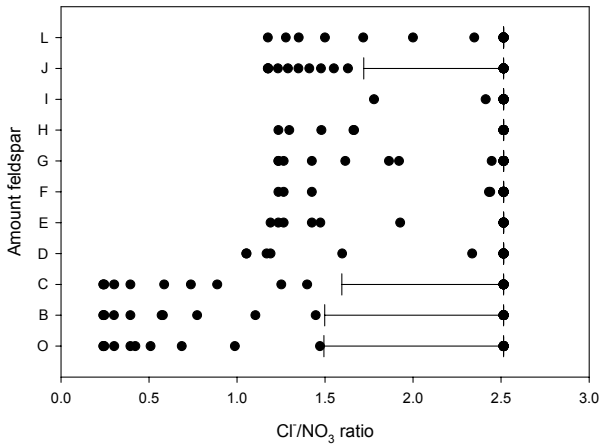
Group 1 Water - Cl/NO_3 vs WRIP
1e-2 pCO_2, 30 °C



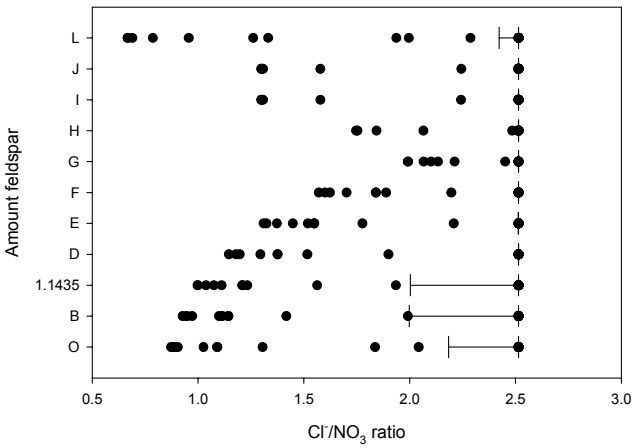
Group 1 Water - Cl/NO_3 Ratio vs WRIP
1e-2 pCO_2, 100 °C



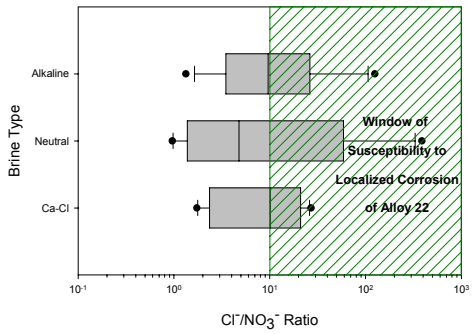
Group 1 Water - Cl/NO_3 Ratio vs WRIP
1e-4 pCO_2, 30 °C



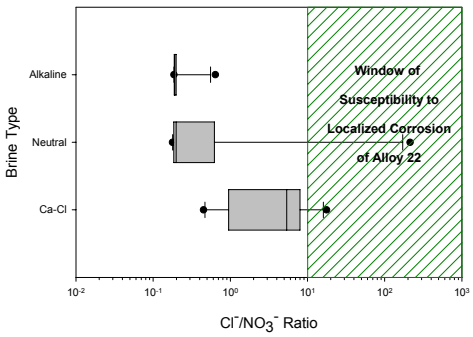
Group 1 Water - Cl/NO_3 Ratio vs WRIP
1e-4 pCO_2, 100 °C



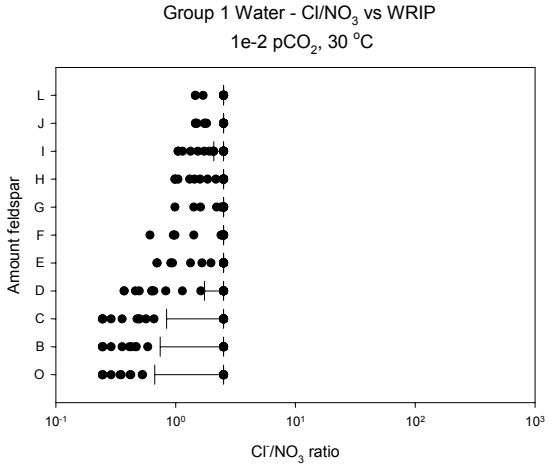
Cl^-/NO_3^- Ratio (at T=30 °C) of Evaporated YM Waters

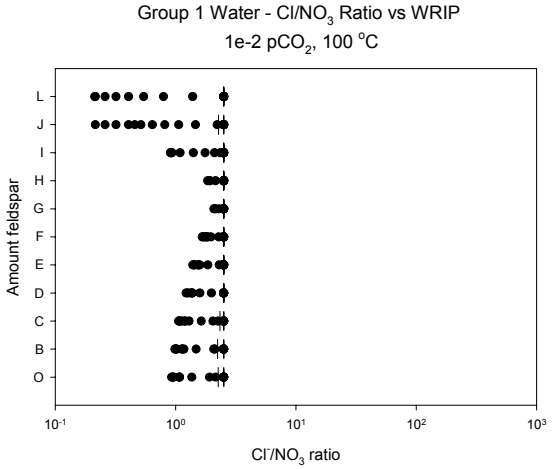


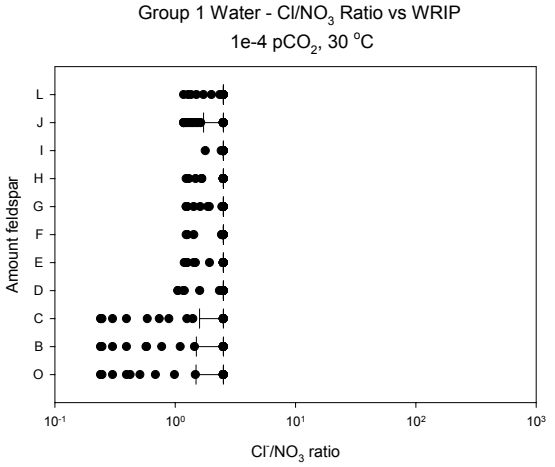
Cl^-/NO_3^- Ratio (at T=90 °C) of Evaporated YM Waters

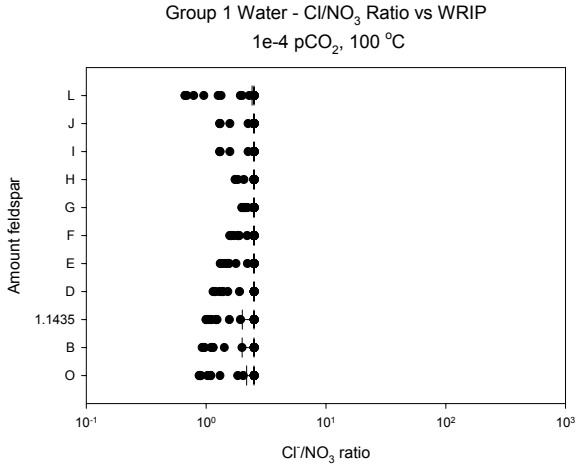


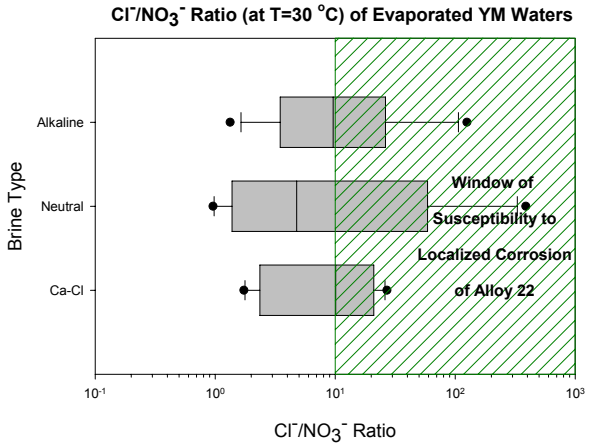
For easier comparison of the range in Cl^-/NO_3^- ratio of Group 1 waters at 30 and 100 °C with the range in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water, the Group 1 results were replotted with the same x-axis scale as that of the YM pore water results.

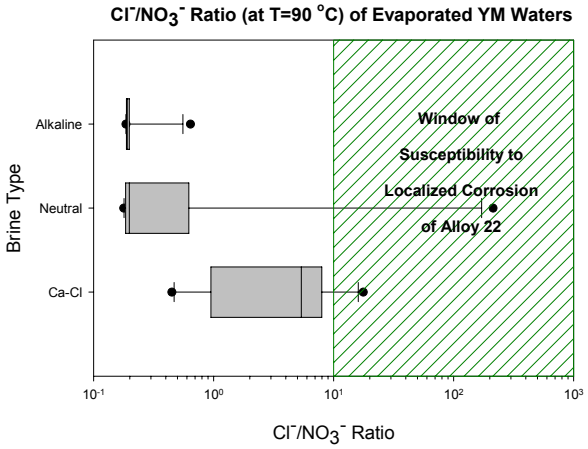




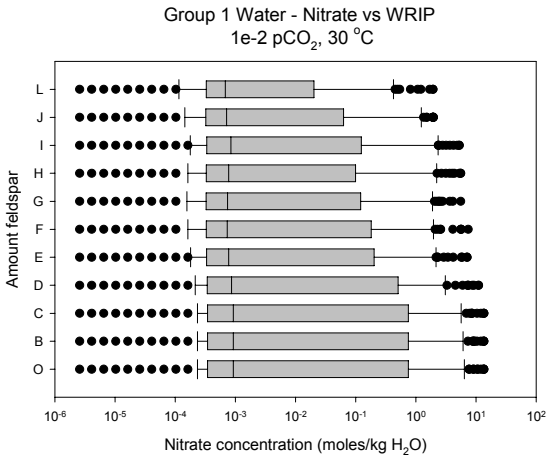


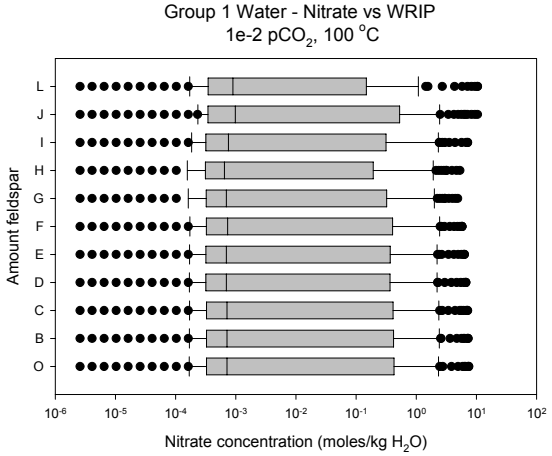


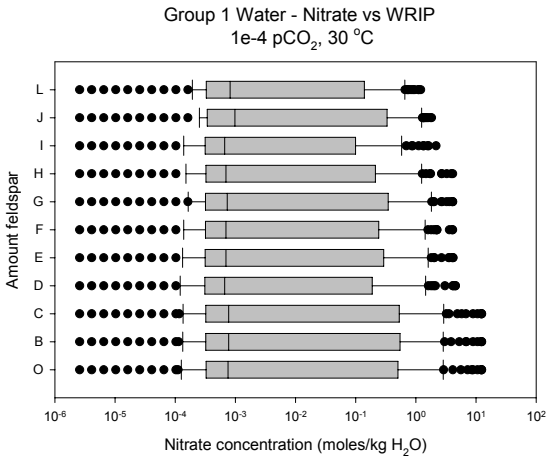


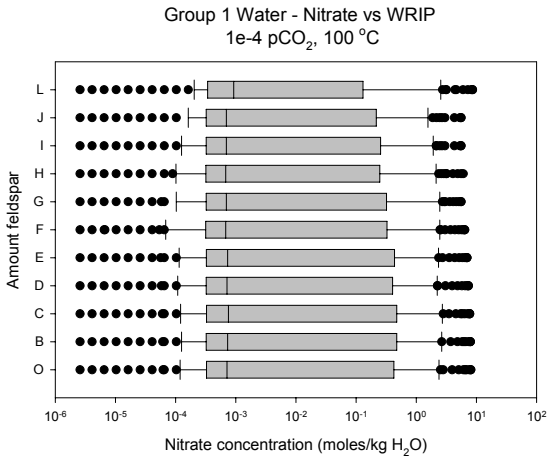


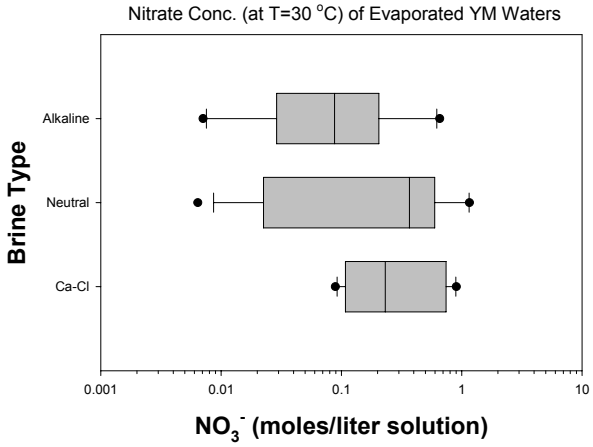
The following compares the range in nitrate concentration of Group 1 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in nitrate concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 244 of this notebook also are shown.

