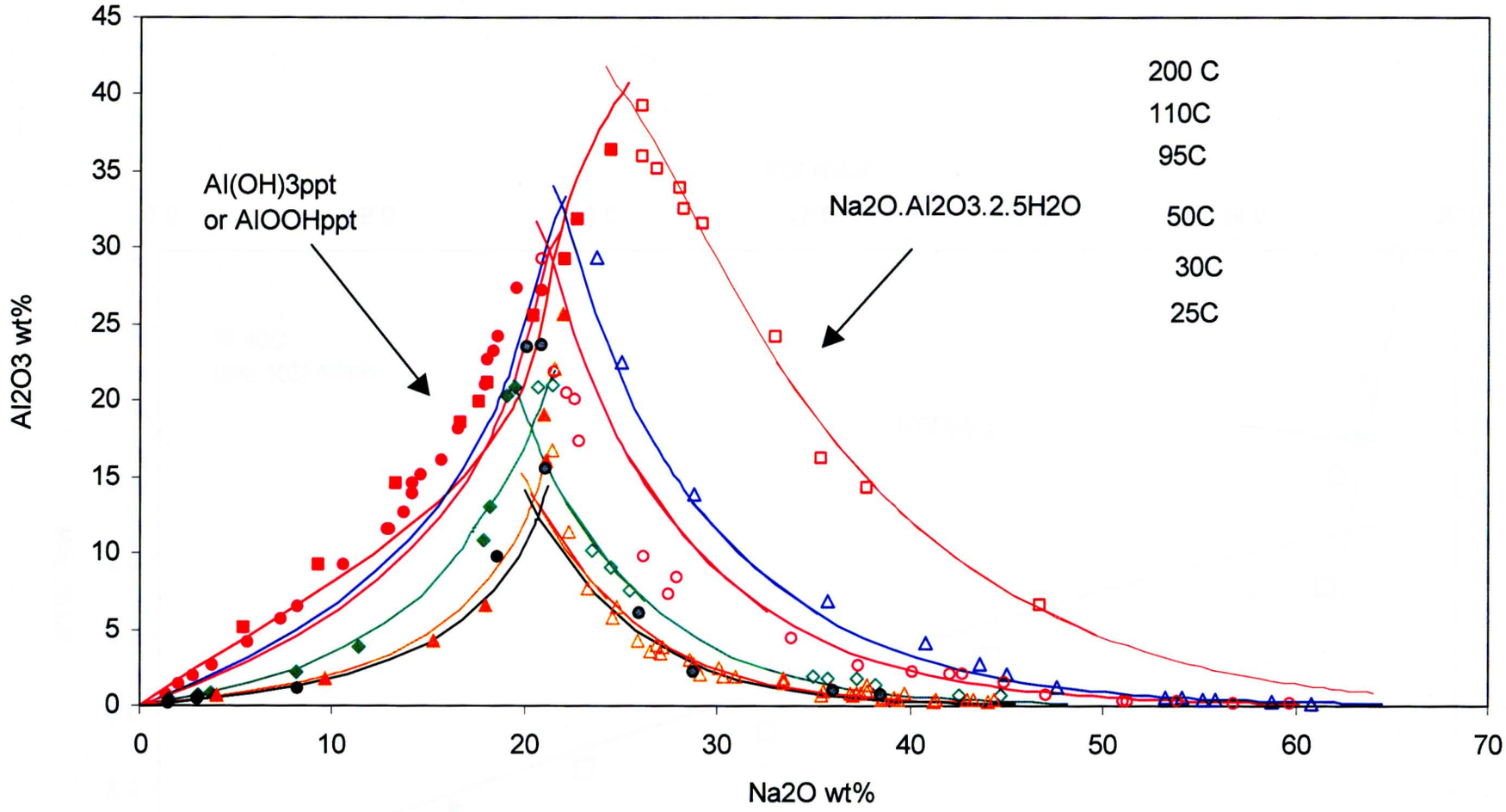
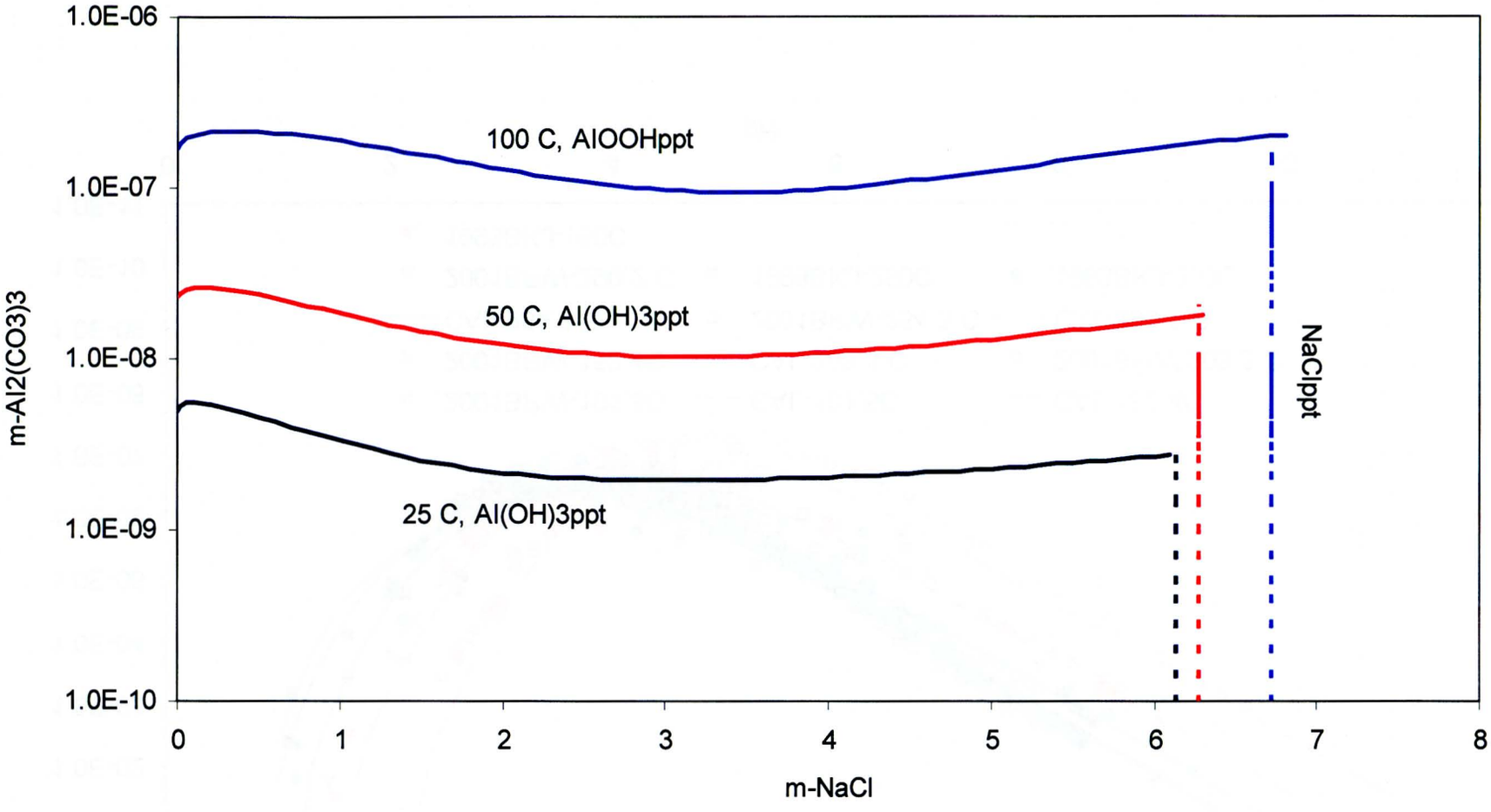
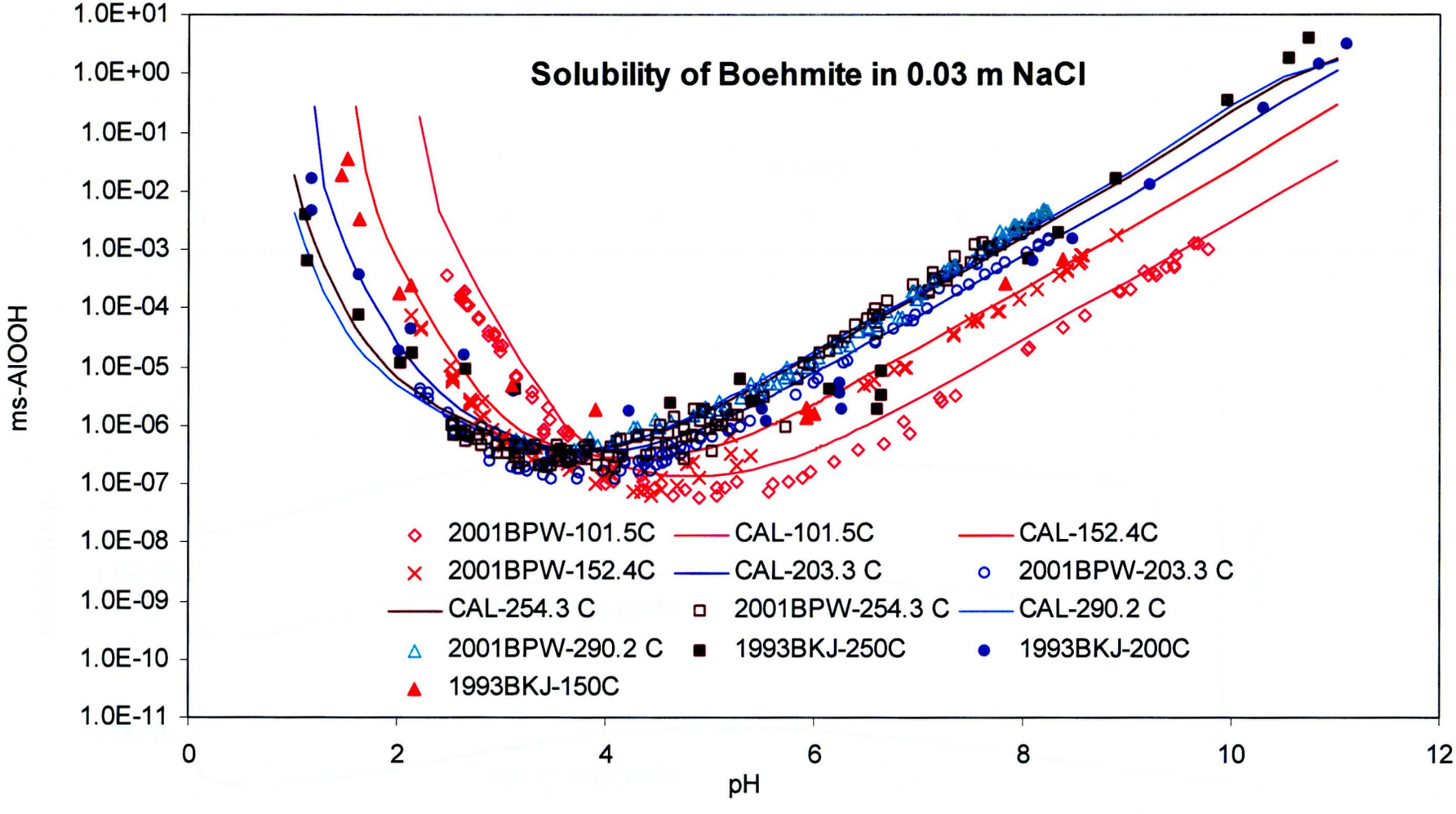
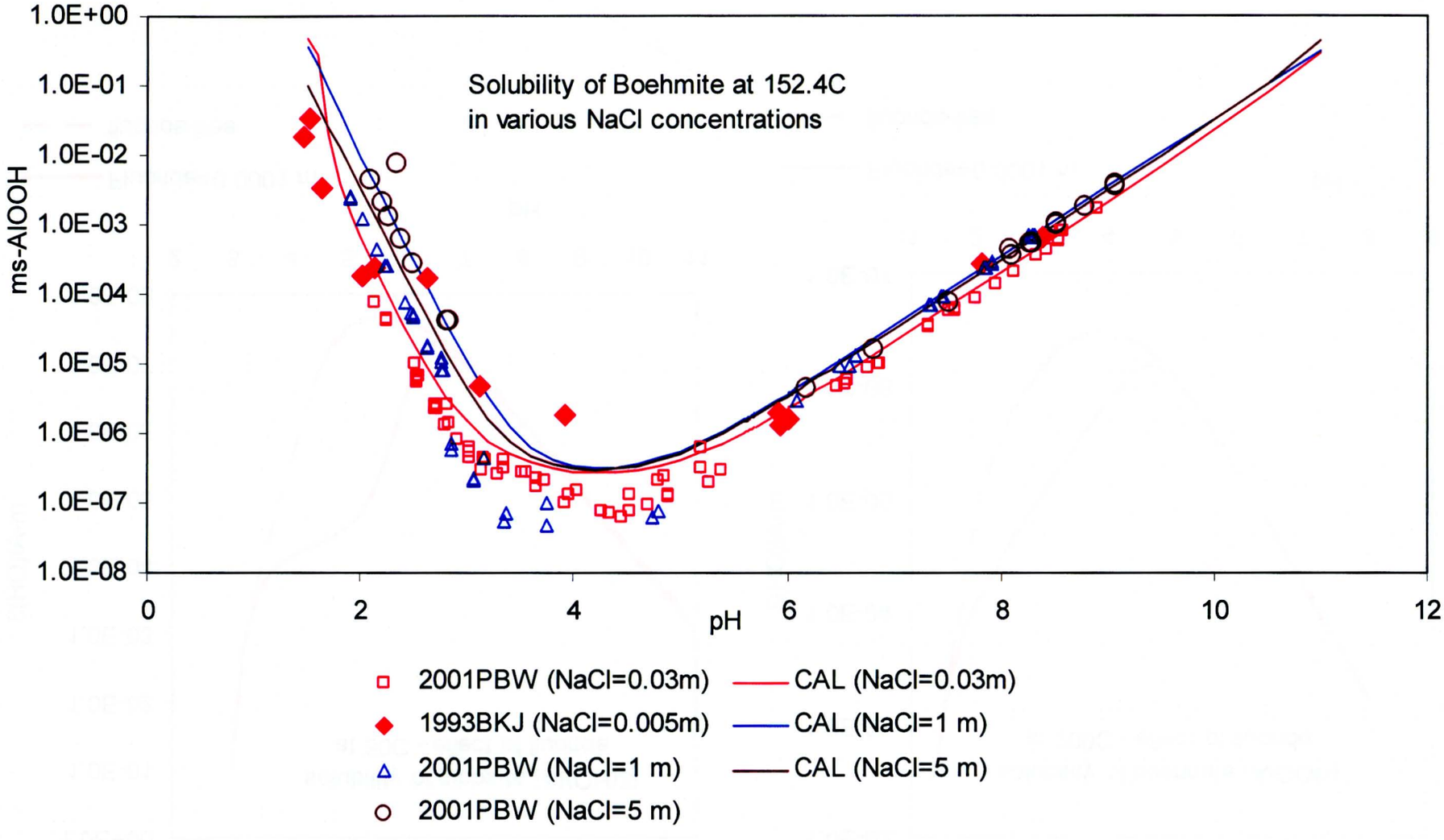
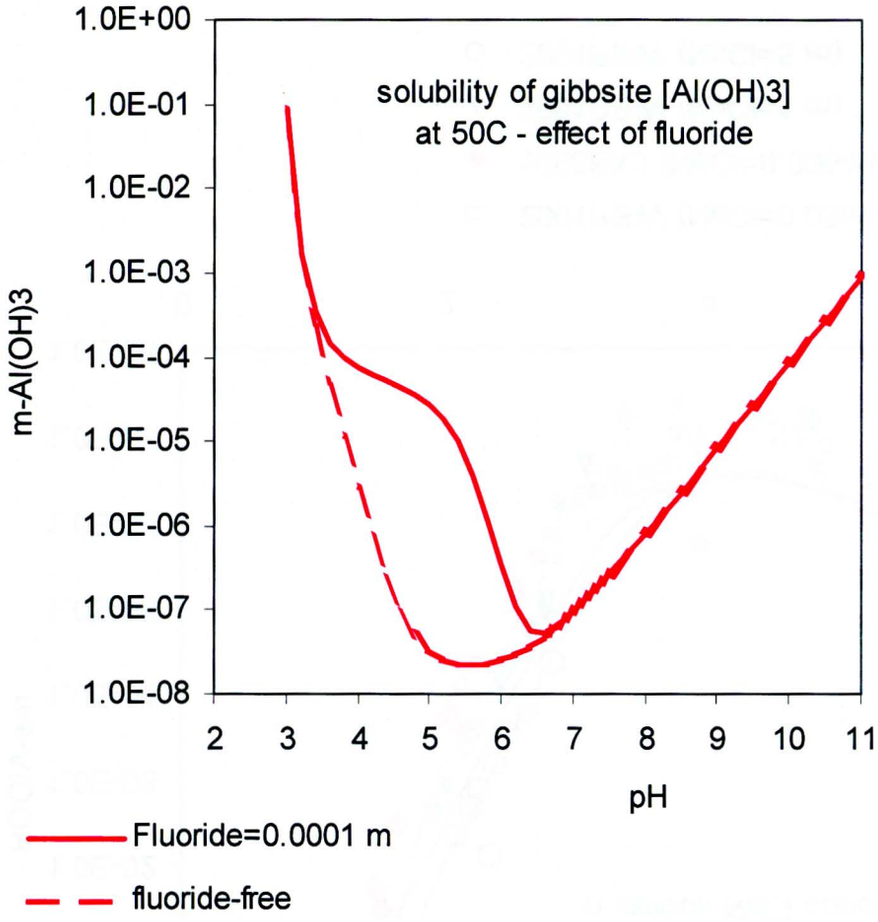
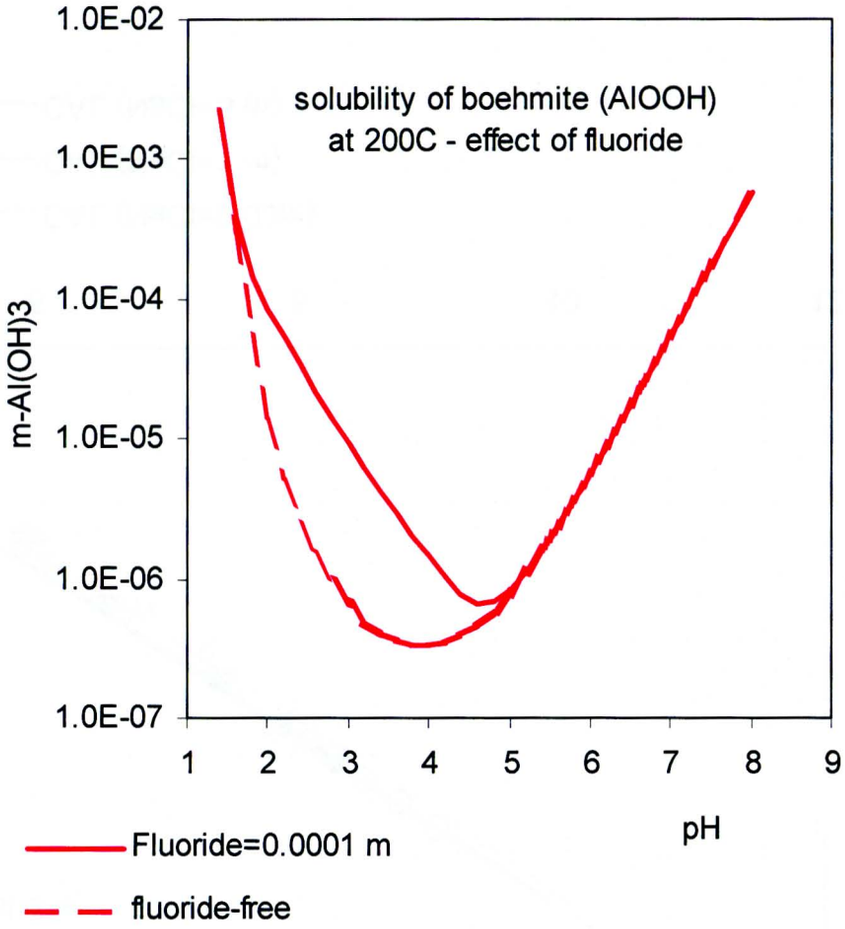

Al(OH)3ppt
or AlOOHppt
Na2O.Al2O3.2.5H2O
200 C
110C
95C
50C
30C
25C
Al2O3 wt%
Na2O wt%
0
5
10
15
20
25
30
35
40
45
0
10
20
30
40
50
60
70

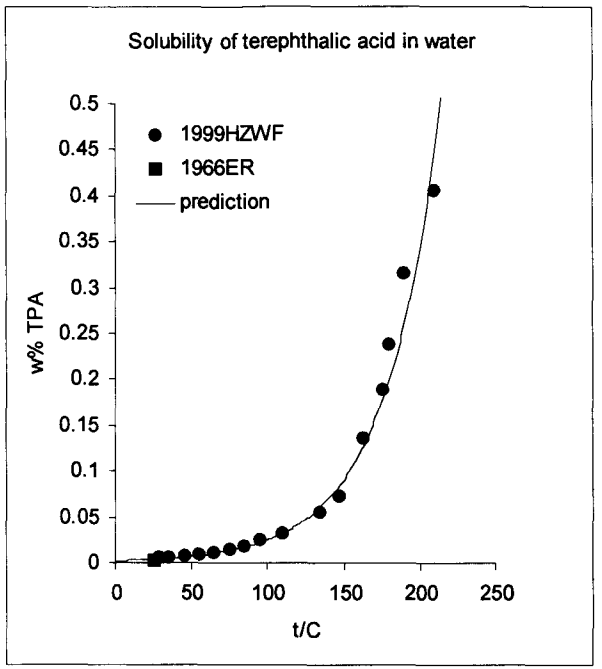

1.0E-06
1.0E-07
1.0E-08
1.0E-09
1.0E-10
m-Al2(CO3)3
100 C, AlOOHppt
50 C, Al(OH)3ppt
25 C, Al(OH)3ppt
NaClppt
0
1
2
3
4
5
6
7
8
m-NaCl

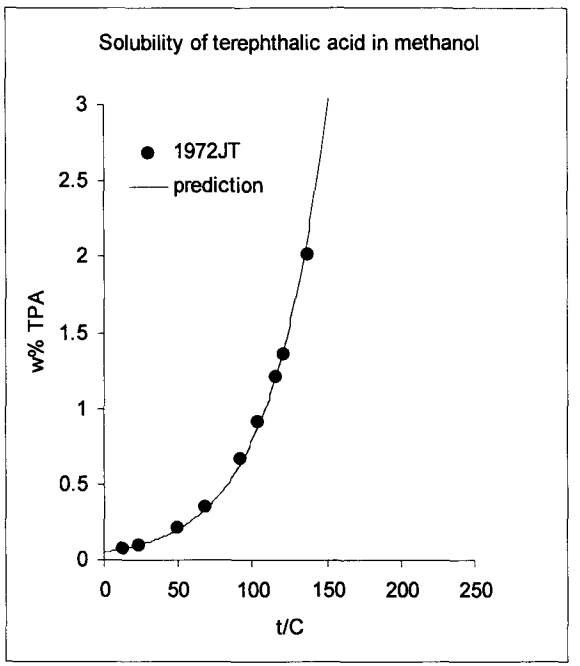

Solubility of Boehmite in 0.03 m NaCl
ms-AlOOH
pH
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1.0E-08
1.0E-09
1.0E-10
1.0E-11
0
2
4
6
8
10
12
2001BPW-101.5C
CAL-101.5C
CAL-152.4C
2001BPW-152.4C
CAL-203.3 C
2001BPW-203.3 C
CAL-254.3 C
2001BPW-254.3 C
CAL-290.2 C
2001BPW-290.2 C
1993BKJ-250C
1993BKJ-200C
1993BKJ-150C

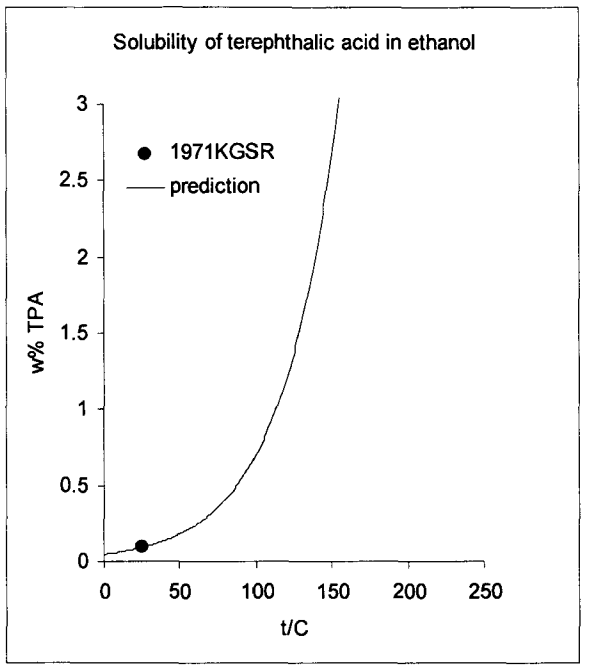

Solubility of Boehmite at 152.4C
in various NaCl concentrations
ms-AlOOH
1.0E+00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1.0E-08
0
2
4
6
8
10
12
pH
2001PBW (NaCl=0.03m)
1993BKJ (NaCl=0.005m)
2001PBW (NaCl=1 m)
2001PBW (NaCl=5 m)
CAL (NaCl=0.03m)
CAL (NaCl=1 m)
CAL (NaCl=5 m)

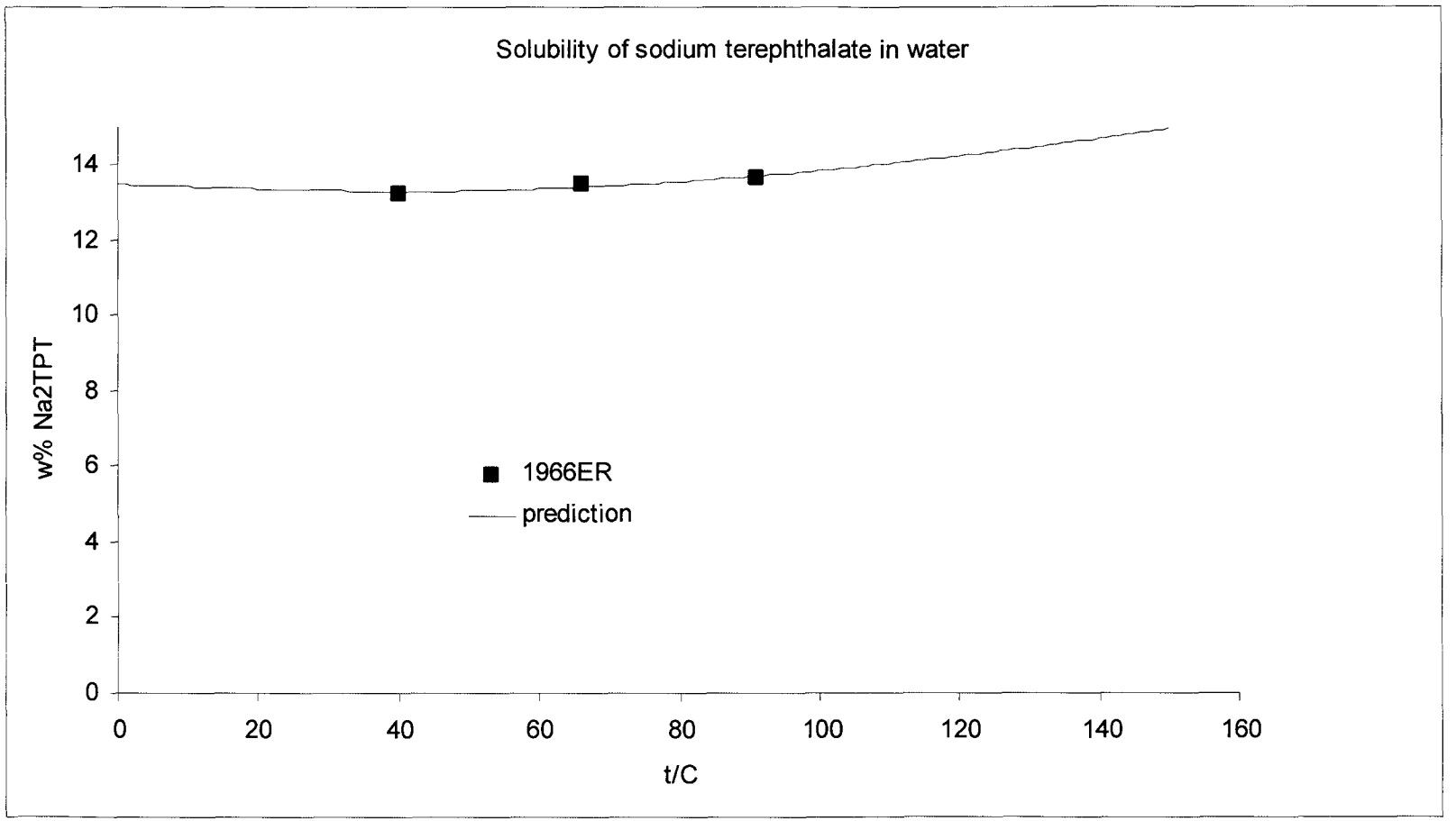

solubility of gibbsite [Al(OH)3]
at 50C - effect of fluoride
m-Al(OH)3
1.0E+00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1.0E-08
2 3 4 5 6 7 8 9 10 11
pH
Fluoride=0.0001 m
fluoride-free