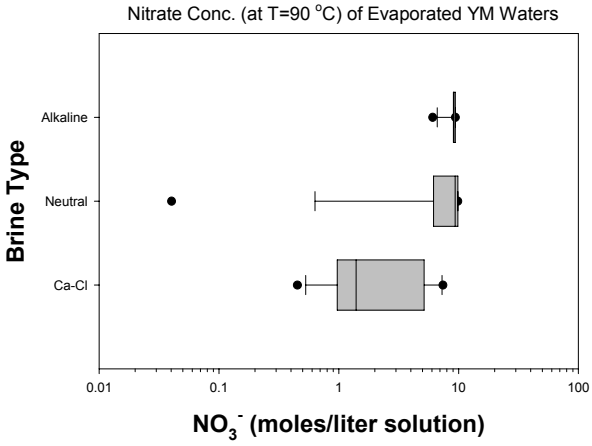




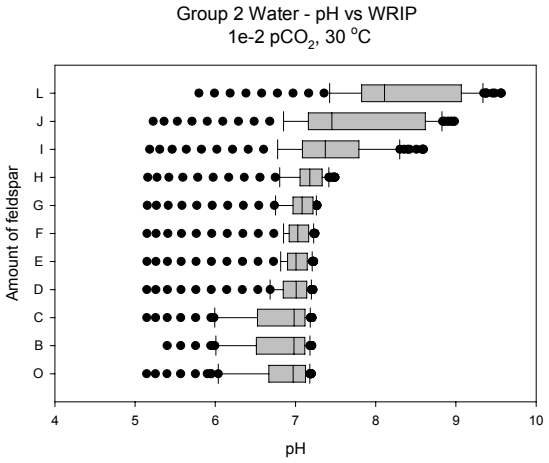


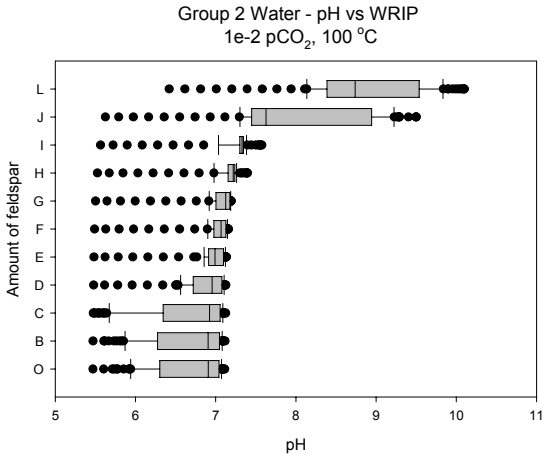


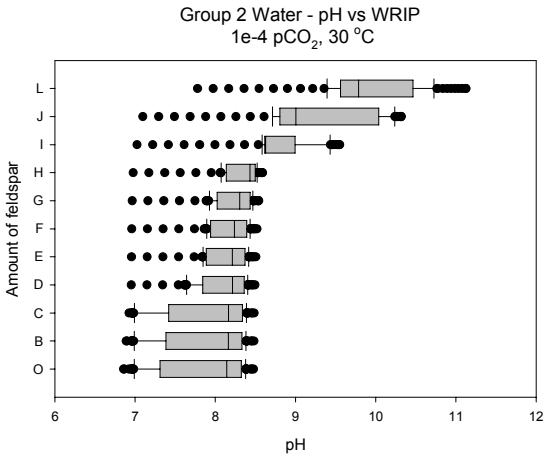


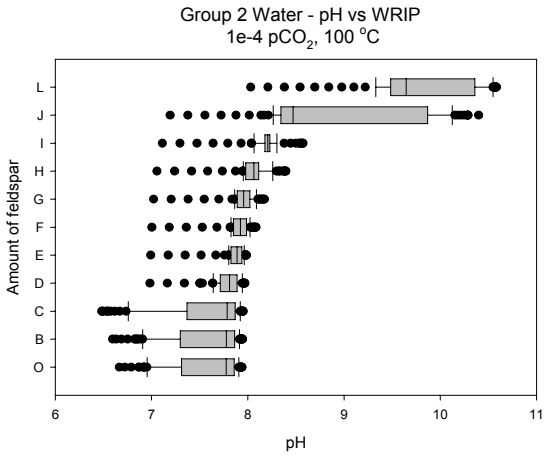


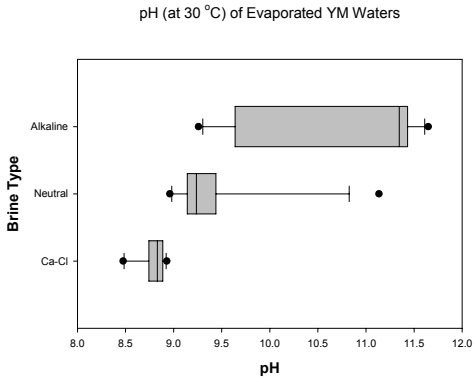
The following compares the pH range of Group 2 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in pH at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 234 of this notebook also are shown.

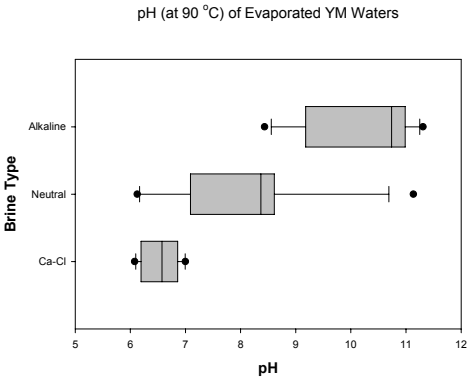




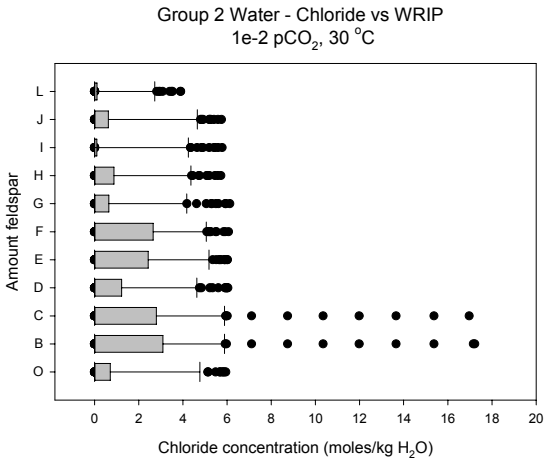


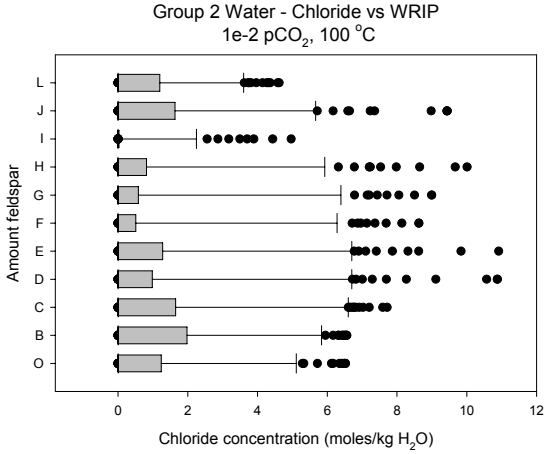


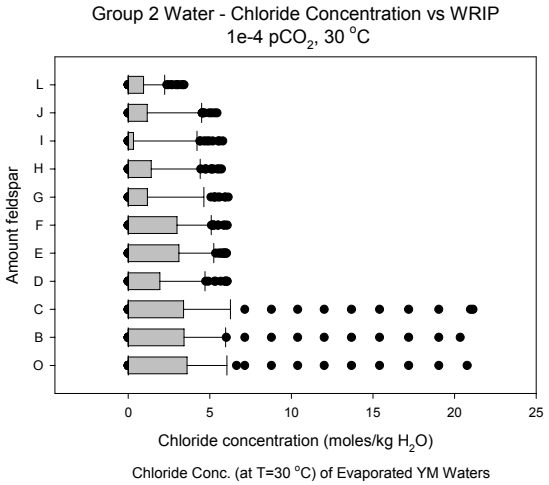




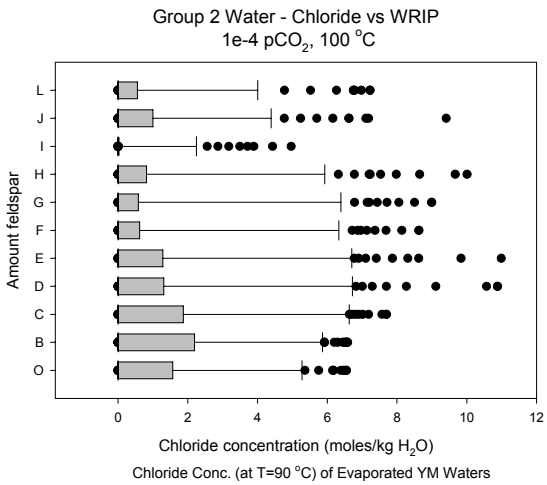
The following compares the chloride concentration range of Group 2 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in chloride concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 235 of this notebook also are shown.



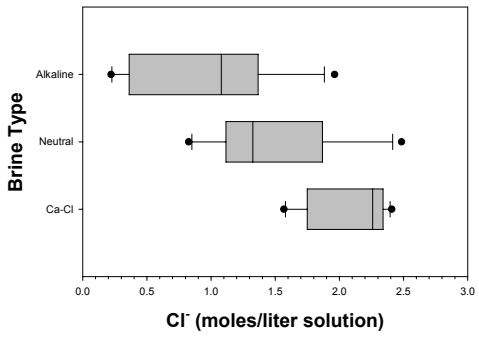


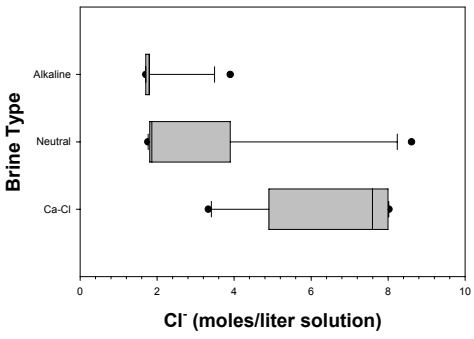


Chloride Conc. (at T=30 °C) of Evaporated YM Waters

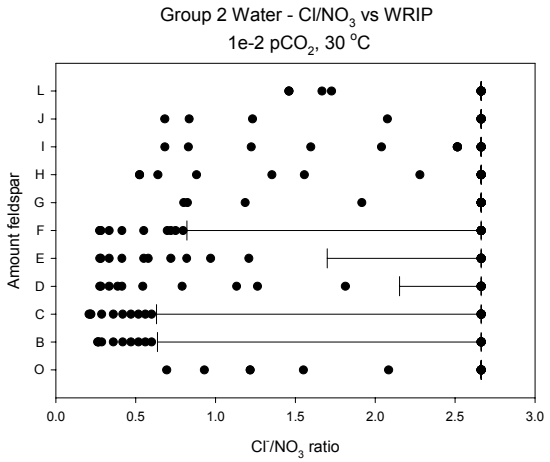


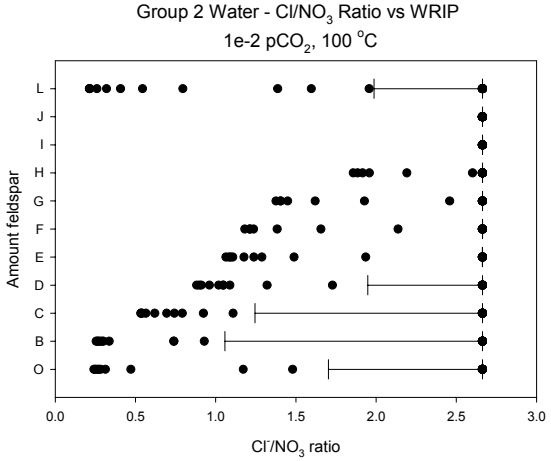
Chloride Conc. (at T=90 °C) of Evaporated YM Waters

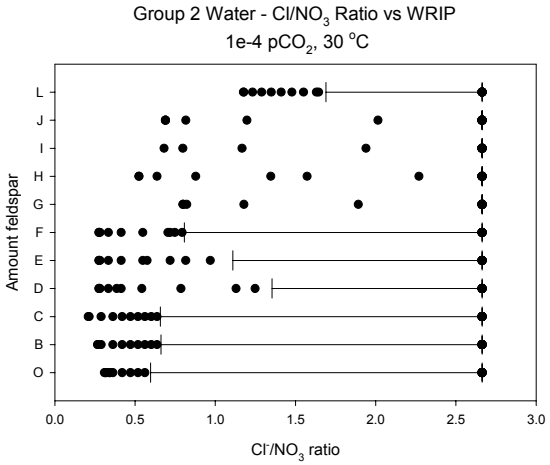


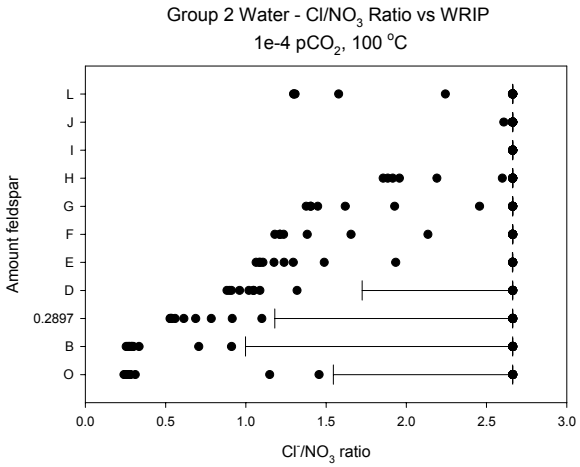


The following compares the range in Cl^-/NO_3^- ratio of Group 2 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 236 of this notebook also are shown.