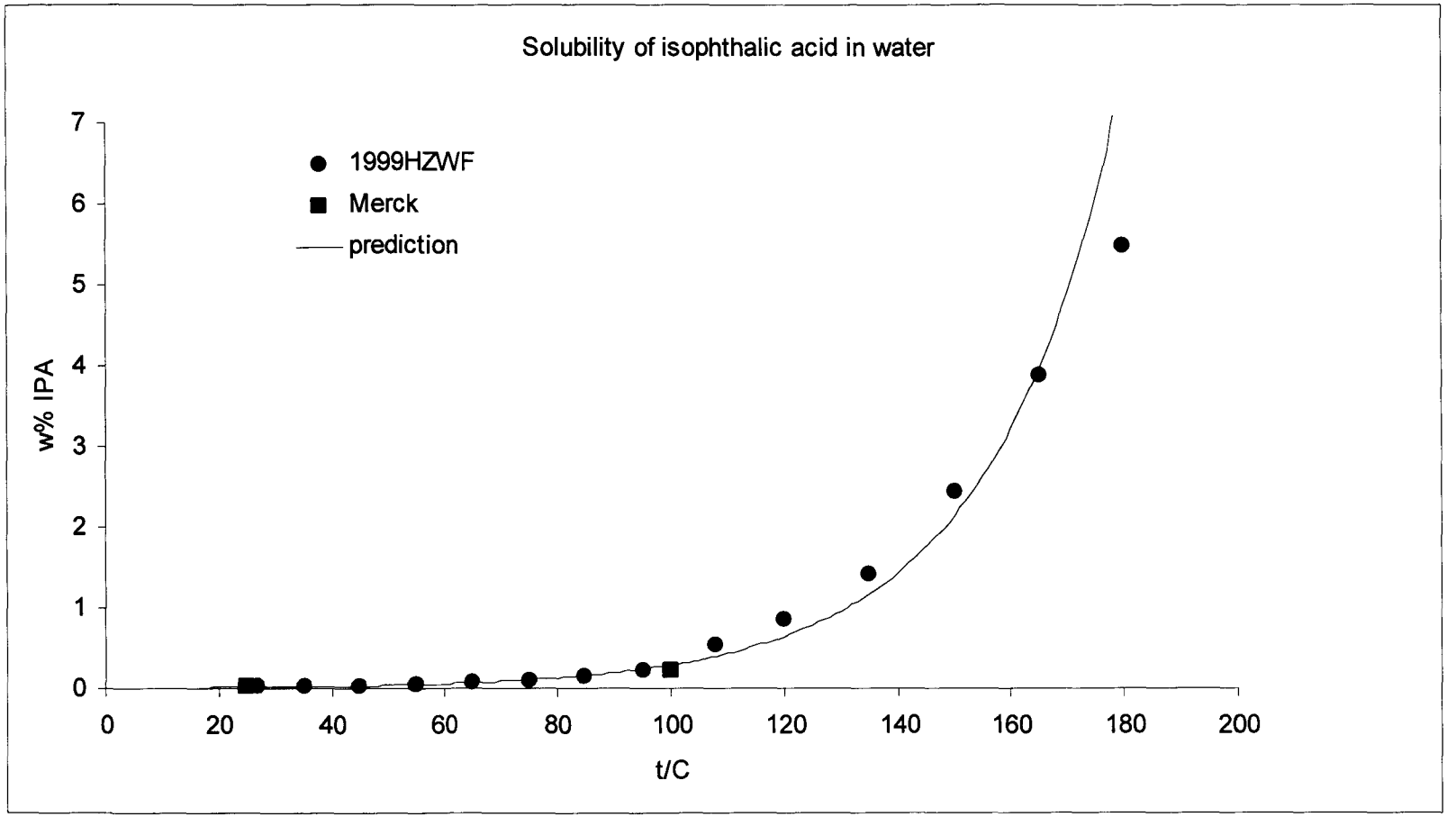

solubility of boehmite (AlOOH)
at 200C - effect of fluoride
m-Al(OH)3
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1 2 3 4 5 6 7 8 9
pH
Fluoride=0.0001 m
fluoride-free

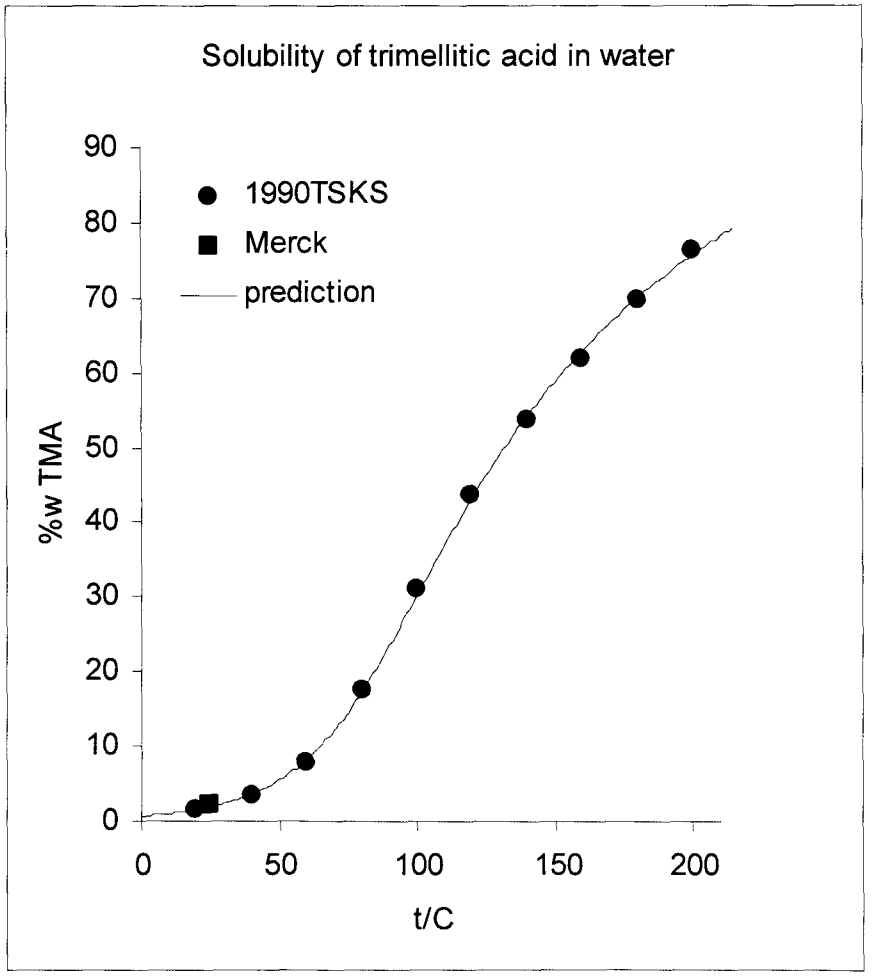

Solubility of terephthalic acid in water
1999HZWF
1966ER
prediction
w% TPA
t/C
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0
50
100
150
200
250

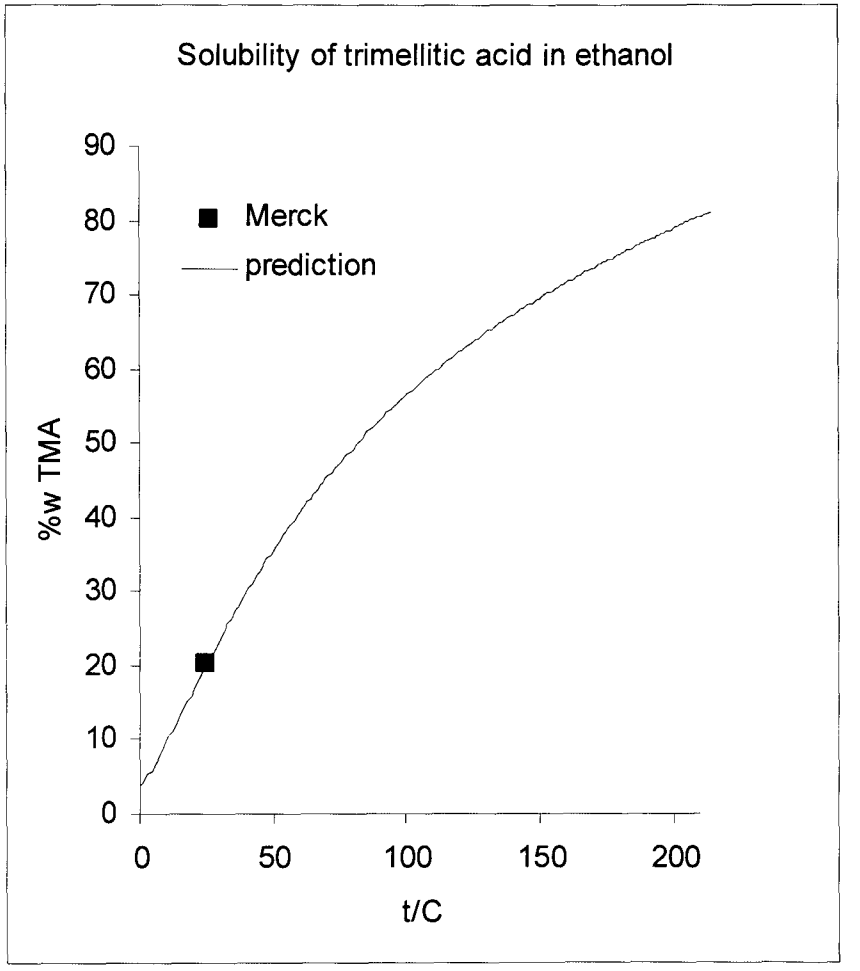

Solubility of terephthalic acid in methanol
1972JT
prediction
w% TPA
t/C
0
0.5
1
1.5
2
2.5
3
0
50
100
150
200
250

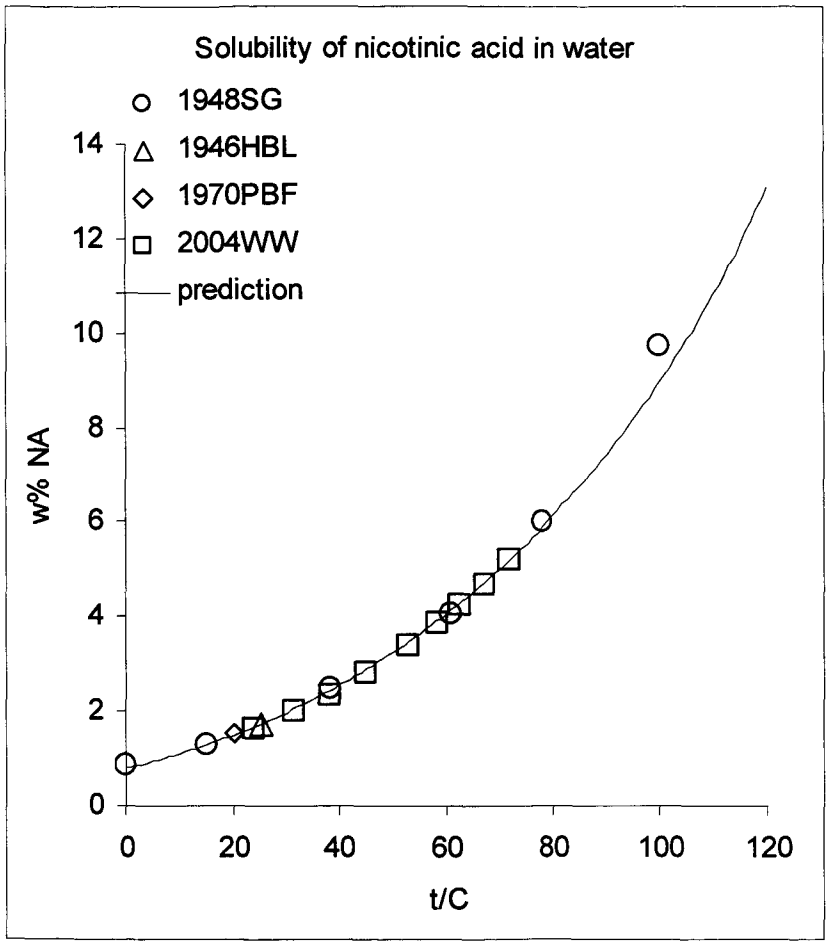

Solubility of terephthalic acid in ethanol
1971KGSR
prediction
w% TPA
t/C
0
0.5
1
1.5
2
2.5
3
0
50
100
150
200
250

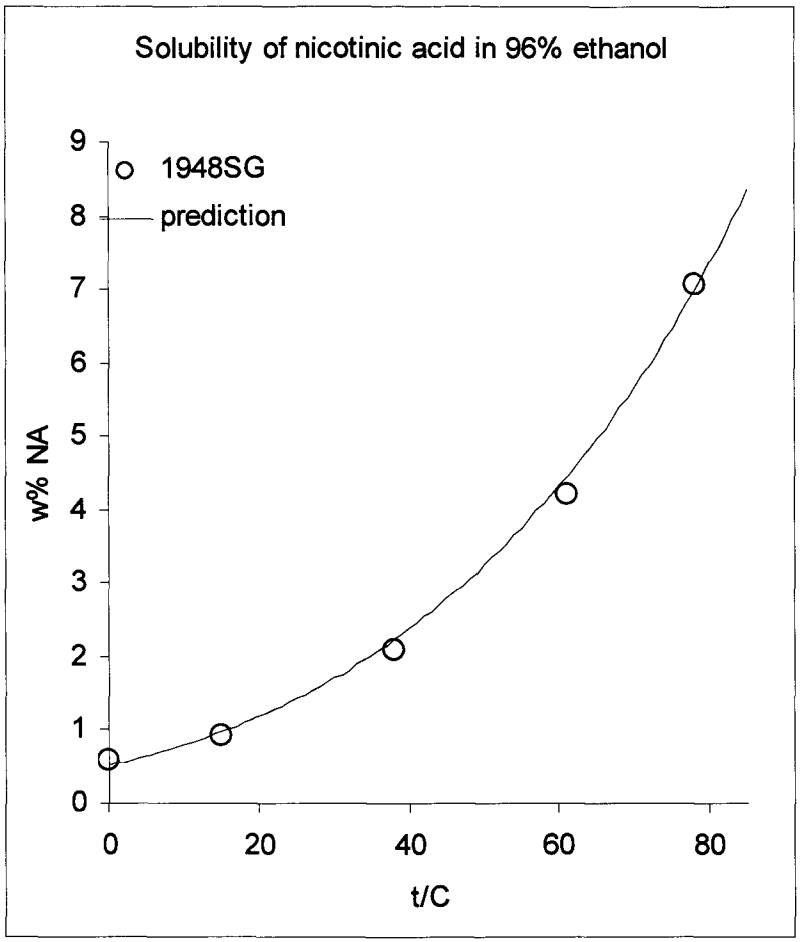

Solubility of sodium terephthalate in water
w% Na2TPT
14
12
10
8
6
4
2
0
0
20
40
60
80
100
120
140
160
t/C
1966ER
prediction