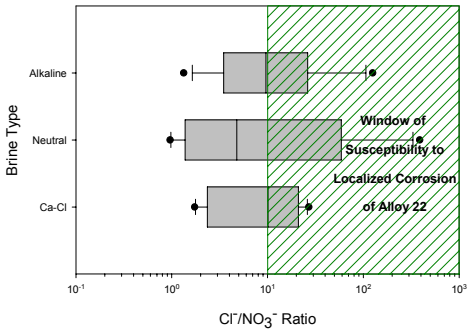




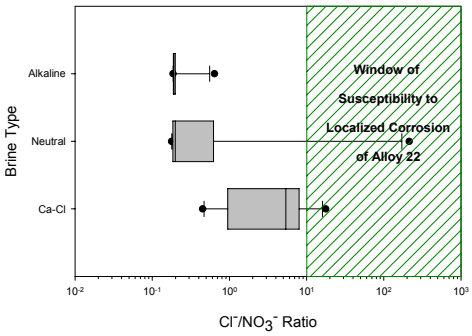




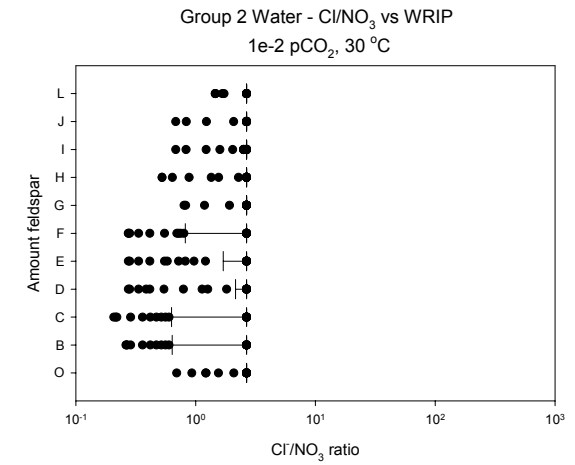
Cl^-/NO_3^- Ratio (at T=30 °C) of Evaporated YM Waters

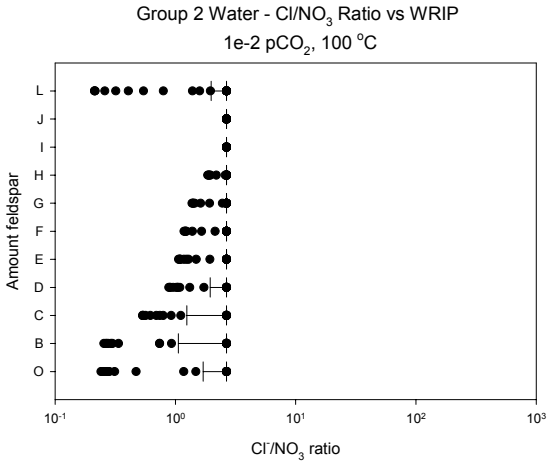


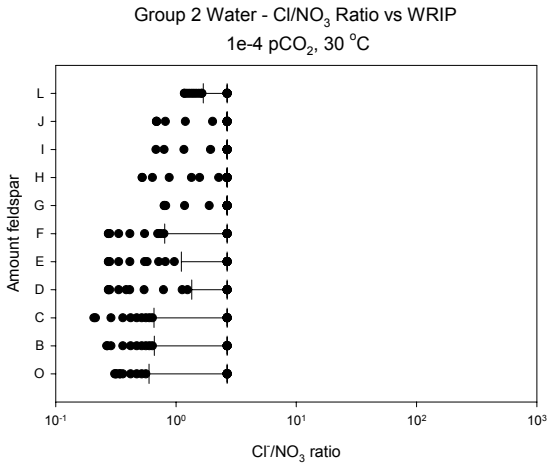
Cl^-/NO_3^- Ratio (at T=90 °C) of Evaporated YM Waters

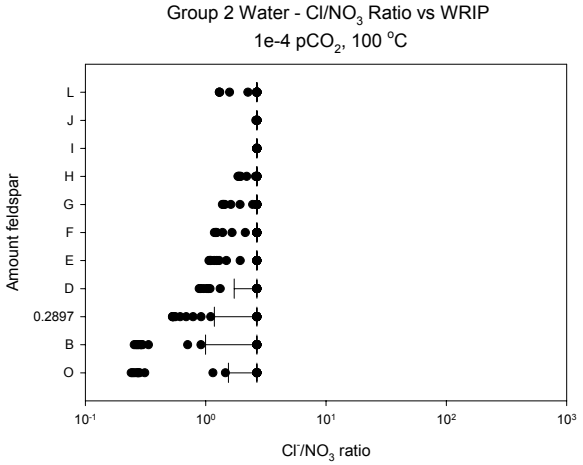


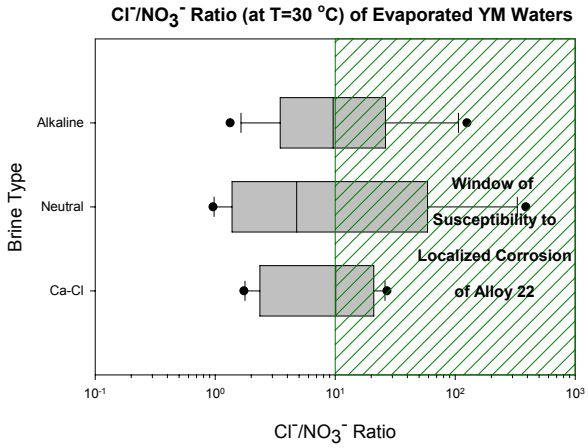
For easier comparison of the range in Cl^-/NO_3^- ratio of Group 2 waters at 30 and 100 °C with the range in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water, the Group 1 results were replotted with the same x-axis scale as that of the YM pore water results.

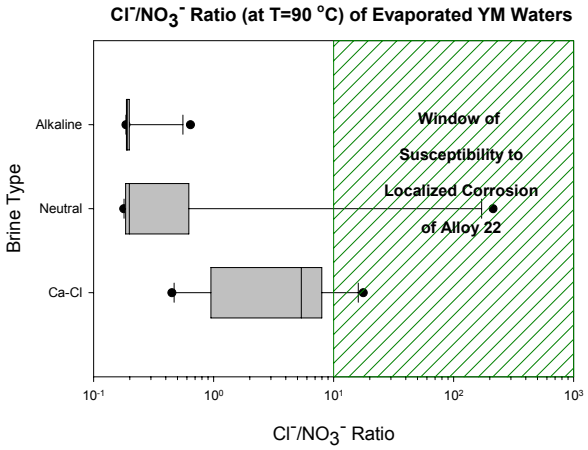




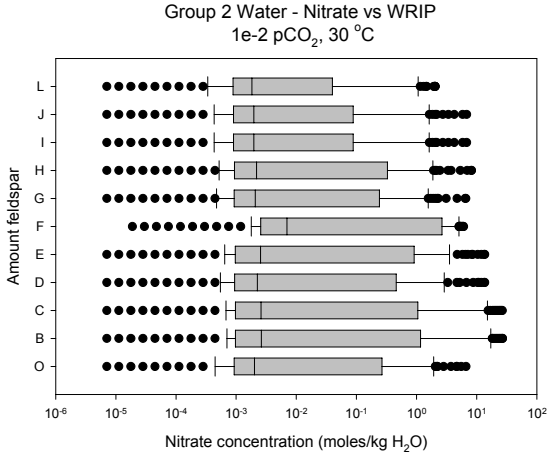


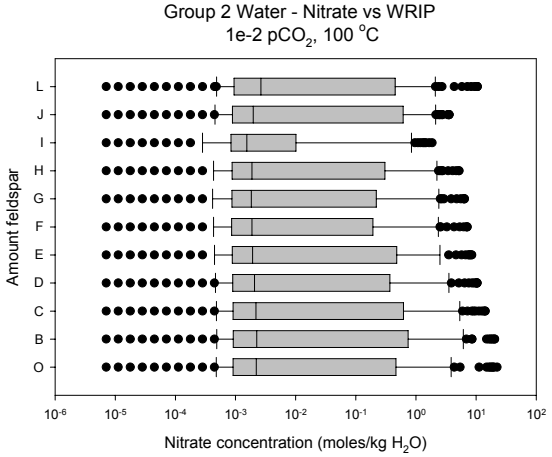


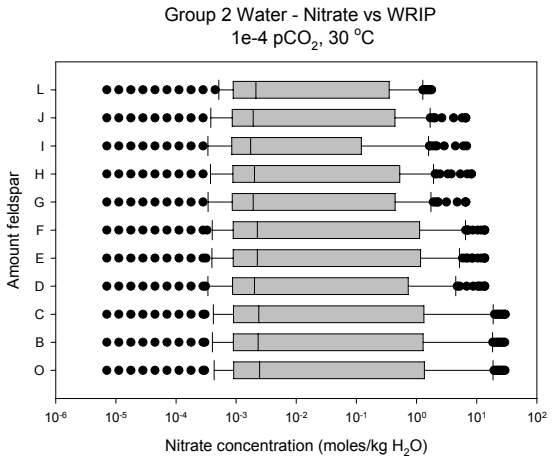


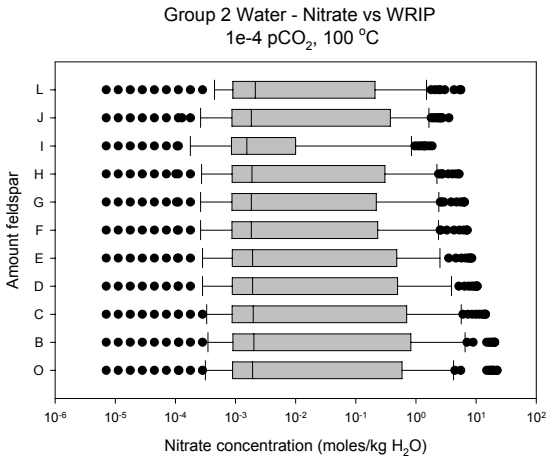


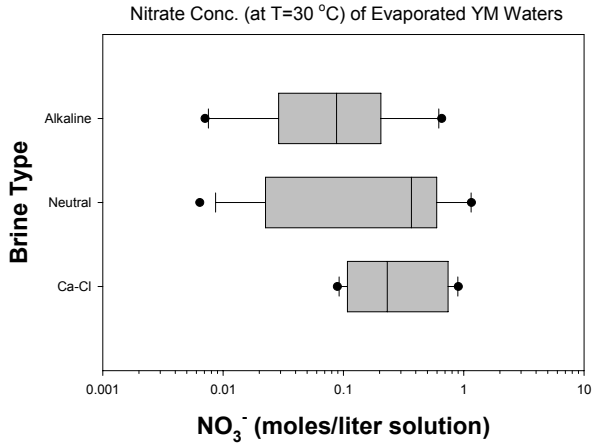
The following compares the range in nitrate concentration of Group 2 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in nitrate concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 244 of this notebook also are shown.