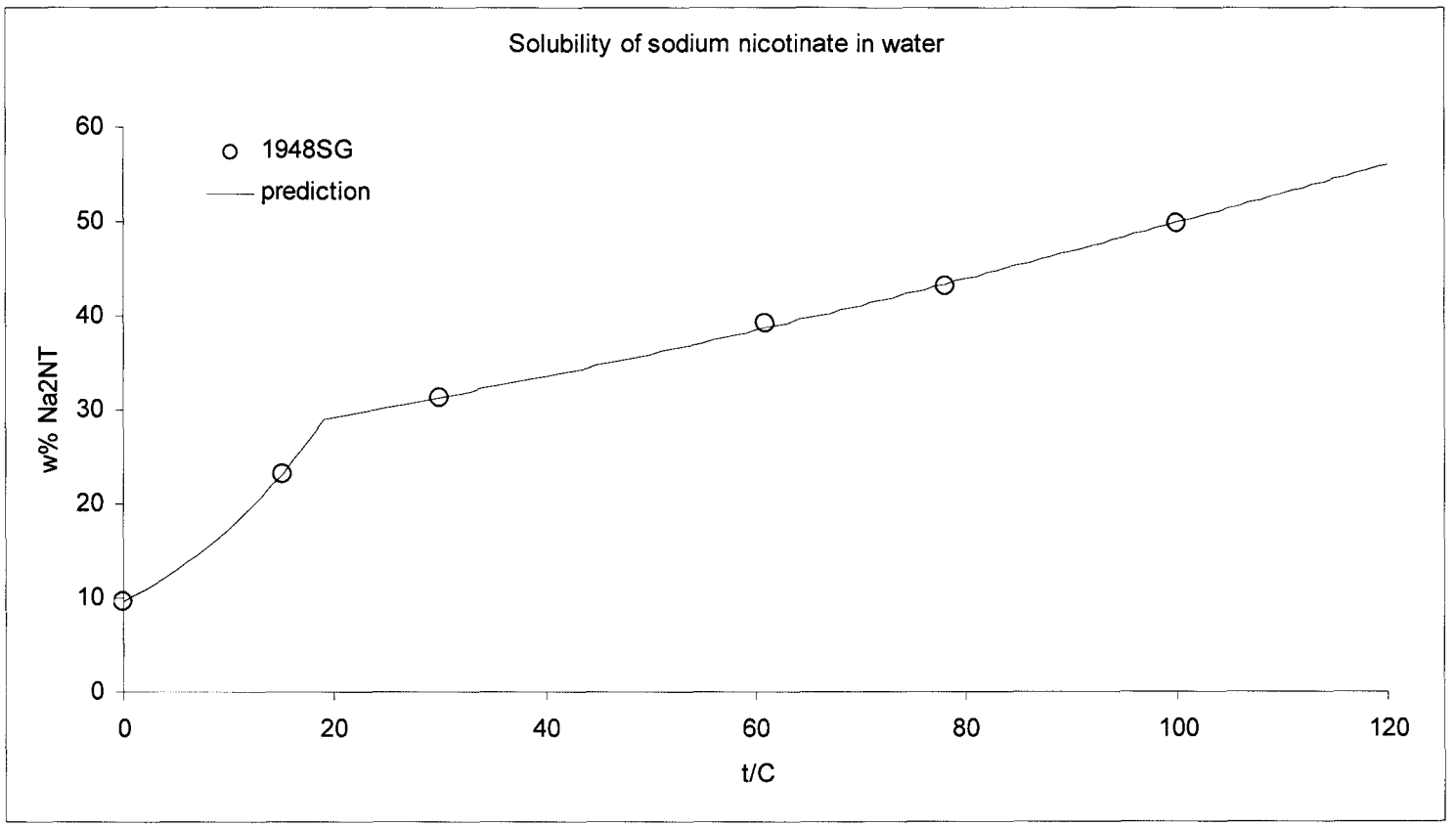

Solubility of isophthalic acid in water
1999HZWF
Merck
prediction
w% IPA
t/C
0
1
2
3
4
5
6
7
0
20
40
60
80
100
120
140
160
180
200

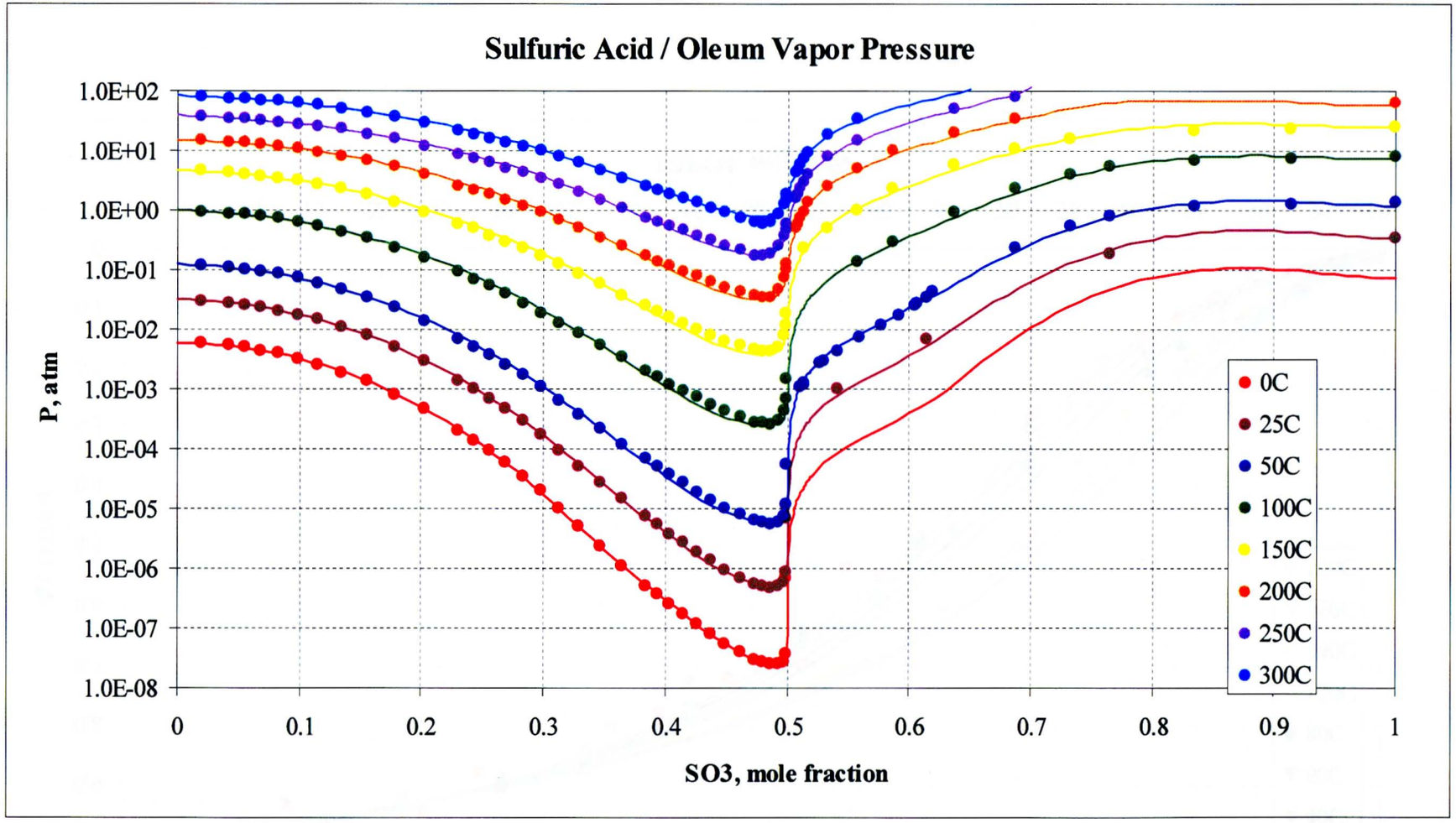

Solubility of trimellitic acid in water
1990TSKS
Merck
prediction
%w TMA
t/C
0
10
20
30
40
50
60
70
80
90
0
50
100
150
200

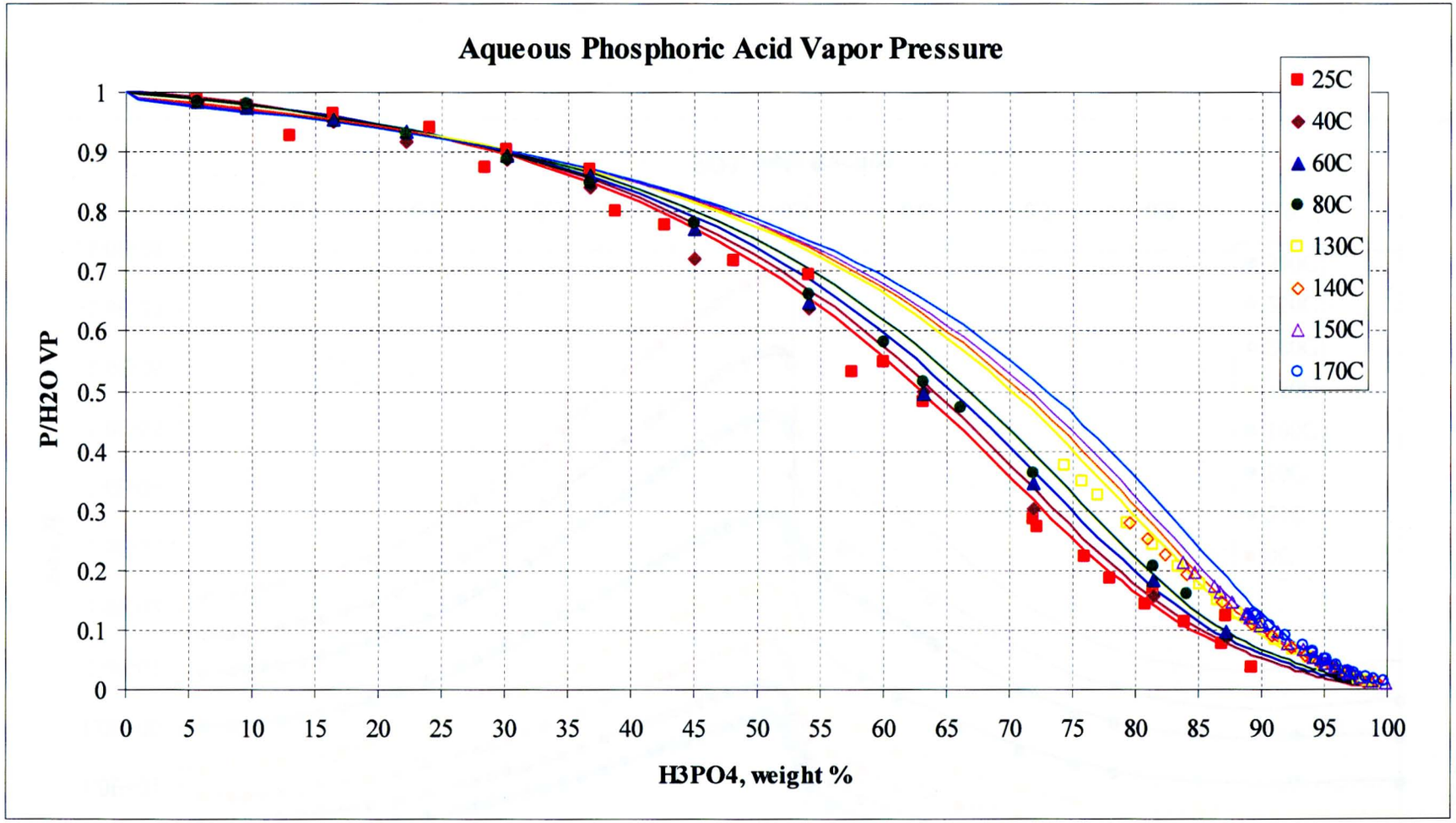

Solubility of trimellitic acid in ethanol
Merck
prediction
%w TMA
t/C
0
10
20
30
40
50
60
70
80
90
0
50
100
150
200


Solubility of nicotinic acid in water
1948SG
1946HBL
1970PBF
2004WW
prediction
w% NA
t/C
0
2
4
6
8
10
12
14
0
20
40
60
80
100
120


Solubility of nicotinic acid in 96% ethanol
1948SG
prediction
w% NA
t/C
0
1
2
3
4
5
6
7
8
9
0
20
40
60
80


Solubility of sodium nicotinate in water
1948SG
prediction
w% Na2NT
t/C
0
10
20
30
40
50
60
0
20
40
60
80
100
120


Sulfuric Acid / Oleum Vapor Pressure
P, atm
1.0E+02
1.0E+01
1.0E+00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1.0E-08
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
SO3, mole fraction
0C
25C
50C
100C
150C
200C
250C
300C


Aqueous Phosphoric Acid Vapor Pressure
P/H2O VP
H3PO4, weight %
25C
40C
60C
80C
130C
140C
150C
170C
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100

December 2, 2004

ESP 7.0 was used to calculate the solubility of NaCl and KCl in the system NaCl-KCl-MgCl2 at 20, 55, and 90 C. The calculated values are compared with experimental data in the following figure. On the next page is a figure showing a comparison of experimental data and calculated values taken from Pabalan and Pitzer (1987; Geochimica et Cosmochimica Acta 51: 2429-2443).

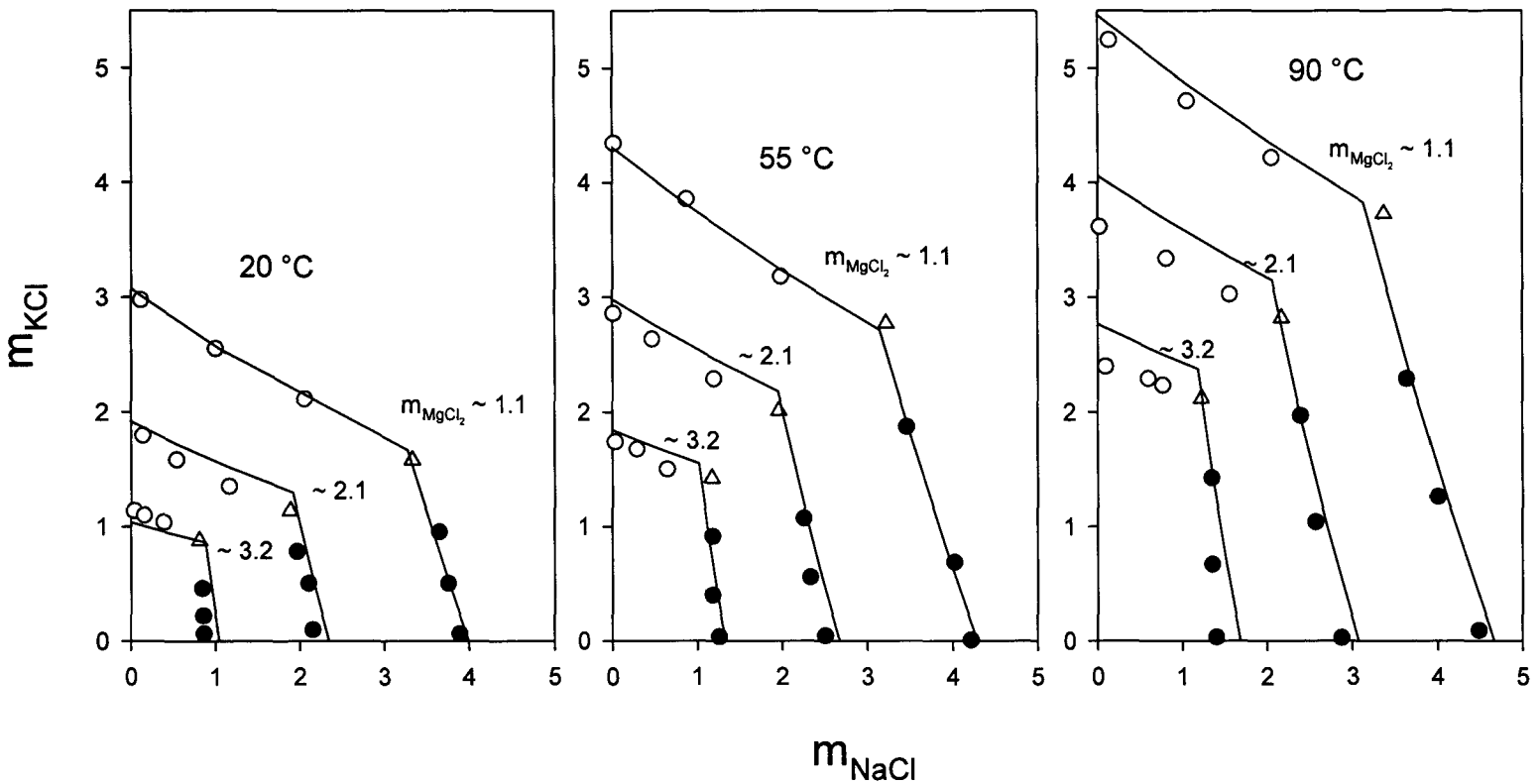


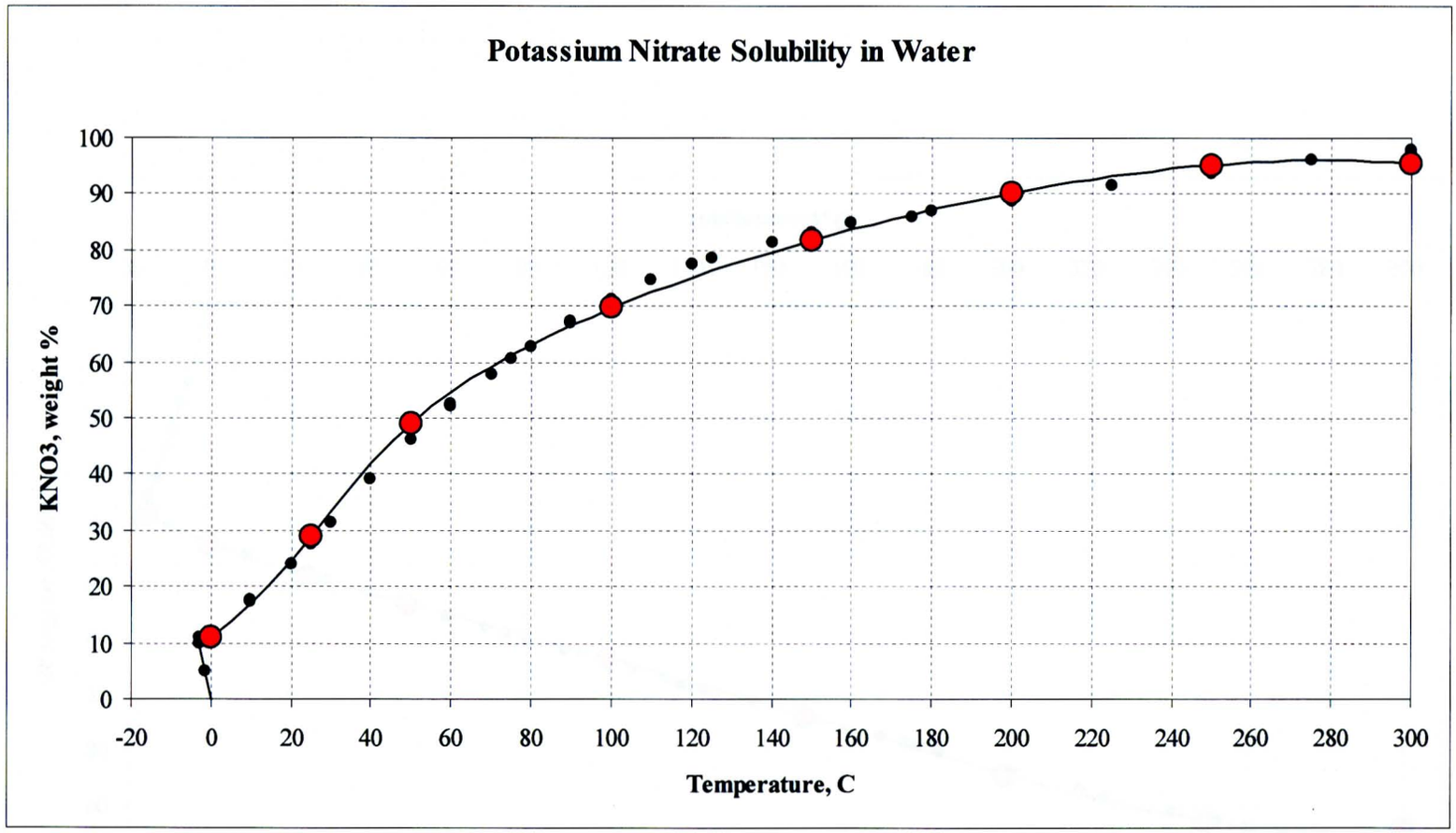
Figure 16 taken from Pabalan and Pitzer (1987) this figure is copyright protected and therefore not included in this notebook.

FIG. 16. Predicted and experimental solubilities of halite and/or sylvite in the quaternary system $NaCl$-KCl-$MgCl_2$-H_2O at 20, 55, and 90°C and at $MgCl_2$ molalities of approximately 1.1, 2.1, and 3.2. Experimental data are from KAYSER (1923).

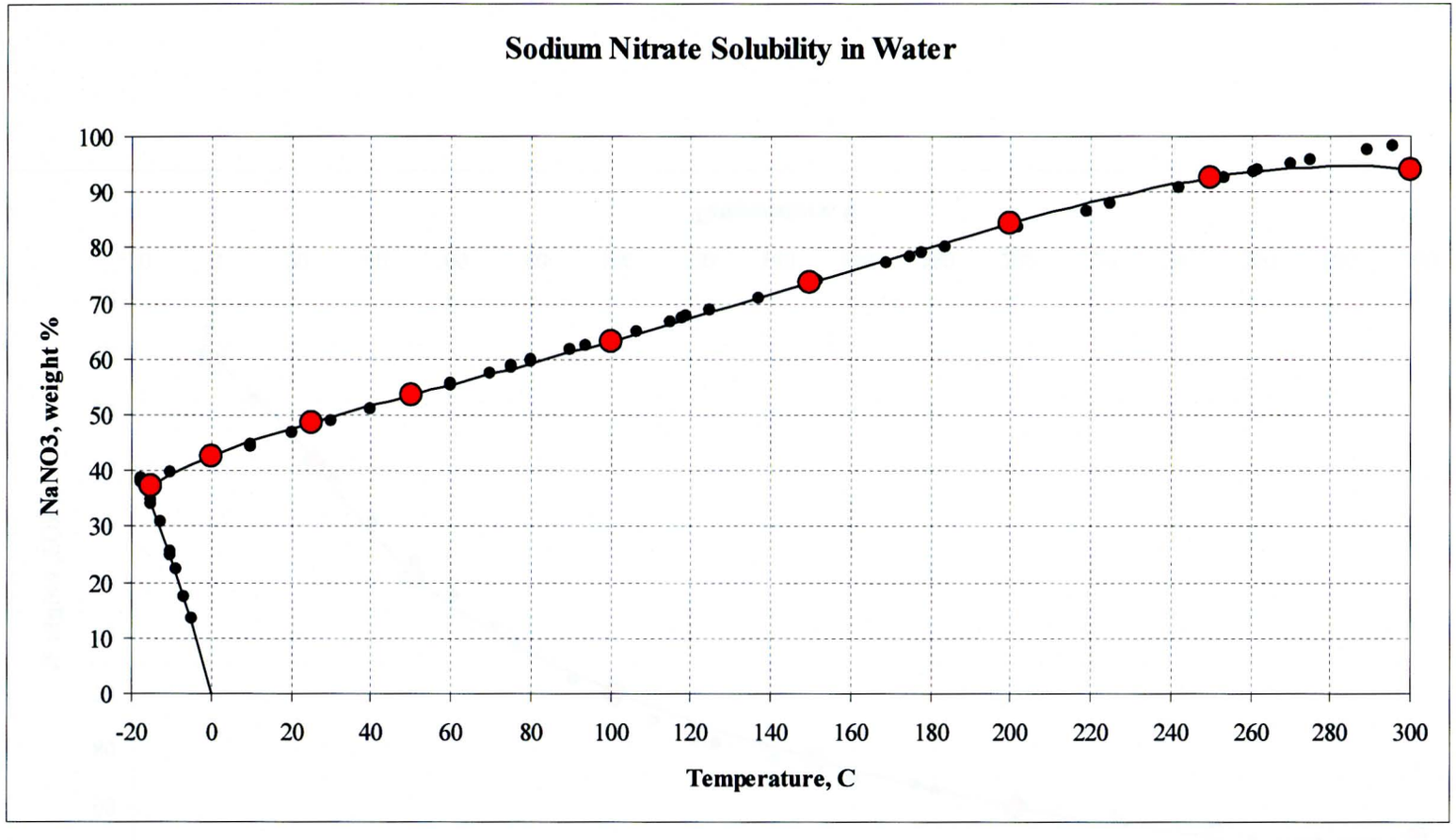
Figure taken from Pabalan and Pitzer (1987)

December 15, 2004

Verification of ESP 7.0 solubility calculation: KNO3 system. Curve: OLI results; black dots: experimental; red dots: RTP results using ESP 7.0.

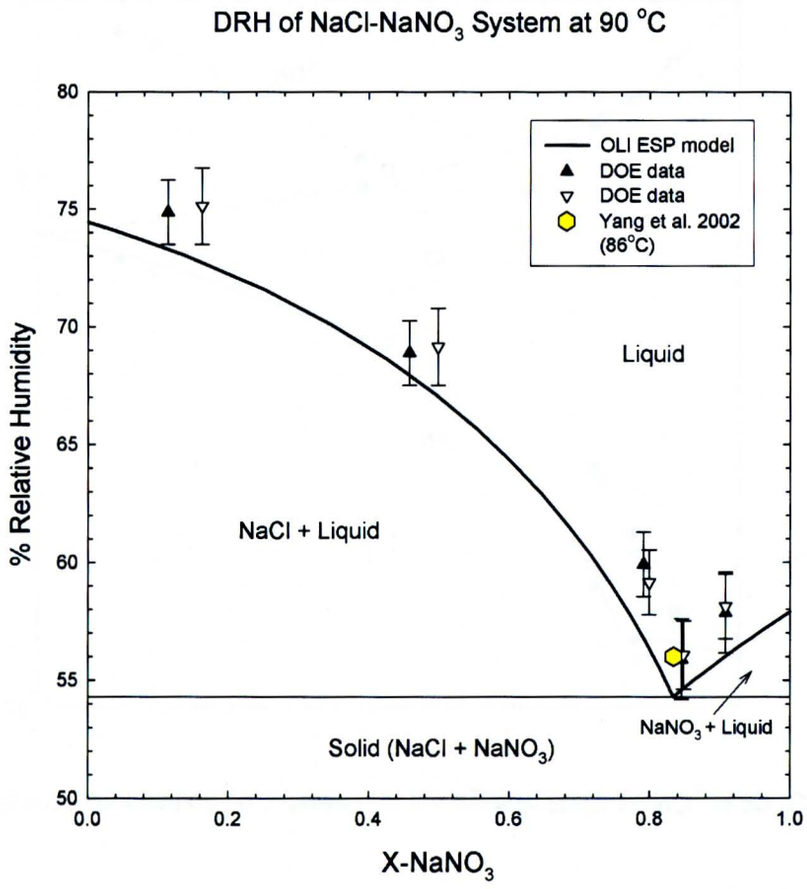


Verification of ESP 7.0 solubility calculations: NaNO3 system: Curve: OLI results; black dots: experimental; red dots: RTP results using ESP 7.0.



December 16, 2004

Figure comparing DOE DRH data for the system NaCl-NaNO3 at 90 C with values calculated using OLI ESP 7.0. Also shown is the figure giving the DOE data (reference: Craig, Carroll, and Wolery, 2004; Water-Rock Interaction; Wanty and Seal, eds., p. 1276). Also shown is the DRH measured by Yang et al. (2002, MRS paper) using a conductivity method. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.