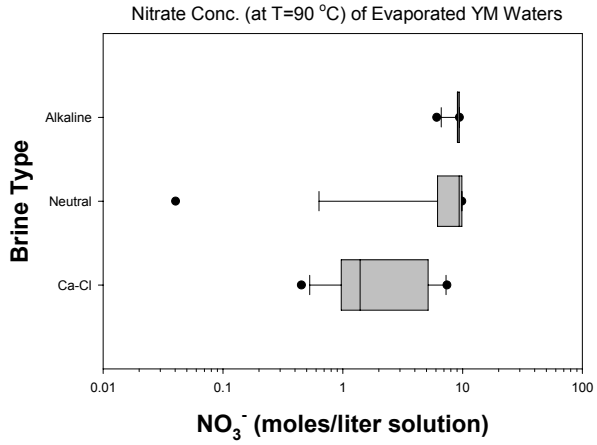




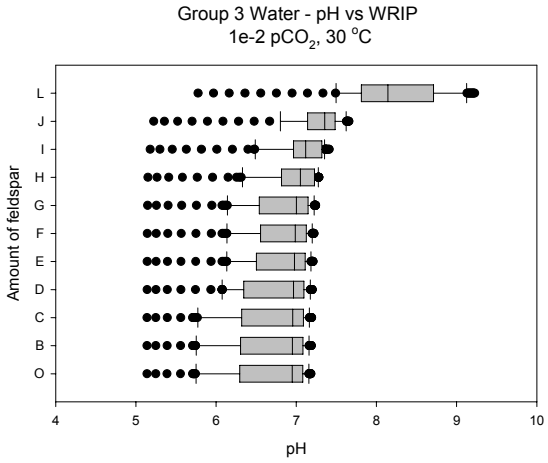


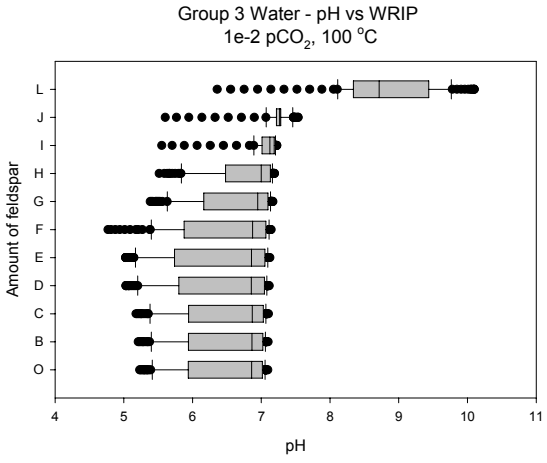


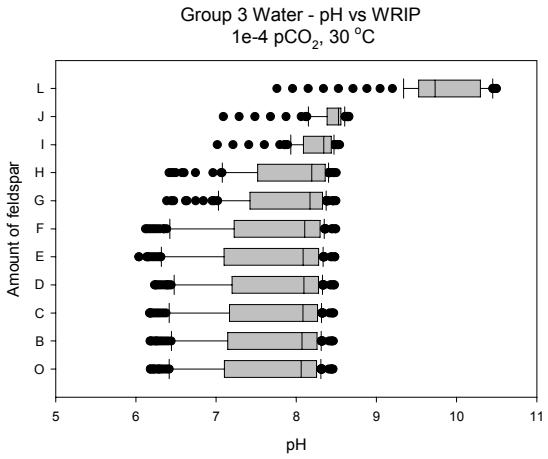


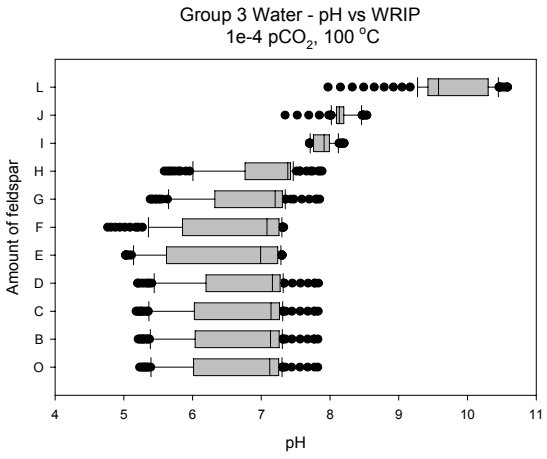


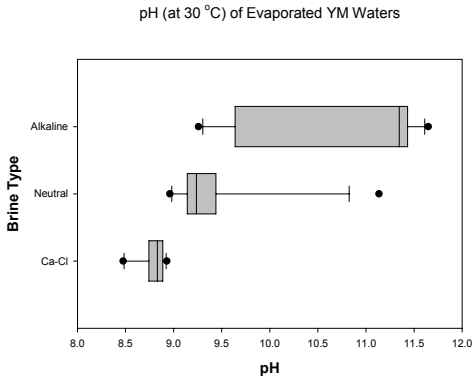
The following compares the pH range of Group 3 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in pH at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 234 of this notebook also are shown.

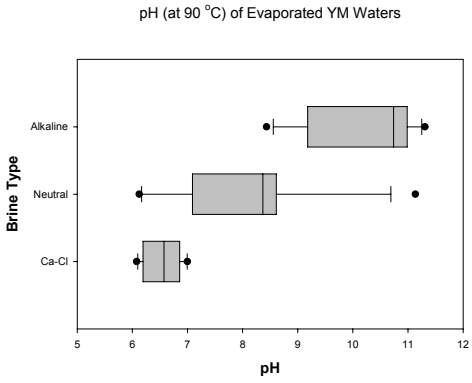




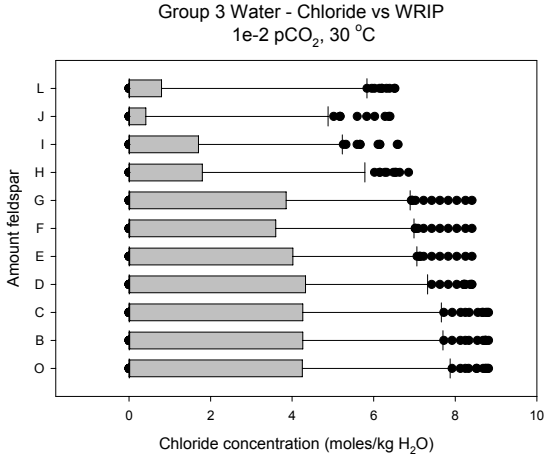


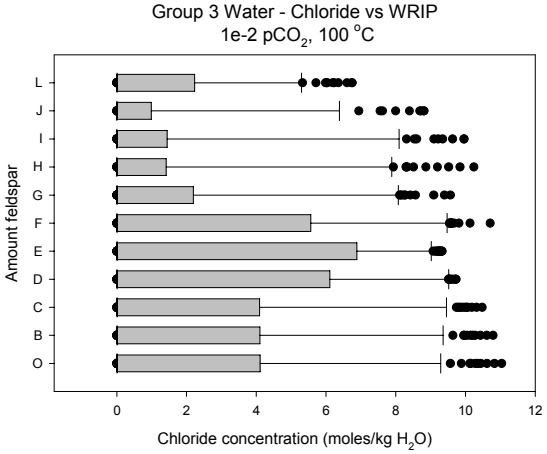


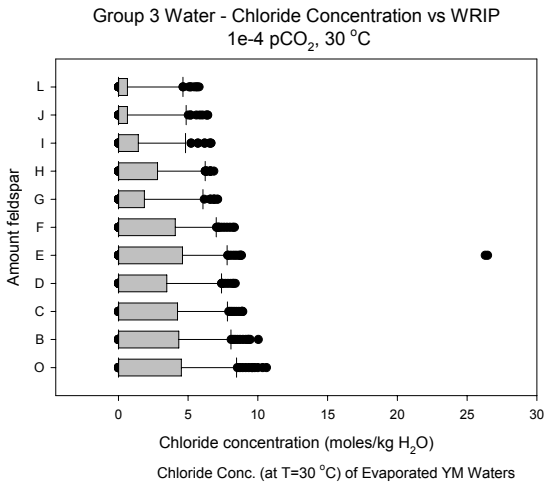


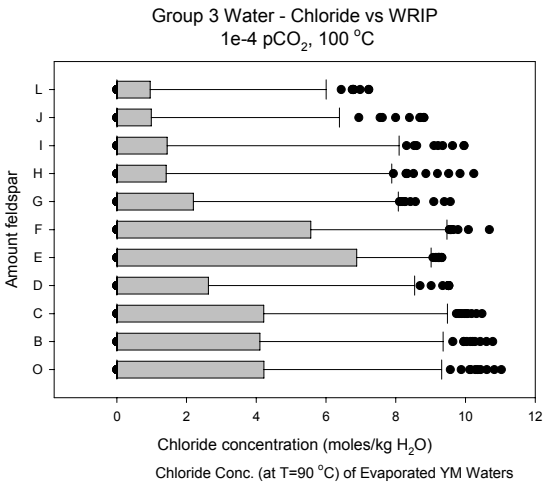


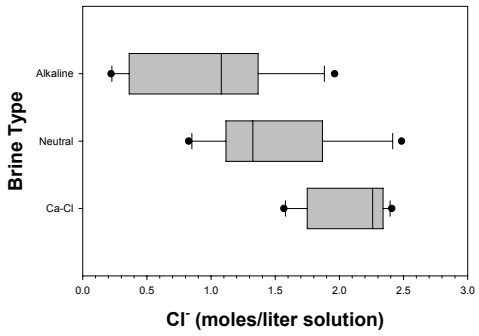
The following compares the chloride concentration range of Group 3 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in chloride concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 235 of this notebook also are shown.

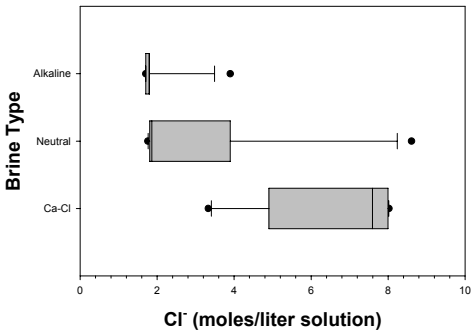




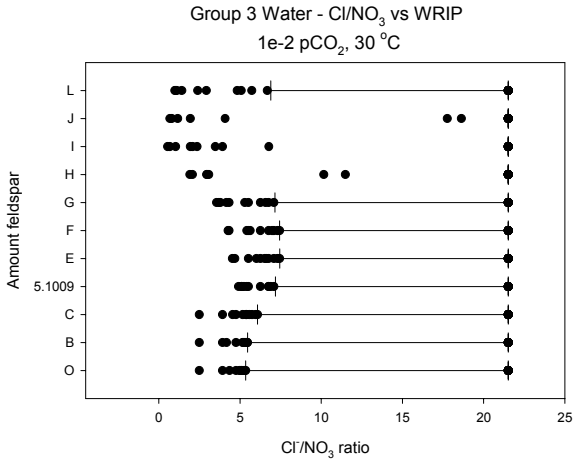


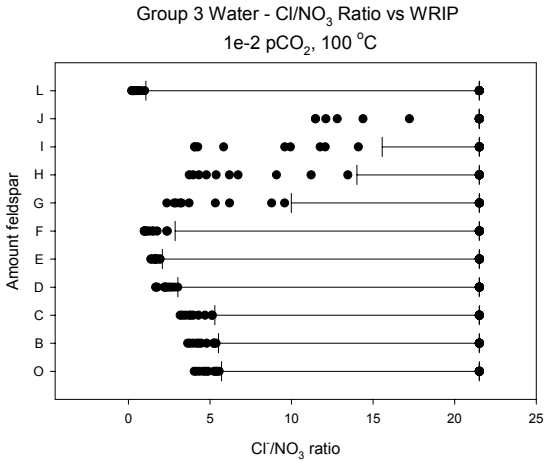


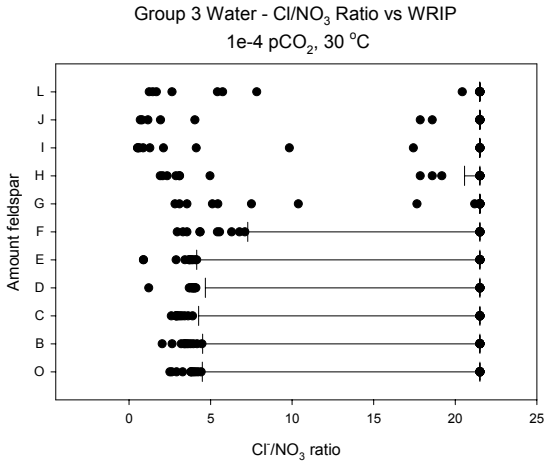


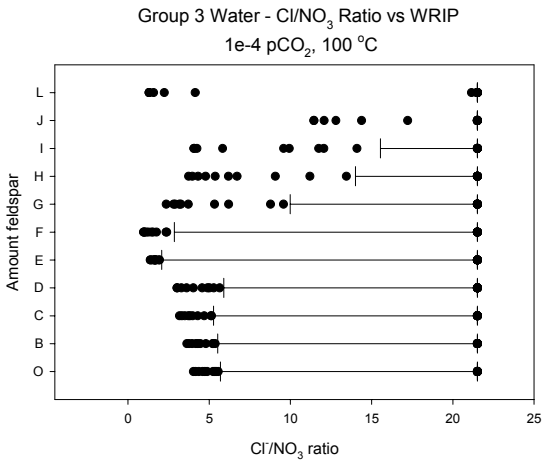


The following compares the range in Cl^-/NO_3^- ratio of Group 3 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 236 of this notebook also are shown.

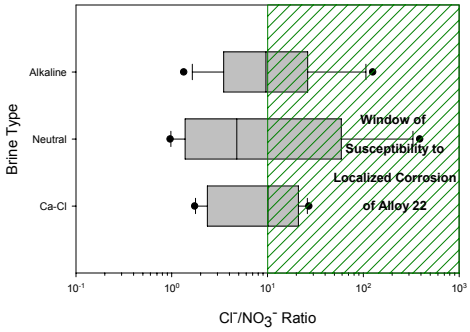




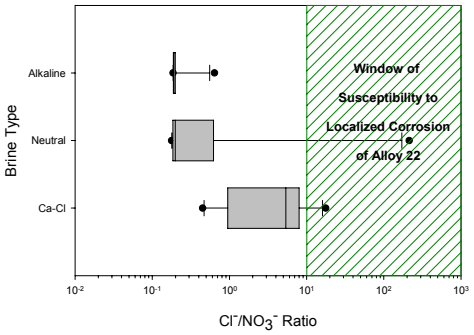




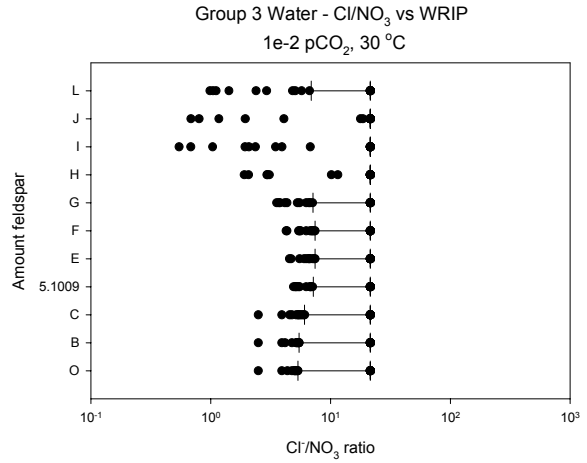
Cl^-/NO_3^- Ratio (at T=30 °C) of Evaporated YM Waters

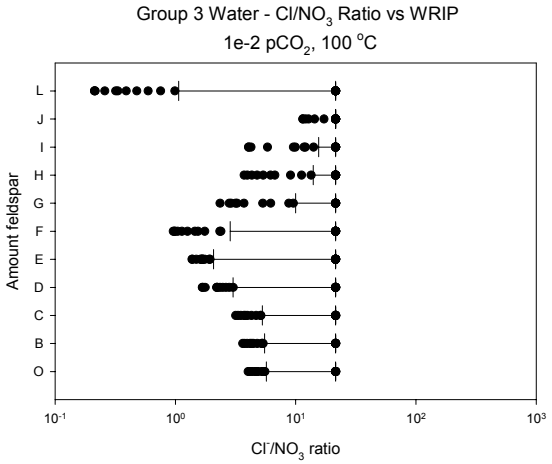


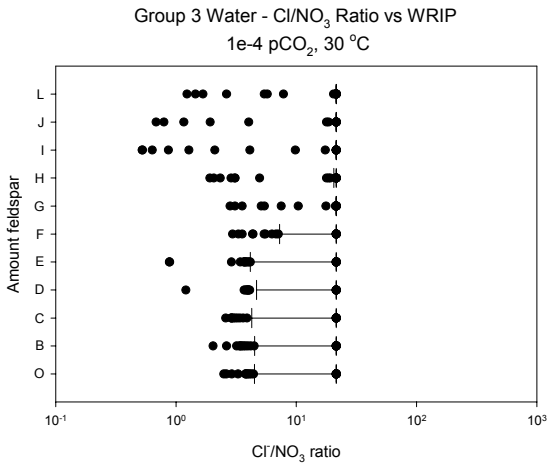
Cl^-/NO_3^- Ratio (at T=90 °C) of Evaporated YM Waters

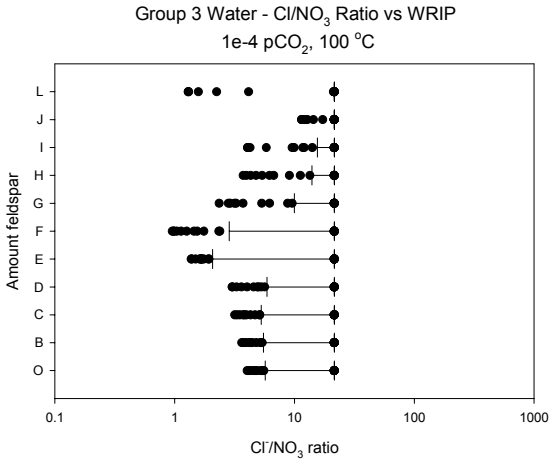


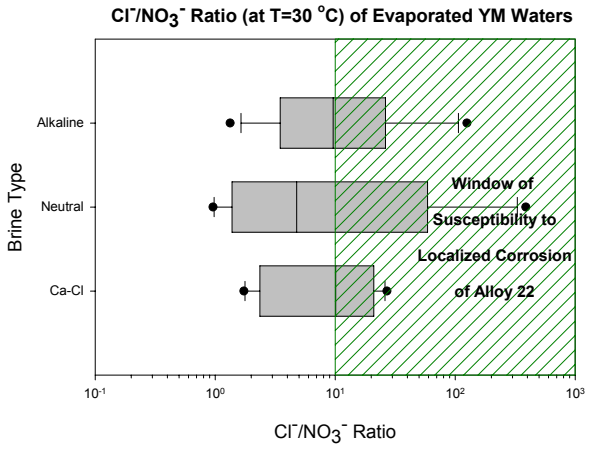
For easier comparison of the range in Cl^-/NO_3^- ratio of Group 3 waters at 30 and 100 °C with the range in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water, the Group 1 results were replotted with the same x-axis scale as that of the YM pore water results.

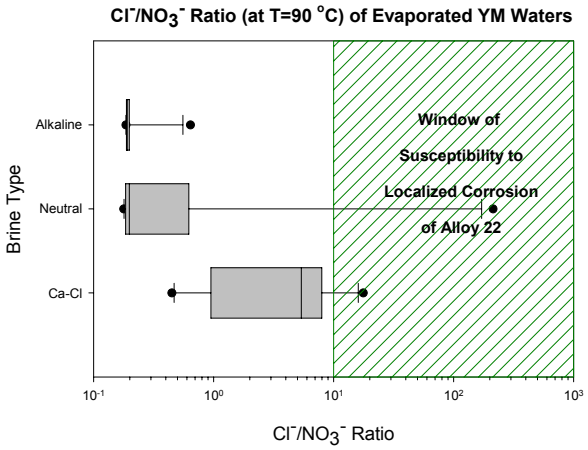




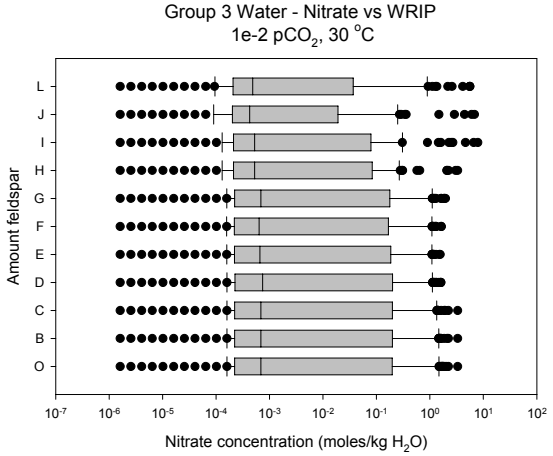


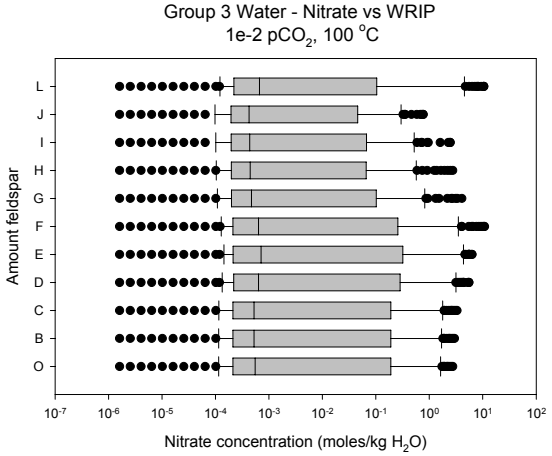


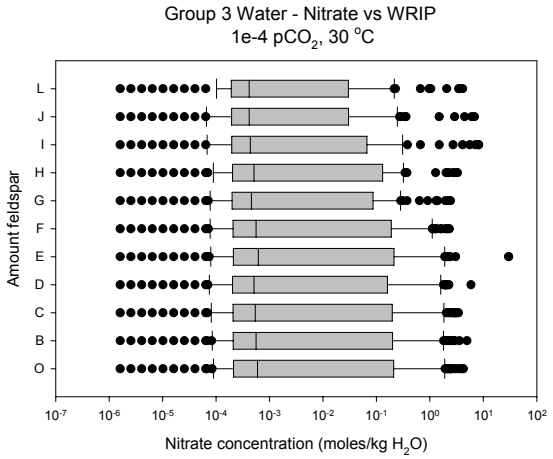


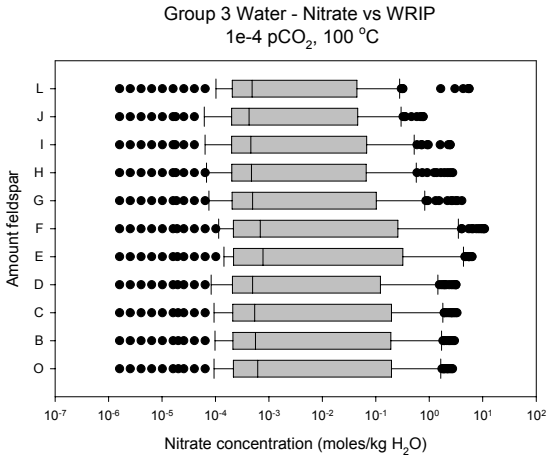


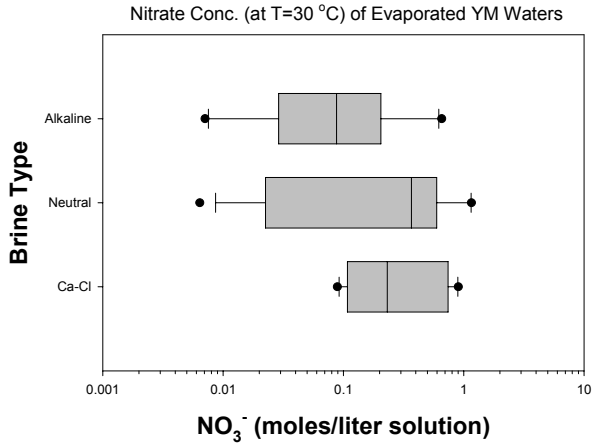
The following compares the range in nitrate concentration of Group 3 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in nitrate concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 244 of this notebook also are shown.

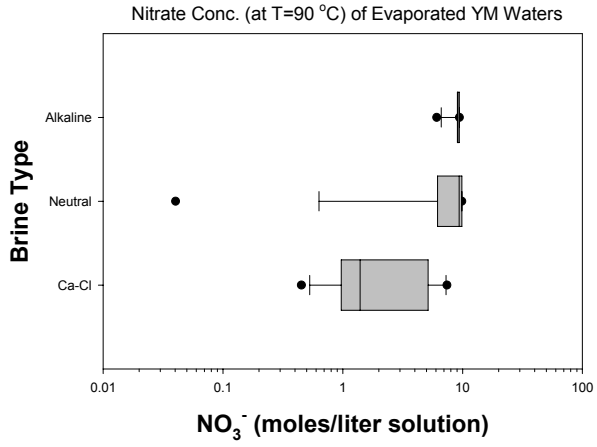




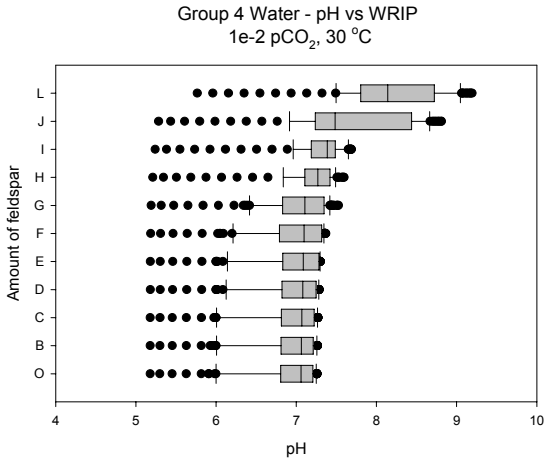


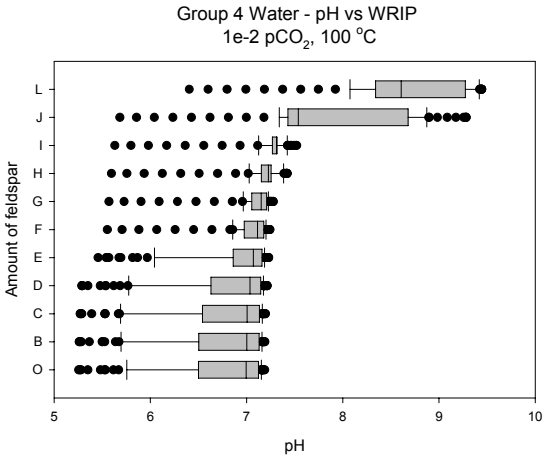


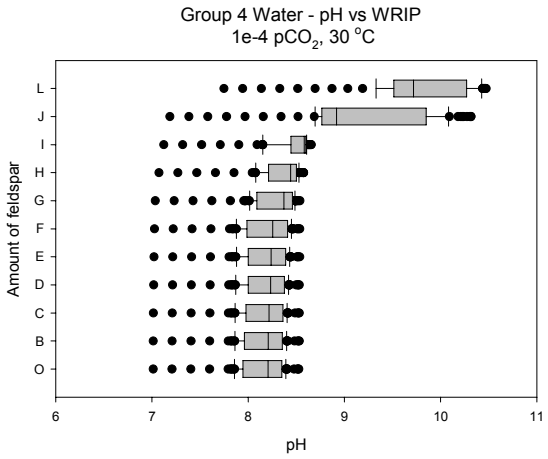


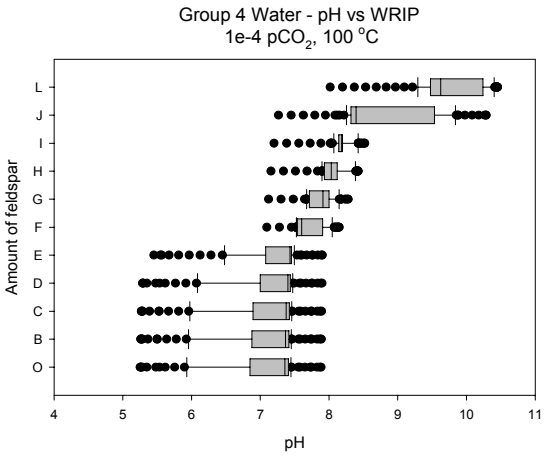


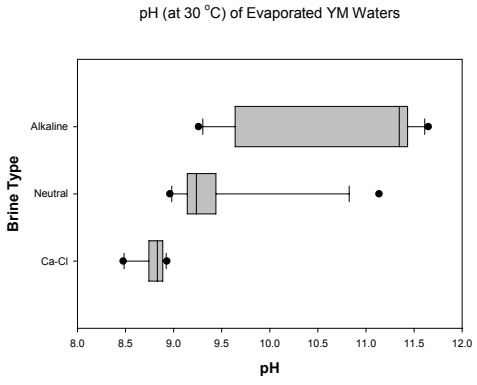
The following compares the pH range of Group 4 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in pH at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 234 of this notebook also are shown.