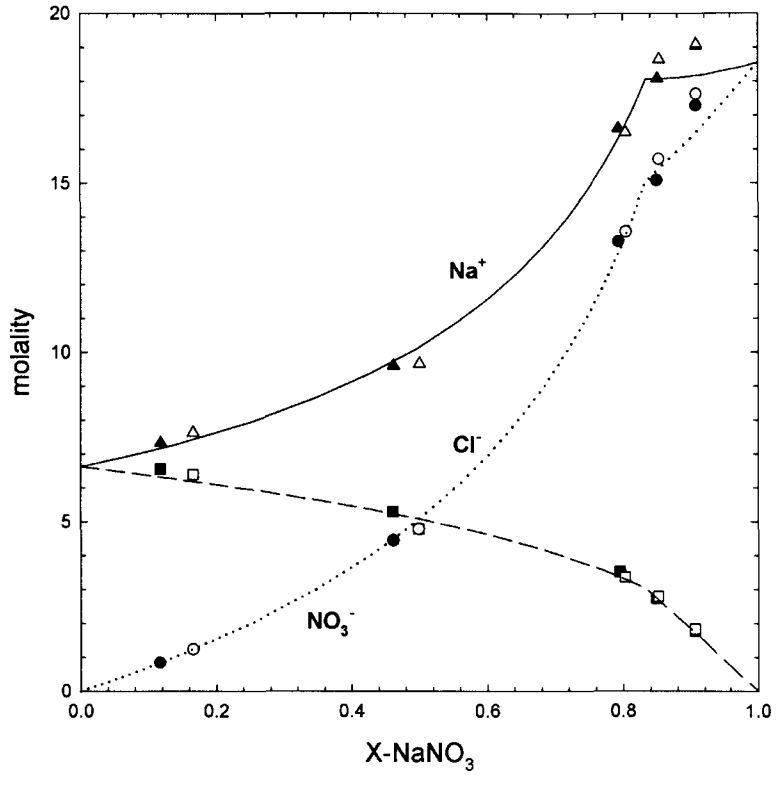


This figure taken from Craig, Carroll, and Wolery; Water-Rock Interaction; Wanty and Seal, eds., p. 1276 (2004) this figure is copyright protected and therefore not included in this notebook.

Craig et al. (2004)

Figure comparing DOE composition data for the system NaCl-NaNO3 at 90 C with values calculated using OLI ESP 7.0. Also shown is the figure giving the DOE data (reference: Craig, Carroll, and Wolery, 2004; Water-Rock Interaction; Wanty and Seal, eds., p. 1276). The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.

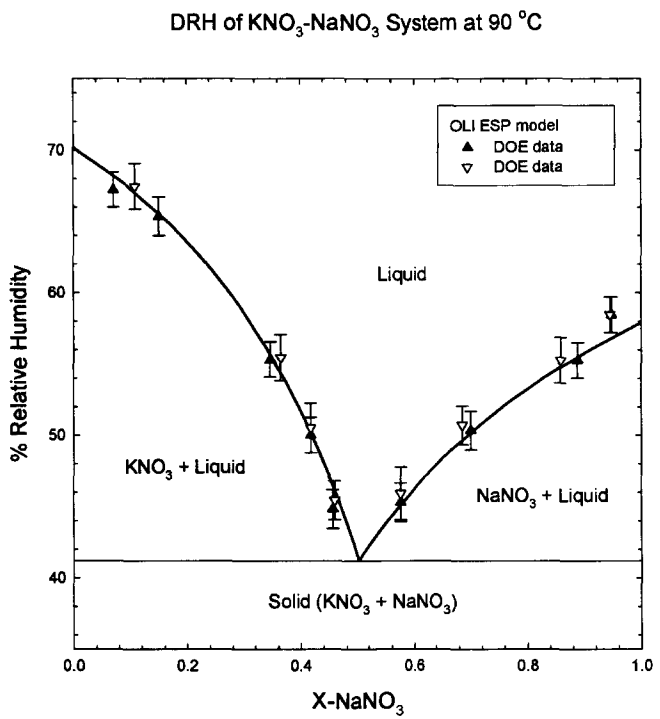
Solution composition vs X-$NaNO_3$ in the system NaCl-$NaNO_3$ at 90 °C



This figure taken from Craig, Carroll, and Wolery; Water-Rock Interaction; Wanty and Seal, eds., p. 1276 (2004) this figure is copyright protected and therefore not included in this notebook.

(Craig et al., 2004)

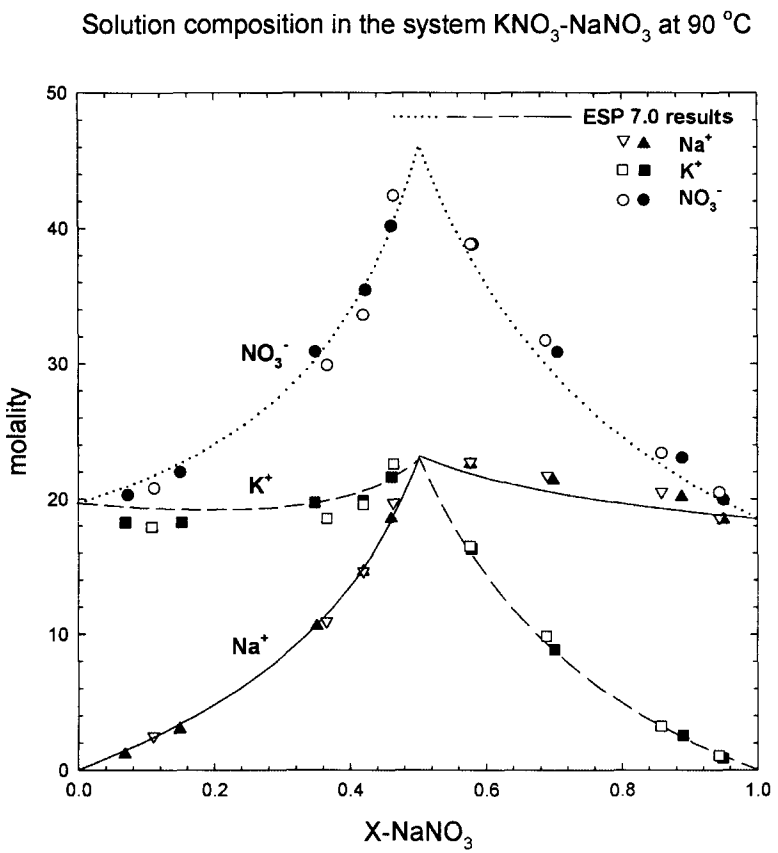
Figure comparing DOE DRH data for the system KNO3-NaNO3 at 90 C with values calculated using OLI ESP 7.0. Also shown is the figure giving the DOE data (reference: Craig, Carroll, and Wolery, 2004; Water-Rock Interaction; Wanty and Seal, eds., p. 1277). The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.



This figure taken from Craig, Carroll, and Wolery; Water-Rock Interaction; Wanty and Seal, eds., p. 1277 (2004) this figure is copyright protected and therefore not included in this notebook.

(Craig et al., 2004)

Figure comparing DOE composition data for the system KNO3-NaNO3 at 90 C with values calculated using OLI ESP 7.0. Also shown is the figure giving the DOE data (reference: Craig, Carroll, and Wolery, 2004; Water-Rock Interaction; Wanty and Seal, eds., p. 1277). The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.

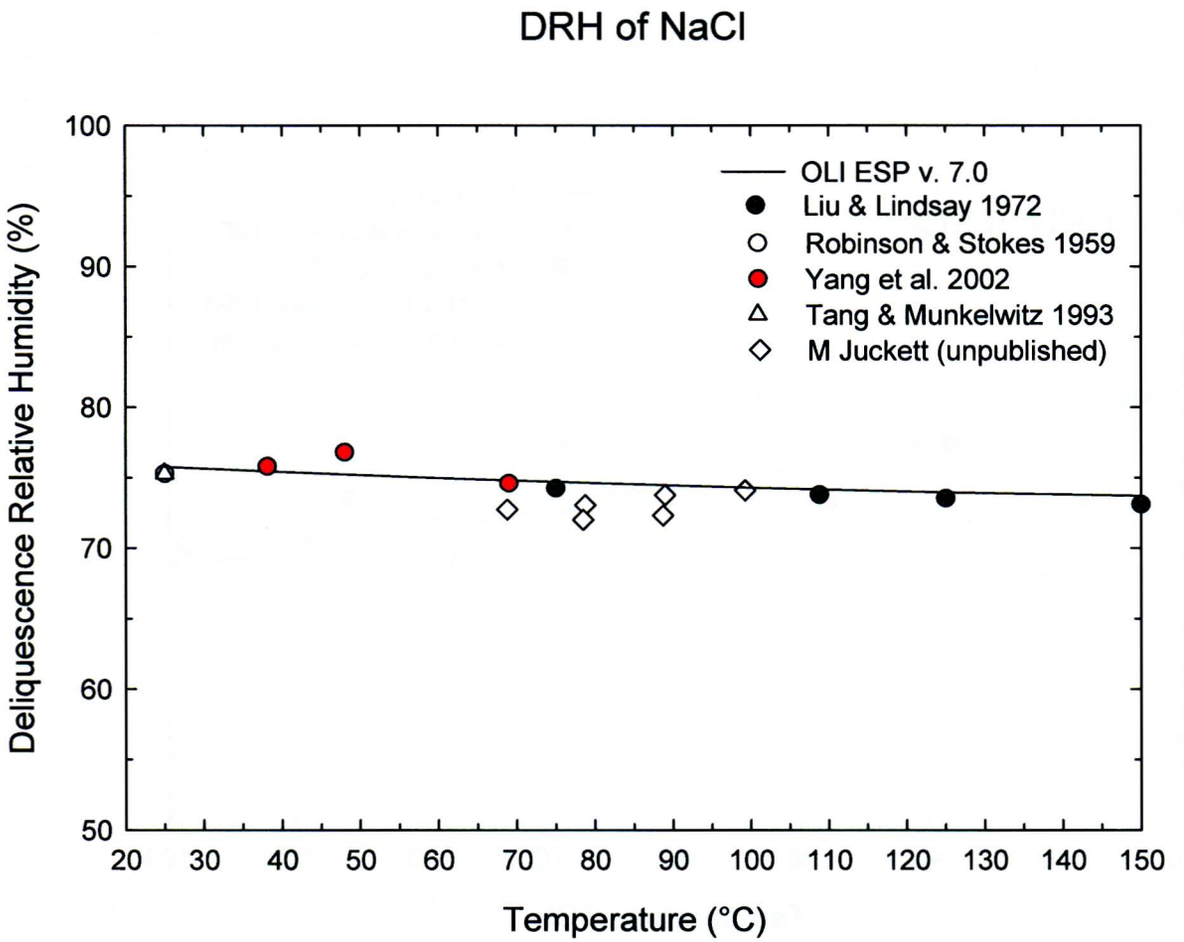


This figure taken from Craig, Carroll, and Wolery; Water-Rock Interaction; Wanty and Seal, eds., p. 1277 (2004) this figure is copyright protected and therefore not included in this notebook.

(Craig et al., 2004)

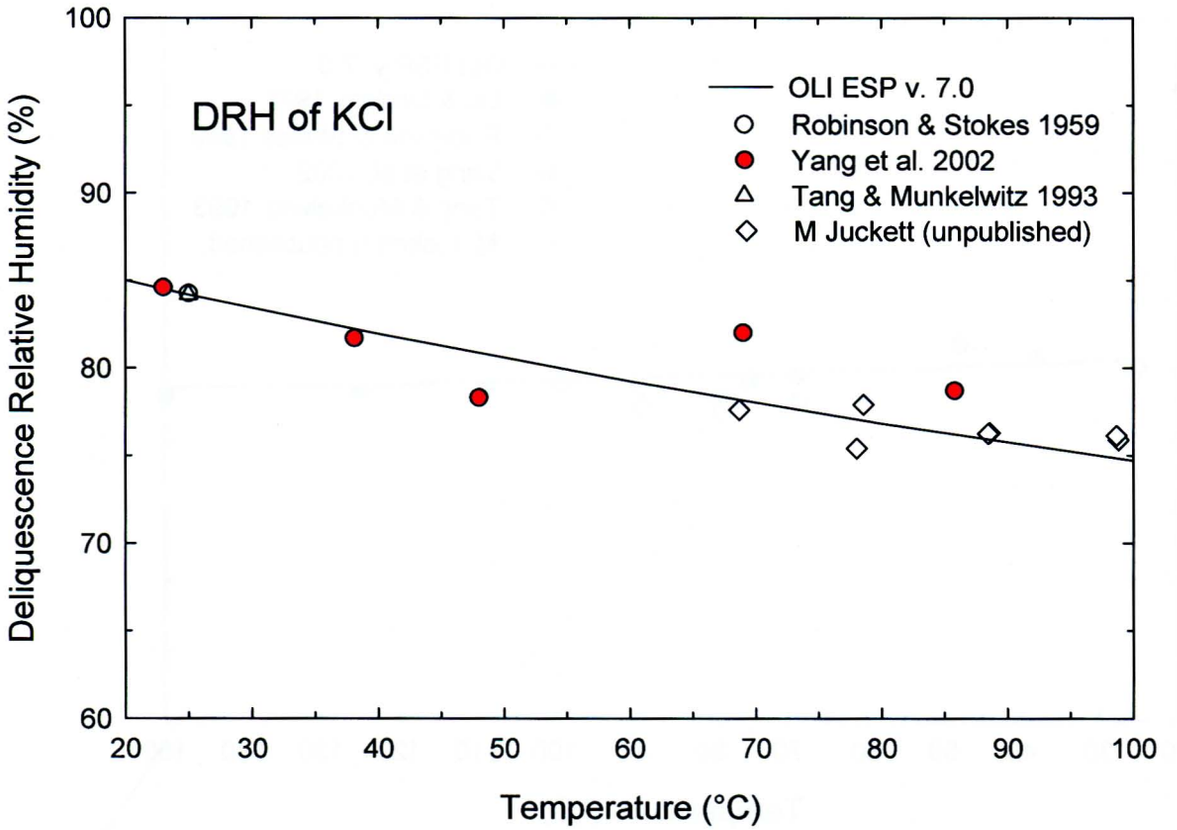
December 27, 2004

The following figure compares DRH values for NaCl taken from several sources:

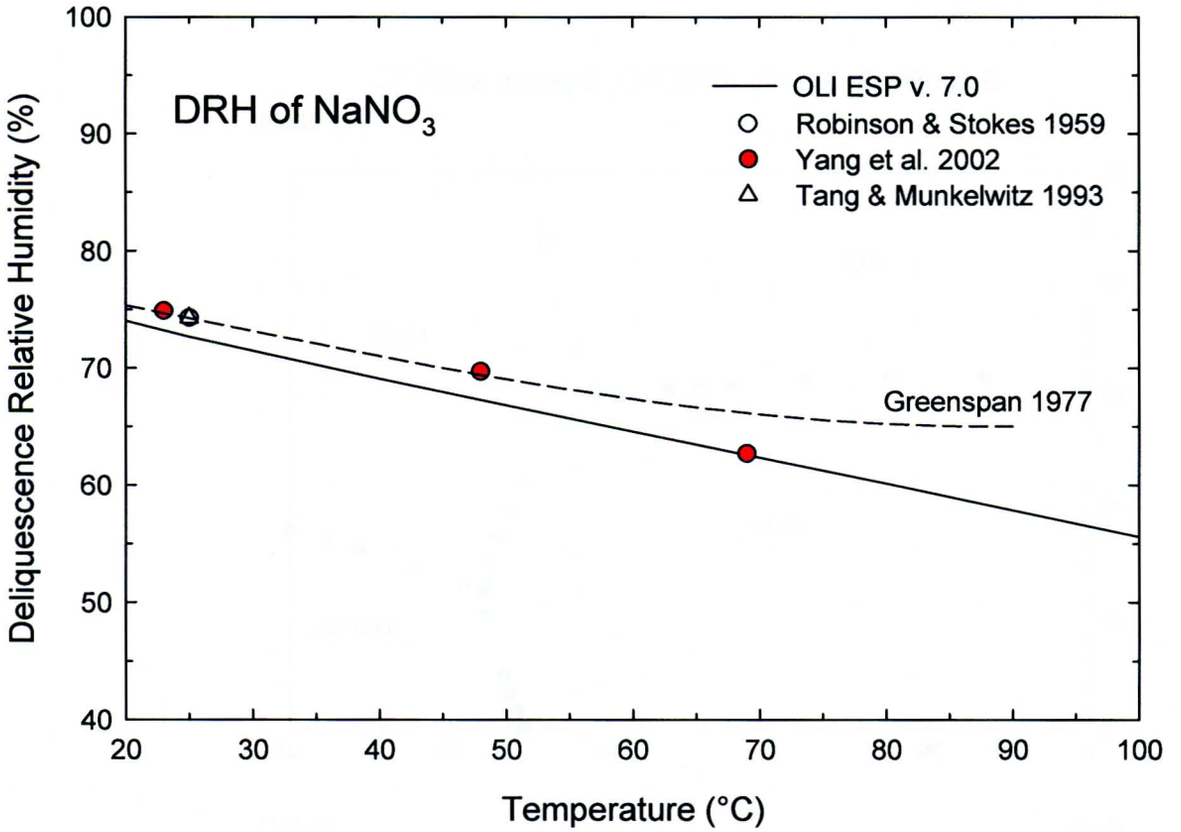


December 28, 2004

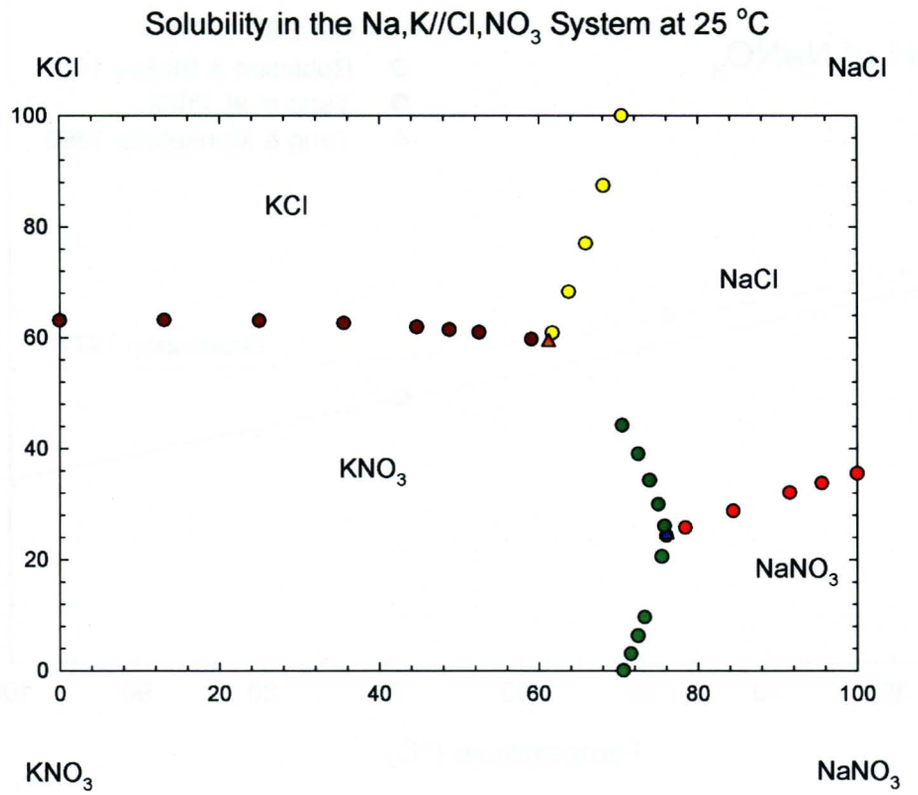
Comparison of KCl DRH from various sources and values calculated with OLI ESP 7.0.

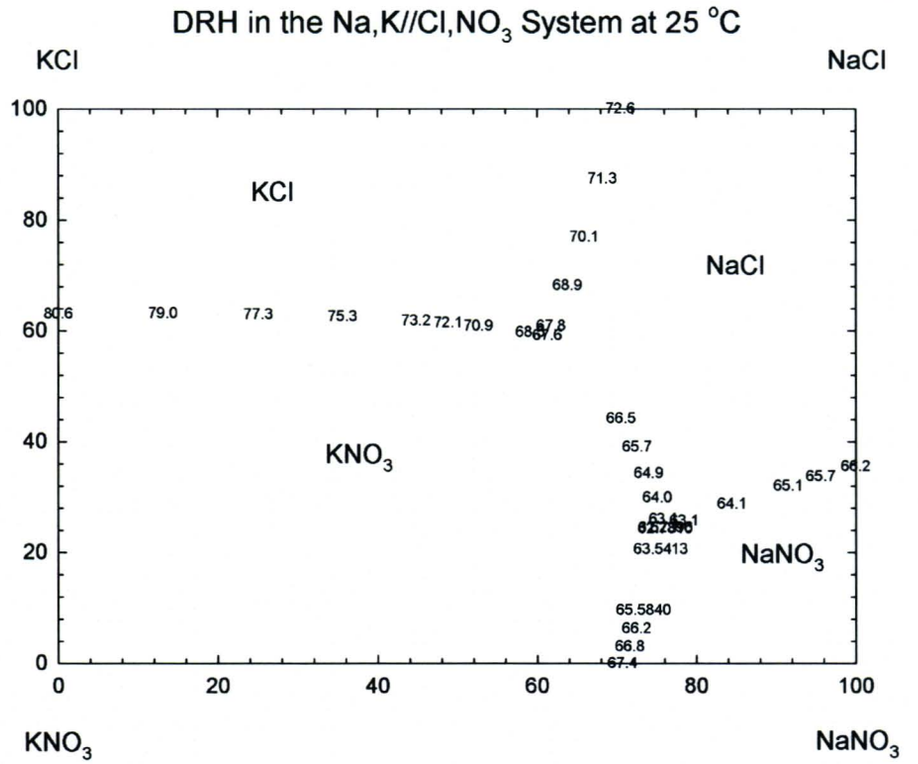


Comparison of NaNO3 DRH from various sources with values calculated using OLI ESP 7.0.

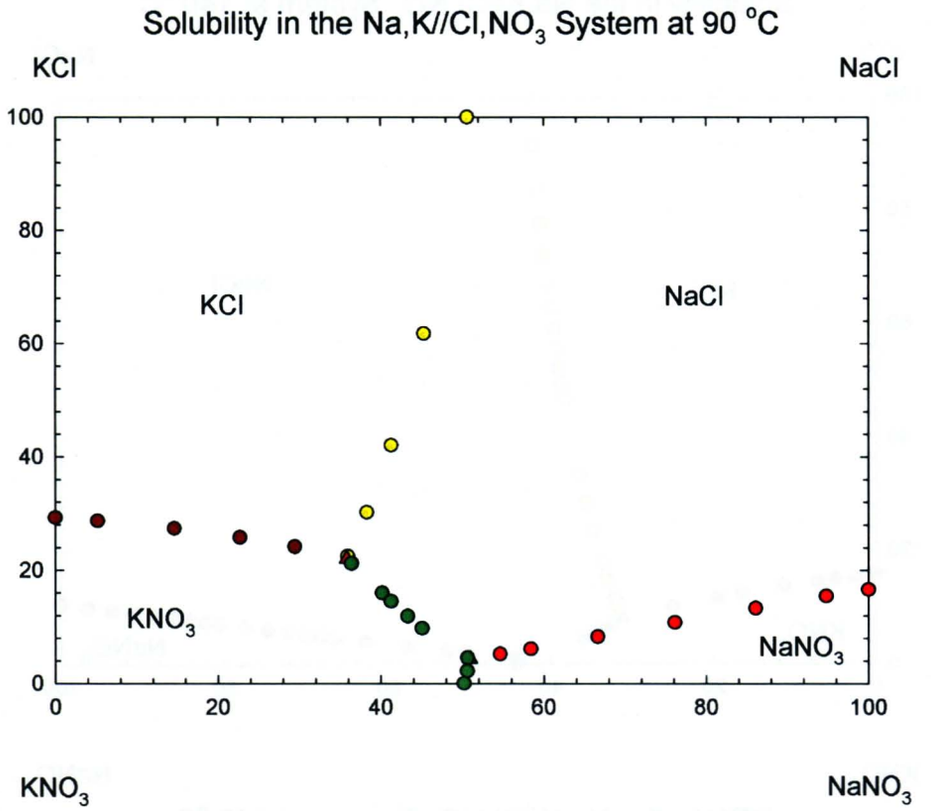


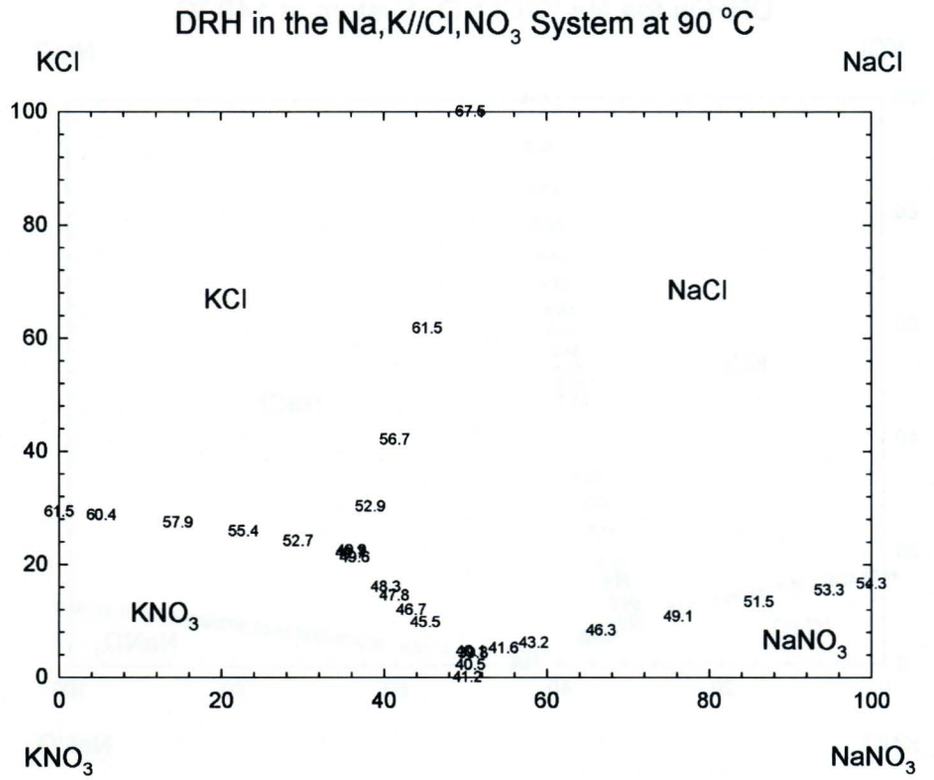
The following figures show the solubility and DRH as a function of composition for the Na,K//Cl,NO3 system at 25 C calculated using ESP 7.0. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.



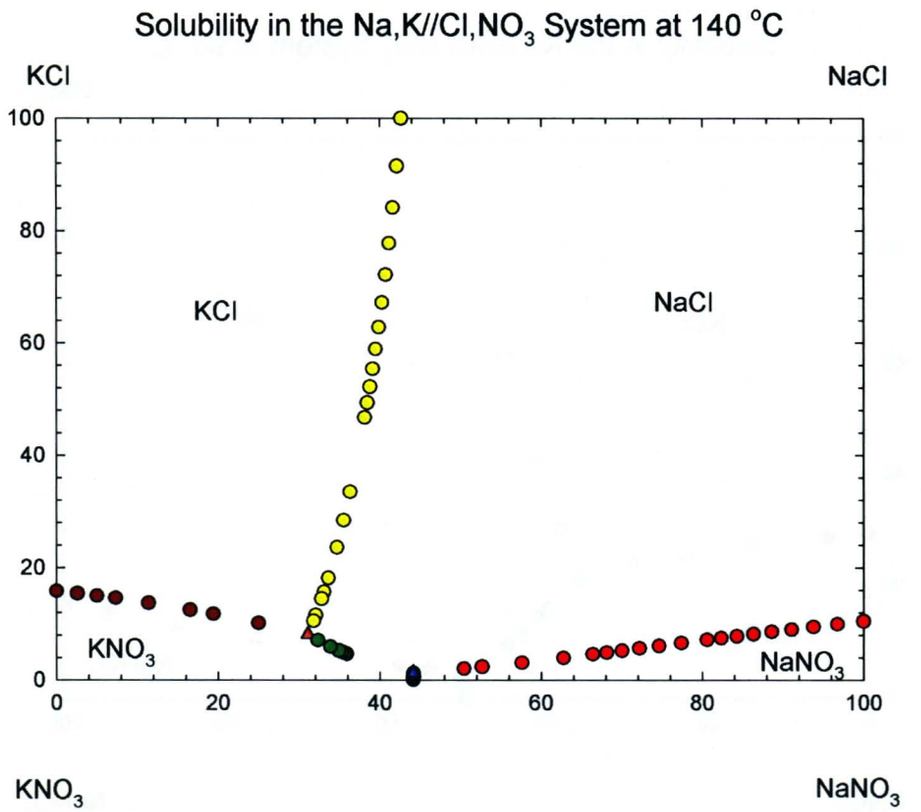


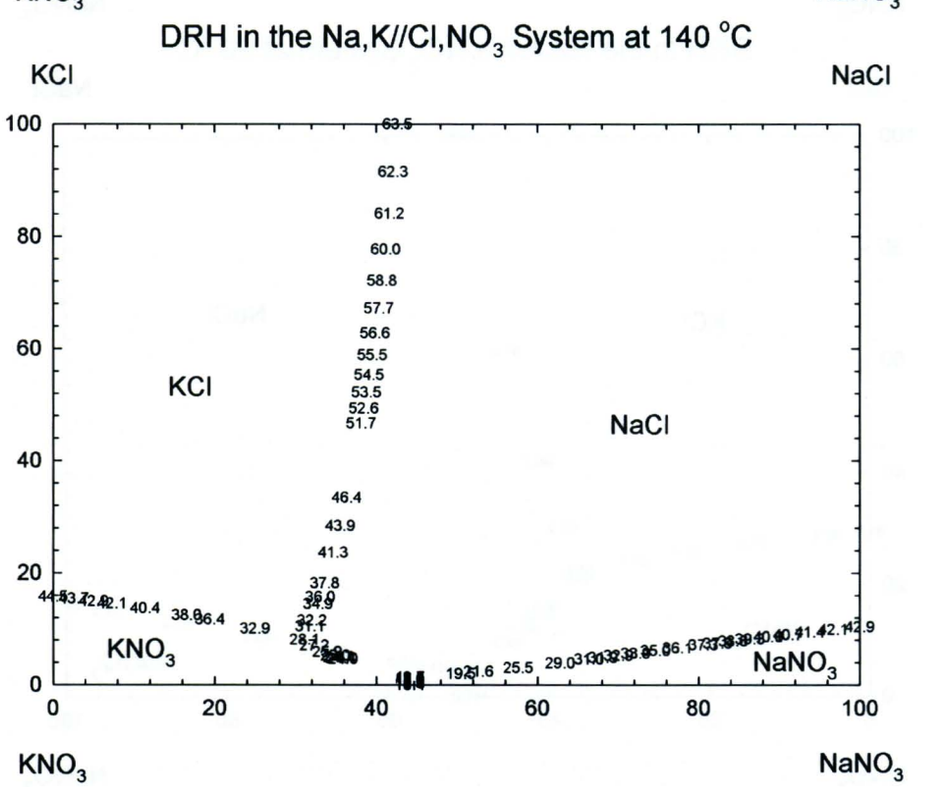
The following figures show the solubility and DRH as a function of composition for the Na,K//Cl,NO3 system at 90 C calculated using ESP 7.0. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.