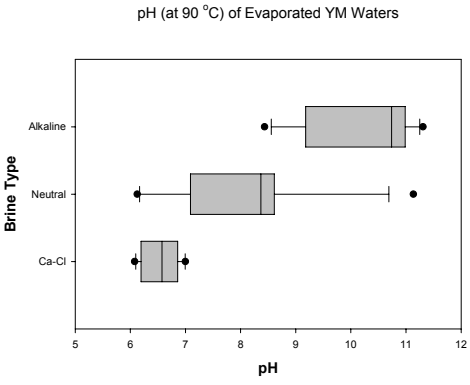




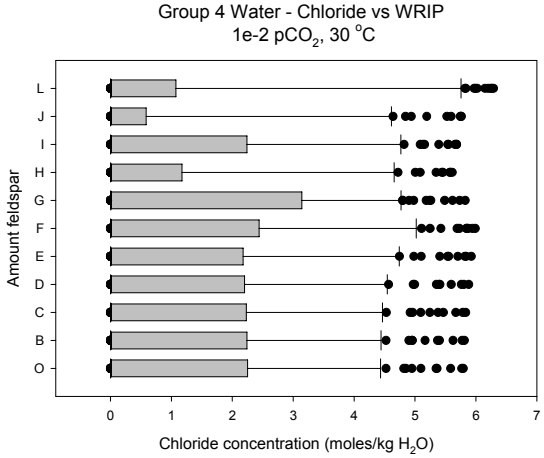


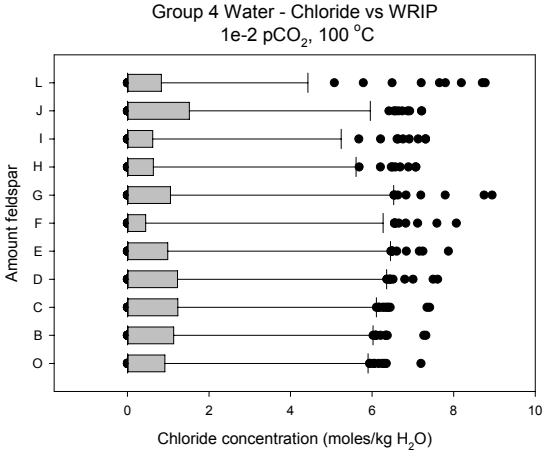


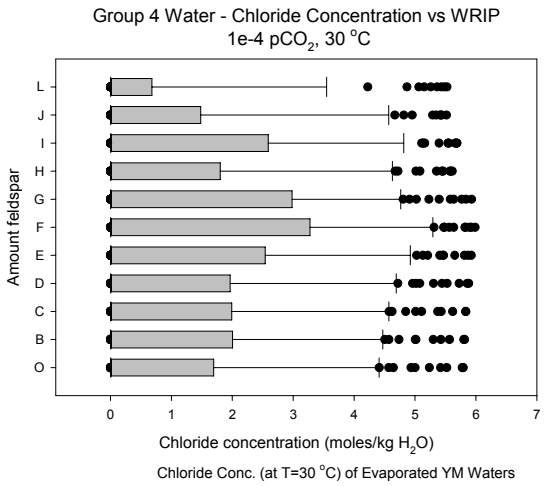


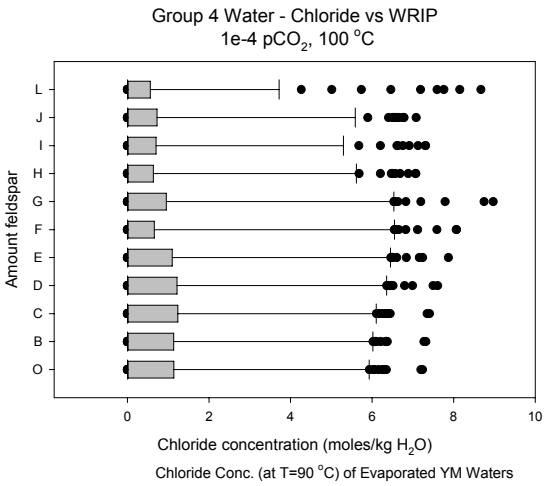


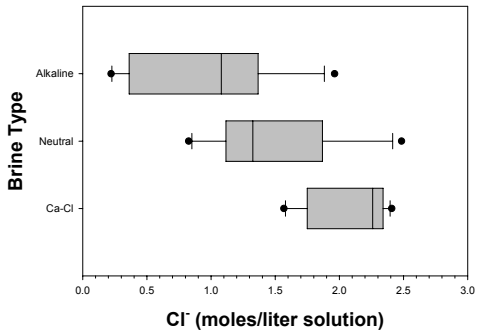
The following compares the chloride concentration range of Group 4 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in chloride concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 235 of this notebook also are shown.

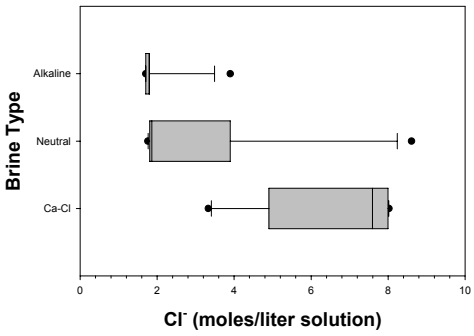




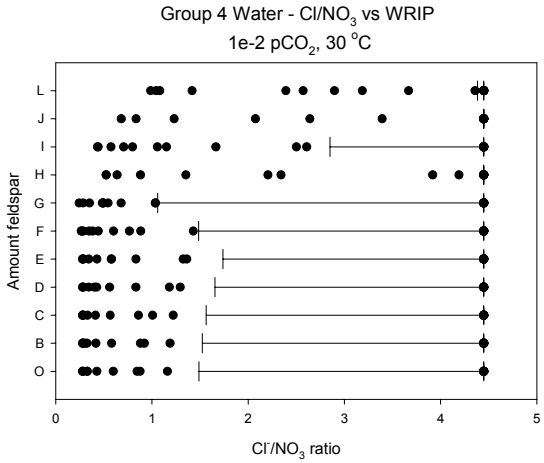


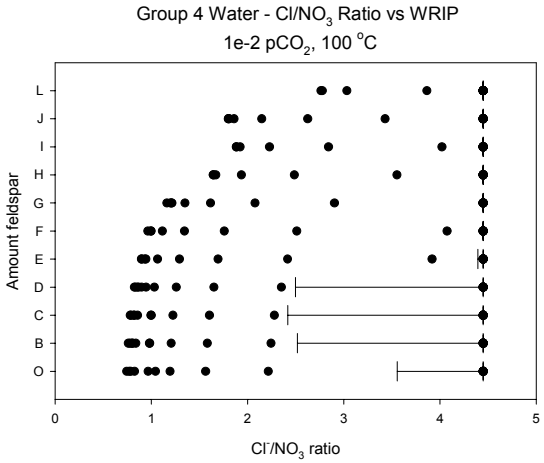


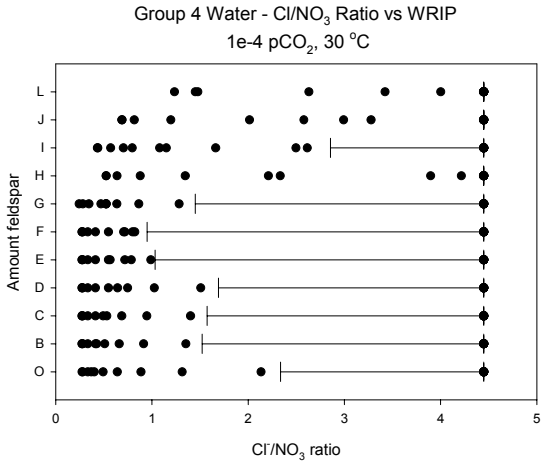


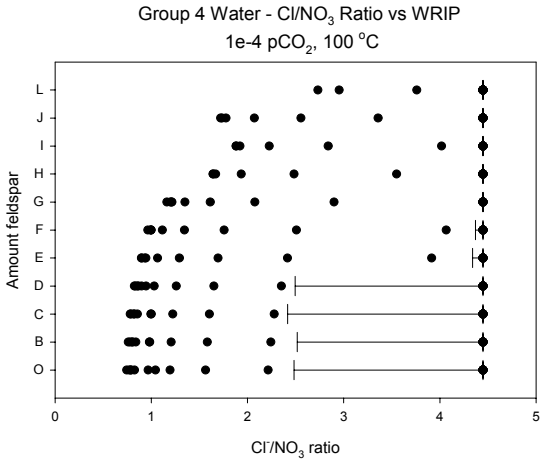


The following compares the range in Cl^-/NO_3^- ratio of Group 4 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 236 of this notebook also are shown.

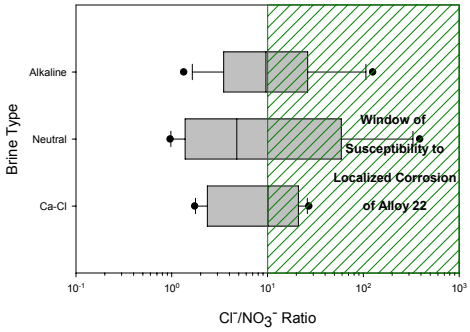




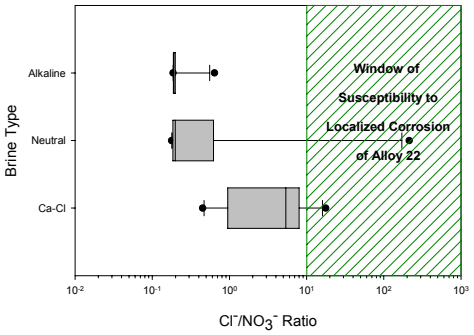




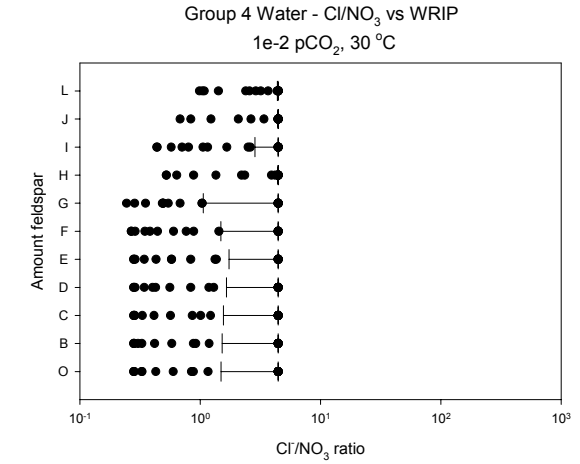
Cl^-/NO_3^- Ratio (at T=30 °C) of Evaporated YM Waters

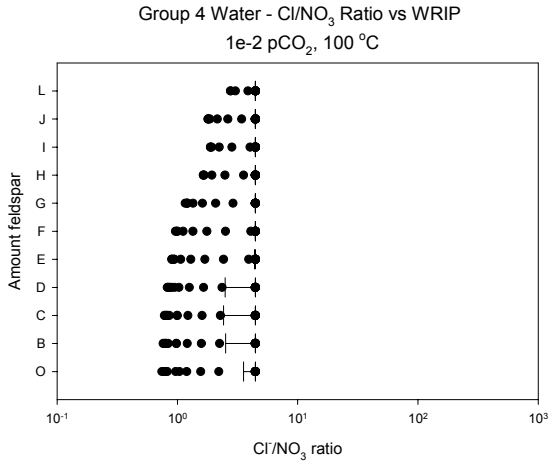


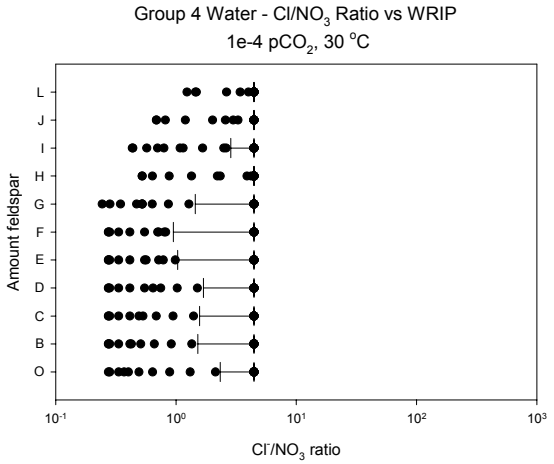
Cl^-/NO_3^- Ratio (at T=90 °C) of Evaporated YM Waters

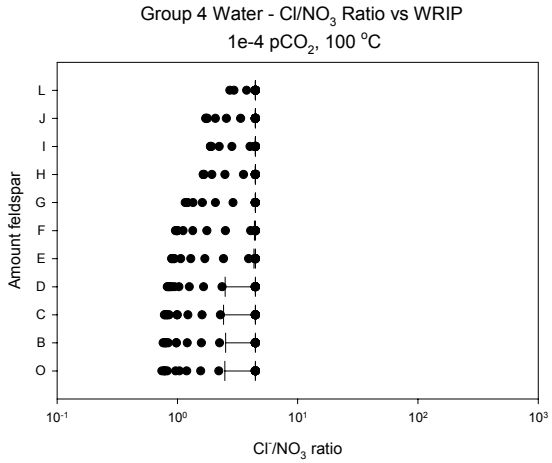


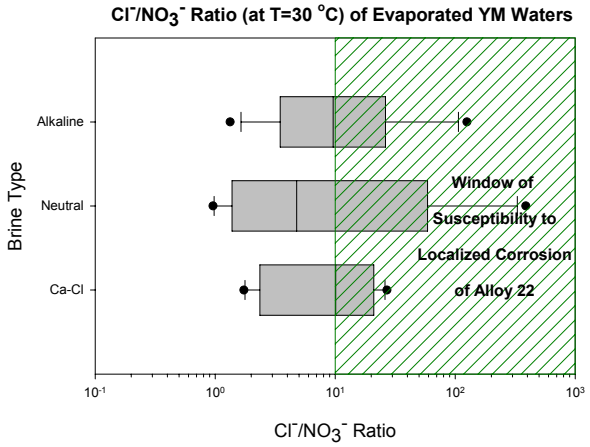
For easier comparison of the range in Cl^-/NO_3^- ratio of Group 4 waters at 30 and 100 °C with the range in Cl^-/NO_3^- ratio at 30 and 90 °C of evaporated YM unsaturated zone pore water, the Group 1 results were replotted with the same x-axis scale as that of the YM pore water results.

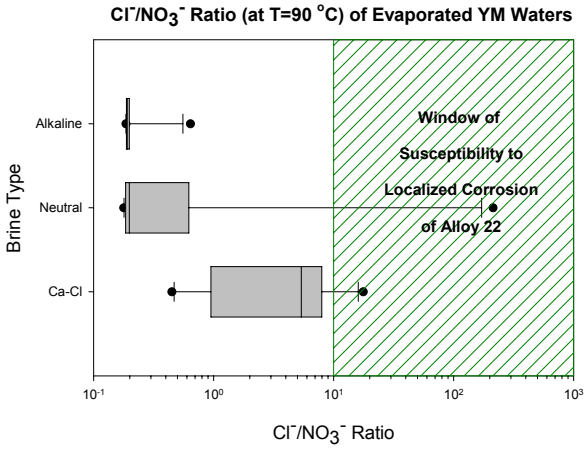




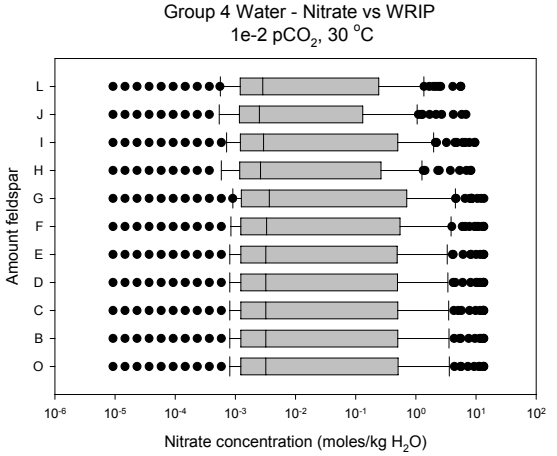


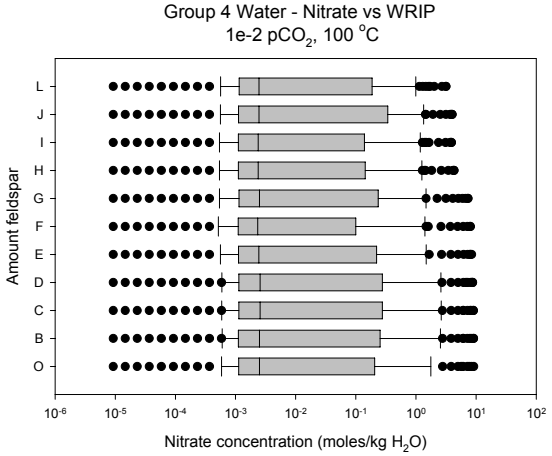


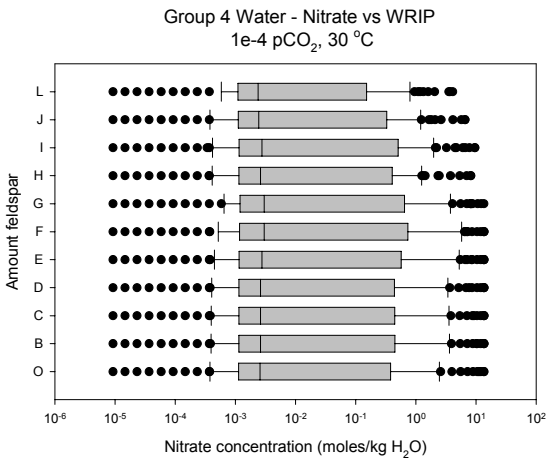


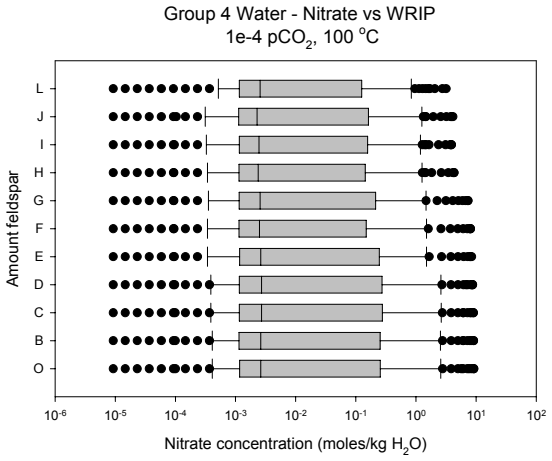


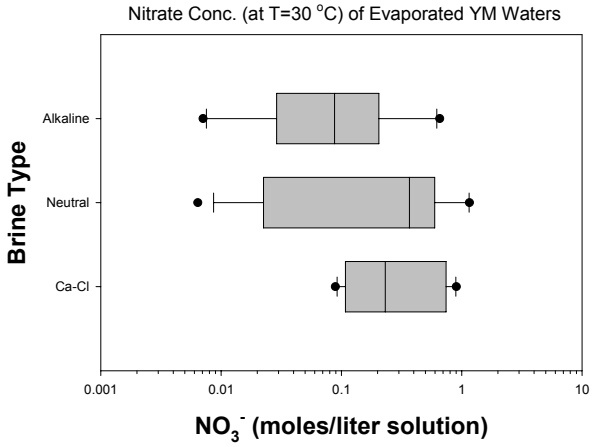
The following compares the range in nitrate concentration of Group 4 waters at 30 and 100 °C at two values of pCO_2 ($1e^{-2}$ and $1e^{-4}$ atm). For comparison, the calculated ranges in nitrate concentration at 30 and 90 °C of evaporated YM unsaturated zone pore water from page 244 of this notebook also are shown.

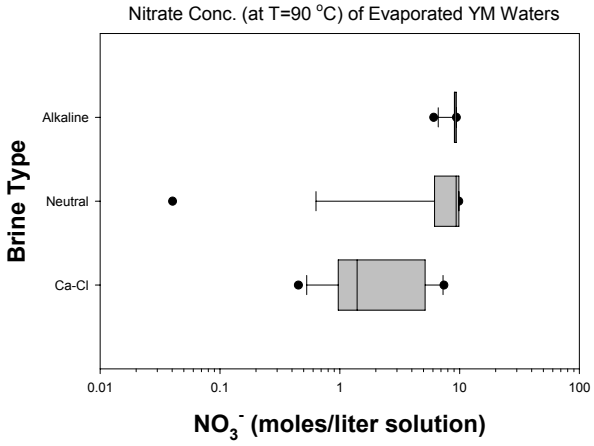












August 24, 2009

The following tables document the results of calculations to validate OLIAnalyzer Version 3.0. The information will be used in preparing a software validation report. The code is considered valid if the calculated values agree with published experimental data to within ±10%. The ±10% criterion is arbitrarily set in the validation test plan because ±10% variation between experimental and calculated values would have no significant effect on the estimated performance of the engineered barrier system in a nuclear waste geologic repository.

OLIAnalyzer Version 3.0 is a suite of process simulation software developed by OLI Systems, Inc. The program suite includes StreamAnalyzer and CorrosionAnalyzer, which in previous versions were stand alone products. CorrosionAnalyzer is used for evaluating the thermodynamic properties that are related to the characteristics of corrosion and the corrosion rate of a metal in a given solution system. OLIAnalyzer is packaged as a stand-alone software with a user-friendly graphic interface for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. OLIAnalyzer Version 3.0 has two options for calculating the thermodynamic parameters: (i) a standard chemistry model and (ii) a Mixed Solvent Electrolyte (MSE) model. The standard chemistry model is applicable to aqueous systems with ionic strengths up to about 30 molal. The MSE model is capable of calculating speciation, chemical, and phase equilibria that are applicable to water-organic-salt systems in the full range of concentrations, as well as aqueous electrolytes from dilute solutions to the fused salt limit. Both chemistry models of OLIAnalyzer Version 3.0 were tested.

The scope of the validation was within the following ranges:

Temperature:	0 to 300 °C [0 to 572 °F]
Pressure:	0 to 1,480 atm [0 to 21,750 psi]
Ionic Strength:	0 to 30 molal with the standard chemistry model
	0 to 130 molal with the MSE chemistry model

Test Case 1—NaCl Solubility as a Function of Temperature

Table 1. Comparison of the Calculated NaCl Solubilities (S) with the Experimental Values

Temp °C		25	50	75	100	125	150	175	200	225	250	275	300
Experimental*	S(m)	6.15	6.28	6.46	6.68	6.94	7.20	7.57	7.97	8.44	8.99	9.65	10.41
OLIAnalyzer Version 3.0 (MSE)	S(m)	6.13	6.27	6.48	6.72	6.97	7.24	7.52	7.88	8.35	8.94	9.67	10.42
	%Dev	-0.33	-0.16	0.31	0.60	0.43	0.56	-0.66	-1.13	-1.07	-0.56	0.21	0.10
OLIAnalyzer Ver. 3.0 (Standard)	S(m)	6.15	6.28	6.47	6.69	6.95	7.25	7.58	7.96	8.39	8.89	9.46	10.16
	%Dev	0	0	0.15	0.15	0.14	0.69	0.13	-0.13	-0.59	-1.11	-1.97	-2.40

*Compiled data are from Pabalan, R.T. Software Validation Report for SOLCALC, Version 1.0. San Antonio, Texas: CNWRA. 2002; original data for T < 75 °C are from Linke, W.F. *Solubilities of Inorganic and Metal Organic Compounds*. Vols. 1 and 2. 4th Edition. Washington, DC: American Chemical Society. 1965. and Liu, C. and W.T. Lindsay. "Thermodynamics of Sodium Chloride Solutions at High Temperatures." *Journal of Solution Chemistry.* No. 1. pp. 45–69. 1972. for T > 75 °C.
†% Dev — deviation

Test Case 2—NaCl and KCl Solubility in Mixed NaCl+KCl Solutions

Table 2. Comparison of Experimental and Calculated Solubility of NaCl and/or KCl in Mixed NaCl-KCl Solutions						
Solubility of NaCl in KCl Solutions						
T (°C)	KCl Conc. (m)	Solubility of NaCl (m)				
		Measured*	OLIAnalyzer Version 3.0 (MSE)		OLIAnalyzer Version 3.0 (Standard)	
			Calc.	%Dev	Calc.	%Dev
40	0	6.217	6.207	−0.16	6.225	0.12
	0.87	5.801	5.794	−0.12	5.795	−0.11
	1.407	5.577	5.545	−0.57	5.540	−0.67
	1.733	5.409	5.397	−0.22	5.389	−0.38
	2.566	5.12	5.027	−1.82	5.065	−1.07
100	0	6.68	6.720	0.60	6.690	0.15
	2.046	5.749	5.753	0.07	5.694	−0.96
	4.024	4.791	4.921	2.71	4.856	1.36
	4.086	4.94	4.896	−0.89	4.832	−2.19
150	0	7.198	7.235	0.51	7.249	0.71
	4.024	5.698	5.604	−1.65	5.439	−4.55
	5.365	5.185	5.142	−0.83	4.953	−4.48
Solubility of KCl in NaCl Solutions						
T (°C)	NaCl Conc. (m)	Solubility of KCl (m)				
		Measured*	OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
			Calc.	%Dev	Calc.	%Dev
40	0	5.37	5.428	−1.08	5.416	0.86
	1.748	4.28	4.328	1.12	4.203	−1.80
	1.827	4.21	4.281	1.69	4.153	−1.35
	3.486	3.32	3.375	1.66	3.193	−3.83
	3.592	3.28	3.323	1.31	3.138	−4.33
100	0	7.54	7.518	−0.29	7.491	−0.65
	1.717	6.44	6.411	−0.45	6.256	−2.86
	1.744	6.32	6.395	1.19	6.238	−1.30
	2.567	5.90	5.915	0.25	5.697	−3.44
	3.422	5.36	5.449	1.66	5.172	−3.51
	3.478	5.34	5.419	1.48	5.139	−3.76
	4.278	4.83	5.014	3.81	4.686	−2.98

Table 2. Comparison of Experimental and Calculated Solubility of NaCl and/or KCl in Mixed NaCl-KCl Solutions (continued)

Solubility of KCl in NaCl Solutions

	NaCl Conc. (M)	Solubility of KCl(m)				
		Measured*	OLIAnalyzer Version 3.0 (MSE)		OLIAnalyser Version 3.0 (Standard)	
			Calc.	%Dev	Calc.	%Dev
150	0	9.02	9.062	0.47	9.045	0.28
	1.711	8.13	8.056	–0.91	7.832	–3.67
	2.567	7.64	7.601	–0.51	7.274	–3.67
	3.422	7.15	7.177	0.38	6.752	–3.67
	4.278	6.71	6.779	1.03	6.266	–3.67

Solubility of NaCl and KCl in a NaCl-KCl Mixture

Calculation	T (°C)	KCl Solubility (m)			NaCl Solubility (m)		
		Measured*	Calc.	%Dev	Measured*	Calc.	%Dev
OLI Analyzer Version 3.0 (MSE)	40	2.627	2.695	2.59	5.008	4.971	–0.74
	100	4.734	4.859	2.64	4.708	4.598	–2.34
	150	6.518	6.657	2.13	4.791	4.758	–0.69
OLI Analyzer Version 3.0 (Standard)	40	2.627	2.453	–6.61	5.008	5.065	1.14
	100	4.734	4.469	–5.60	4.708	4.685	–0.49
	150	6.518	6.021	–7.63	4.791	4.737	–1.14

*Data are from Pabalan, R.T. Software Validation Report for SOLCALC, Version 1.0. San Antonio, Texas: CNWRA. 2002; original data from Linke, W.F. *Solubilities of Inorganic and Metal Organic Compounds*. Vols. 1 and 2. 4th Edition. Washington, DC: American Chemical Society. 1965.

Test Case 3—Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

Table 3. Comparison of Experimental and Calculated Solubility of $MgCl_2$ in $CaCl_2$-KCl-NaCl Solutions								
Temp (°C)	Fixed Salt Concentrations (m)			Solubility of $MgCl_2$ (m)				
					OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
	$CaCl_2$	KCl	NaCl	Measured*	Calc.	%Dev	Calc.	%Dev
50	0.000	0.021	0.050	6.457	6.093	–5.64	6.192	–4.11
	0.086	0.022	0.049	6.366	6.148	–3.42	6.144	–3.49
	0.182	0.022	0.050	6.279	6.093	–2.96	6.094	–2.95
	0.376	0.023	0.051	5.981	5.983	0.03	5.989	0.13
	0.620	0.024	0.052	5.680	5.848	2.96	5.865	3.25
	0.768	0.025	0.051	5.391	5.769	7.01	5.792	7.44
	1.226	0.028	0.058	4.833	5.530	14.42	5.576	15.40
0	0.000	0.005	0.039	5.954	5.537	–7.00	5.547	–6.82
	0.127	0.005	0.040	5.754	5.439	–5.47	5.459	–5.14
	0.274	0.005	0.040	5.519	5.326	–3.50	5.357	–2.93
	0.538	0.005	0.042	5.175	5.124	–0.99	5.176	0.02
	0.880	0.006	0.041	4.697	4.866	3.60	4.946	5.31
	1.042	0.006	0.044	4.546	4.745	4.38	4.838	6.44
	1.146	0.007	0.048	4.401	4.667	6.04	4.769	8.36

*Korin, E.J. and A.S. Roy. "Heterogeneous Equilibrium in the Quinary System NaCl-KCl-$MgCl_2$-$CaCl_2$-H_2O in 0–50 °C Temperature Range." *Journal of Chemical Engineering Data*. Vol. 33. pp. 60–64. 1988.

Test Case 4—Vapor Pressure of KCl Solutions at 300 °C [572 °F] as a Function of Concentration

Table 4. Comparison of Experimental and Calculated Vapor Pressure of KCl Solutions at 300 °C [572 °F]					
	Vapor Pressure (Bar)				
		OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
KCl Concentration (m)	Measured*	Calc.	%Dev	Calc.	%Dev
0.549	85.70	84.07	−1.90	83.54	−2.52
0.966	84.78	82.92	−2.19	82.42	−2.78
1.392	83.32	81.79	−1.84	81.32	−2.40
1.904	81.78	80.48	−1.59	80.05	−2.12
2.954	79.02	77.93	−1.38	77.65	−1.73
3.388	77.62	76.90	−0.93	76.74	−1.13
4.283	75.26	74.78	−0.64	74.99	−0.36
4.528	74.56	74.20	−0.48	74.54	−0.03

*Data are from Pabalan, R.T. Software Validation Report for SOLCALC, Version 1.0. San Antonio, Texas: CNWRA. 2002; original data are from Zarembo, V.I., N.A. Antonov, V.N. Gilyarov, and M.K. Fedorov. "Activity Coefficients of KCl in the System KCl-H_2O at Temperatures of 150–350 °C and Pressures up to 1500 kg/cm^2." *Journal of Applied Chemistry*. Vol. 49. pp. 1,259–1,263. 1976.

Test Case 5—Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C [212 °F] as a Function of Concentration

Table 5. Comparison of Experimental and Calculated Vapor Pressure of $CaCl_2$ Solutions at 100 °C [212 °F]					
	Vapor Pressure (atm)				
		OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
$CaCl_2$ Concentration (m)	Measured*	Calc.	%Dev	Calc.	%Dev
0.5	0.978	0.991	1.33	0.987	0.92
1	0.948	0.962	1.48	0.959	1.16
2	0.875	0.886	1.26	0.883	0.91
3	0.781	0.790	1.15	0.787	0.77
4	0.682	0.686	0.59	0.680	−0.29
5	0.580	0.584	0.69	0.576	−0.69

Lide, D.R. *CRC Handbook of Chemistry and Physics*. D.R. Lide, ed. 77th Edition. Boston, Massachusetts: CRC Press. 1997.

Test Case 6—Lowering of Vapor Pressure by $NaNO_3$, NaOH, and $NaHSO_4$, in Aqueous Solutions at 100 °C [212 °F]

Table 6. Comparison of Experimental and Calculated Vapor Pressure of $NaNO_3$, NaOH, and $NaHSO_4$ Solutions at 100 °C [212 °F]					
	Vapor Pressure of $NaNO_3$ Solution (atm)				
		OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
$NaNO_3$ Concentration (m)	Measured*	Calc.	%Dev	Calc.	%Dev
2	0.939	0.948	0.96	0.950	1.17
4	0.881	0.888	0.79	0.891	1.14
6	0.827	0.835	0.97	0.836	1.09
8	0.779	0.788	1.16	0.786	0.90
10	0.738	0.746	1.08	0.740	0.27
	Vapor Pressure of NaOH Solution (atm)				
		OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
NaOH Concentration (m)	Measured*	Calc.	%Dev	Calc.	%Dev
2	0.937	0.943	0.64	0.940	0.32
4	0.859	0.865	0.7	0.854	–0.58
6	0.773	0.781	1.03	0.761	–1.55
8	0.680	0.695	2.21	0.669	–1.62
10	0.587	0.611	4.09	0.582	–0.85
	Vapor Pressure of $NaHSO_4$ Solution (atm)				
		OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
$NaHSO_4$ Concentration (m)	Measured*	Calc.	%Dev	Calc.	%Dev
2	0.938	0.943	0.53	0.941	0.32
4	0.868	0.872	0.46	0.859	–1.04
6	0.805	0.805	0	0.772	–4.10
8	0.750	0.741	–1.20	0.698	–6.93
10	0.696	0.683	–1.87	0.631	–9.34
*Lide, D.R. *CRC Handbook of Chemistry and Physics*. D.R. Lide, ed. 77th Edition. Boston, Massachusetts: CRC Press. 1997.					

Test Case 7—Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

Table 7. Comparison of Experimental and Calculated Deliquescence Relative Humidity of $NaNO_3$-NaCl-KNO_3 Mixture at 86 °C [186.8 °F]				
Deliquescence Relative Humidity of $NaNO_3$-NaCl-KNO_3 Saturated Solution (%)				
	OLIAnalyzer 3.0 (MSE)		OLIAnalyzer 3.0 (Standard)	
Measured*	Calc.	%Dev	Calc.	%Dev
43.4	41.3	–4.8	48.8	12.4
*Yang, et al. (2002)				

Test Case 8—Solubility of $NaNO_3$ and NaOH Up to Concentrations Beyond 30 M

Table 8. Comparison of the Calculated Solubilities (molal) with the Experimental Values for Concentrated $NaNO_3$ and NaOH Solutions

Salt	Temp (□C)	94.05	106.8	114.9	136.9	151.6	178	183.8	201.6
$NaNO_3$	Expt*	19.5	21.9	23.5	28.9	33.6	44.6	47.8	59.8
	Calc.	19.5	21.9	23.5	29.0	33.7	44.8	47.9	59.6
	%Dev	0	0	0	. 0.34	. 0.30	0.45	0.21	. 0.33
NaOH	Temp (□C)	30	40	50	60	80	110	192	—
	Expt*	29.8	32.3	36.3	43.5	78.3	91.3	130.3	—
	Calc.	29.2	32.0	36.0	43.3	77.5	90.1	140.4	—
	%Dev	–2.0	–0.93	–0.83	–0.46	–1.0	–1.3	7.8	—

*Linke (1965)

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ELECTRONIC NOTEBOOK #930E

October 1, 2009 through March 31, 2010

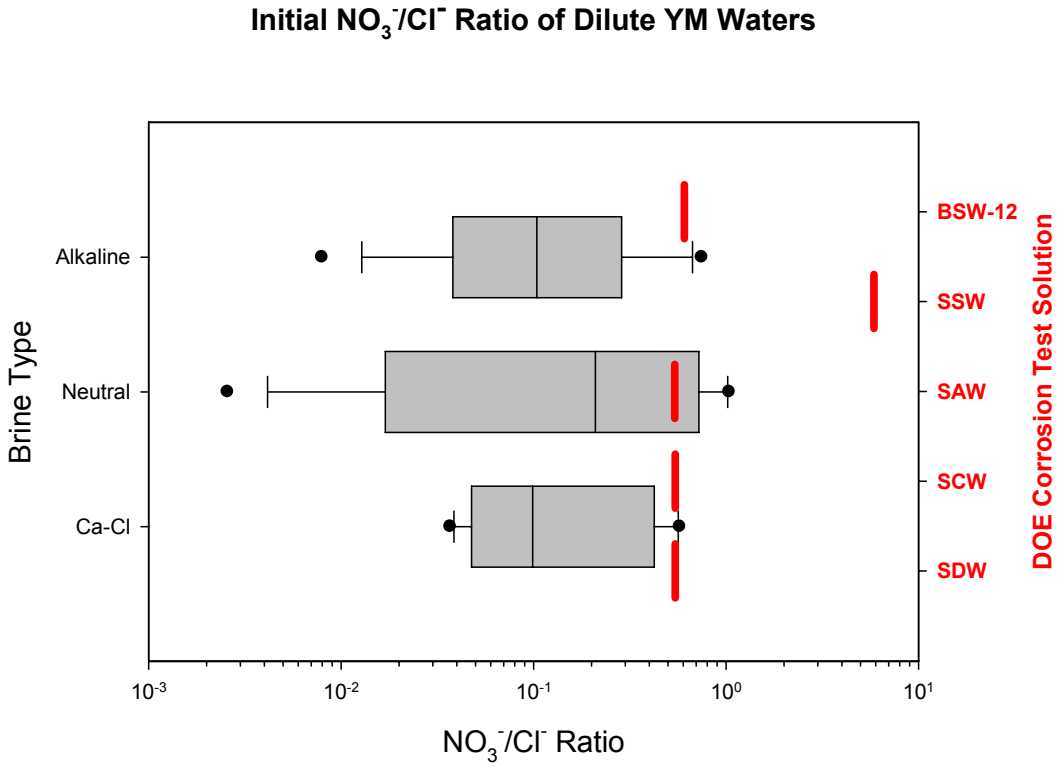
20.14002.01.353

Roberto T. Pabalan

The entries in this electronic scientific notebook #930E document activities conducted during the period October 1, 2009, through March 31, 2010, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.14002.01.353).

February 3, 2010

The following figure is a plot of the initial NO3/Cl ratio of the 33 dilute YM pore waters used in evaporation simulations (see page 183 of notebook #930E). The compositions of the YM pore waters are the same as those in the table on pages 155 and 156 of notebook # 679E. Also plotted are the NO3/Cl ratios of the solutions DOE used in its corrosion tests (test solution names SDW, SCW, SAW, SSW, and BSW-12). The test solution compositions are listed on page 170 of notebook #930E.



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