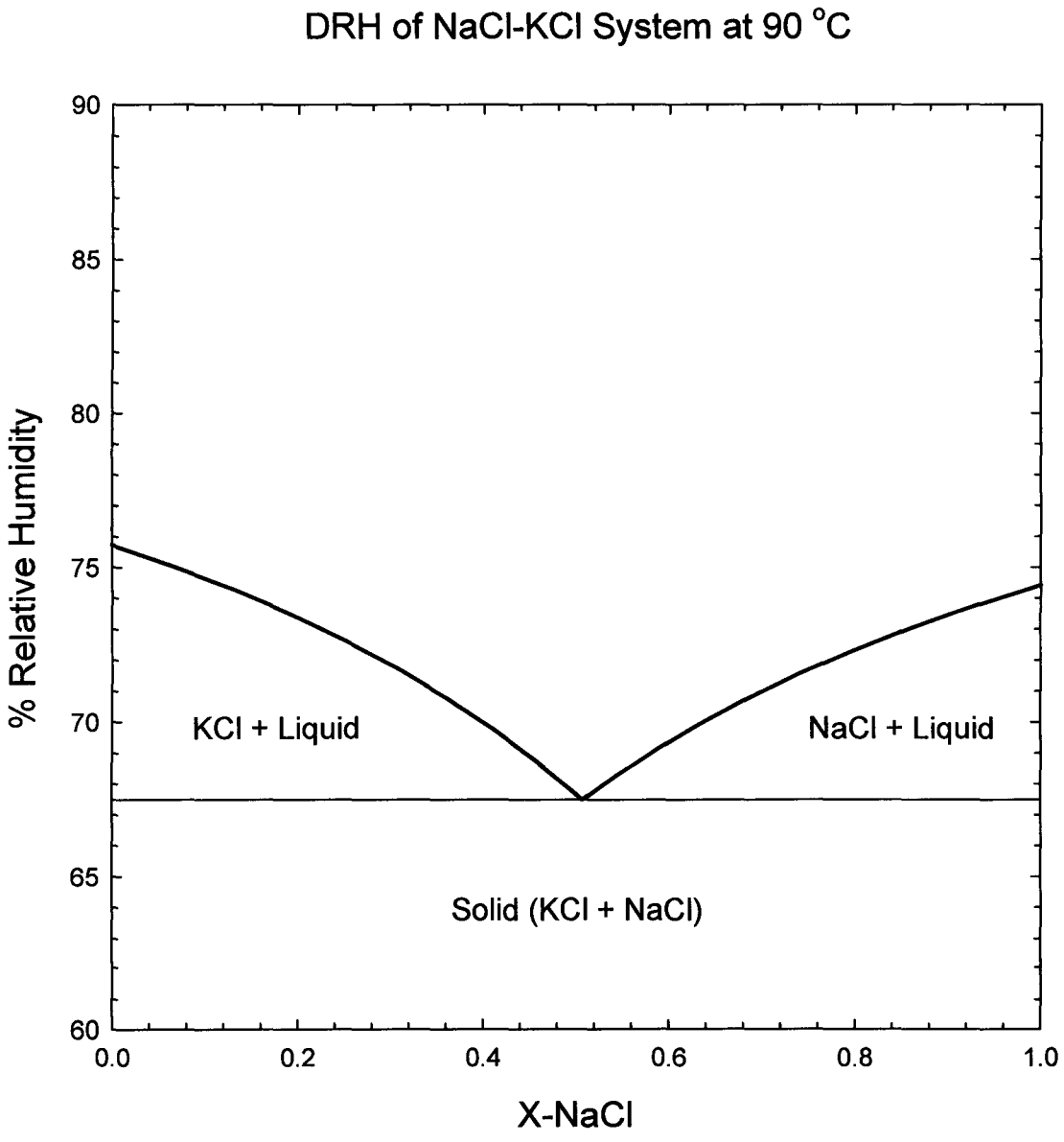
The following figures show the solubility and DRH as a function of composition for the Na,K//Cl,NO3 system at 140 C calculated using ESP 7.0. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.



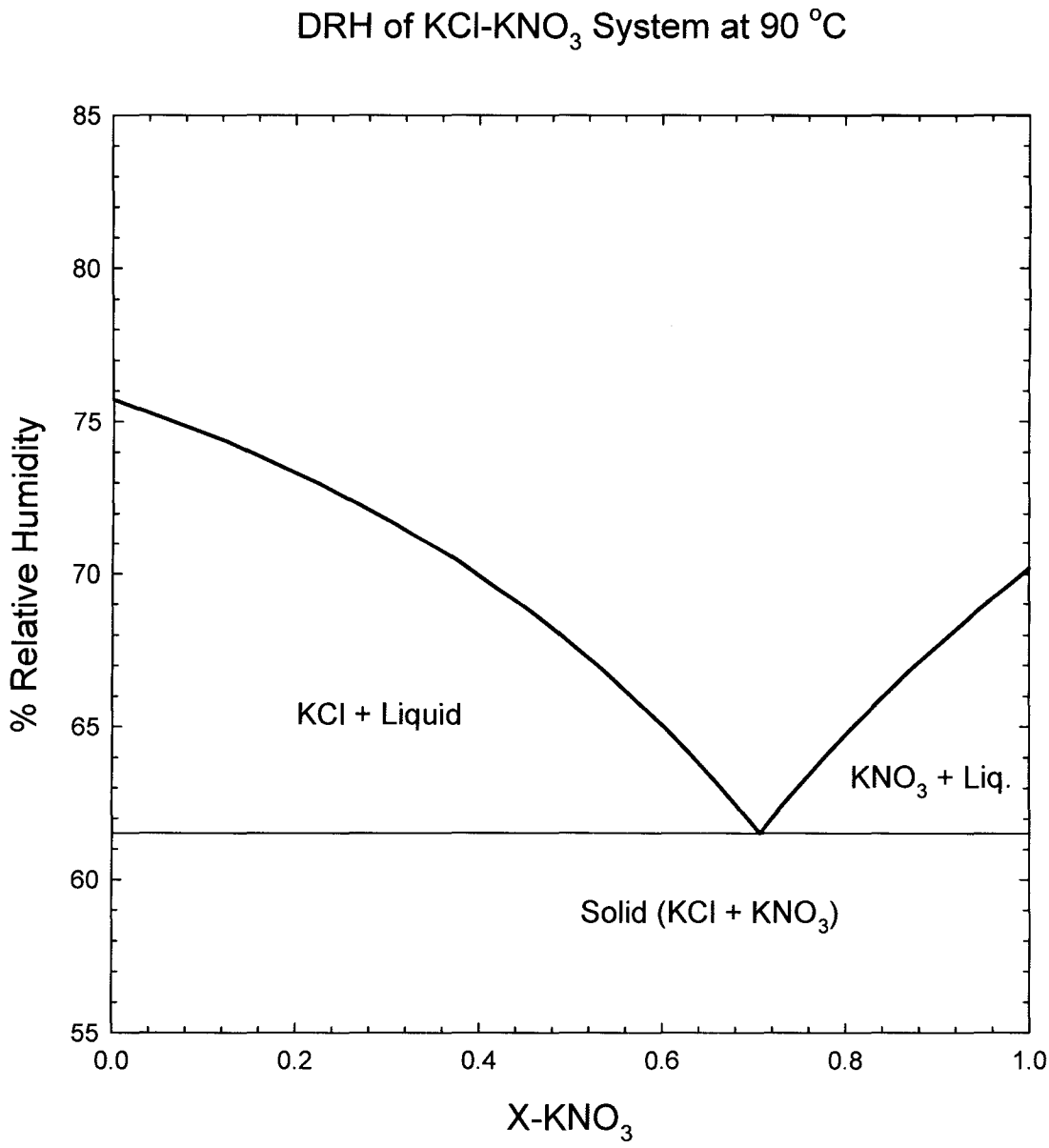


December 29, 2004

DRH in the system NaCl-KCl at 90 C calculated using OLI ESP v. 7.0. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.



DRH in the system KCl-KNO3 at 90 C calculated using OLI ESP v. 7.0. The ESP 7.0 output results are summarized in the Excel file "Quaternary Na-K-Cl-NO3.xls" included in CD ESN679-CD-1.



Entries into Scientific Notebook No. 679 for the period September 1, 2004, through February 28, 2005, have been made by

3/7/2008

Roberto T. Pabalan / Date

No original entry into this Scientific Notebook has been removed.

3/7/2008

Roberto T. Pabalan / Date

ELECTRONIC NOTEBOOK #679

October 1, 2005 through September 30, 2006

20.06002.01.212

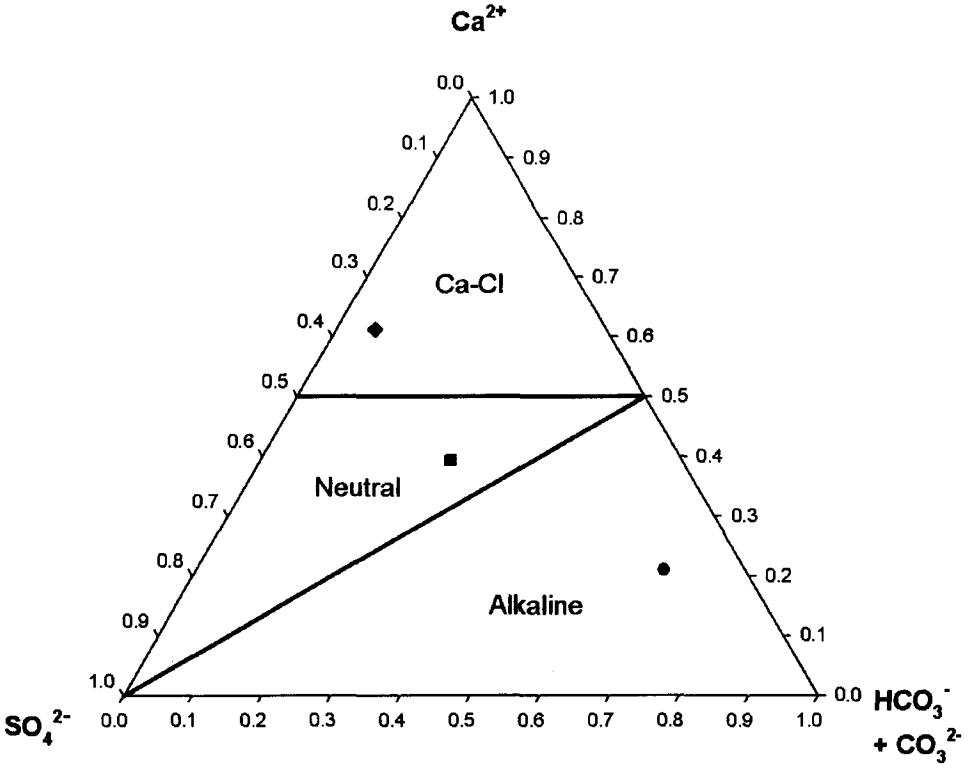
Roberto T. Pabalan

February 21, 2006

From: Darrell Dunn [darrell.dunn@swri.org]
Sent: Tuesday, February 21, 2006 9:05 AM
To: roberto.pabalan@swri.org
Subject: Water chemistries
Can you provide a representative starting water chemistry for neutral, alkaline, and Ca-Cl brines? We have all of the equipment we need to initiate the integrated tests except water composition.

Darrell S. Dunn
Principal Engineer
Mechanical and Materials Engineering Division
Southwest Research Institute
6220 Culebra Road
San Antonio, Texas 78238-5166
Tel: (210) 522-6090
Fax: (210) 522-6965

Three compositions representing Ca-Cl, neutral, and alkaline waters were selected from the USGS unsaturated zone porewater data (Yang et al., 1996, 1998, 2003), which have been input into an Aquachem 5.0 database. The three compositions, with sample I.D.s SD-6/443.5 – 443.8/U (neutral), UE-25_NRG-6/158.2-15 (Ca-Cl), and UE-25_UZ#16/1343.7 (alkaline), are plotted in a ternary Ca-carbonate-SO4 diagram as follows:



The three water compositions are as follows:

SAMPLEID		SD-6/443.5 – 443.8/U	UE-25 NRG-6/ 158.2-158.6	UE-25 UZ#16/1343.7
Water type		Neutral	Ca-Cl	Allkaline
REFERENCE		Yang et al. 2003	Yang et al. 1996	Yang et al. 1996
PHLAB		7.4	6.8	8.4
SAMPLE_DEPTH		135.2	48.28	409.62
NA	mg/l	65.5	35.6	99
K	mg/l	4	0	0
MG	mg/l	11.7	23.3	2.4
CA	mg/l	48.2	122	17
F	mg/l	6.3		
CL	mg/l	47.3	185	56
SO4	mg/l	98	159	23
NO3	mg/l	86	32	18
HCO3	mg/l	101	34	47.6
CO3	mg/l	1	0	58.8
SI	mg/l	84.4	97.4	62.1
AL	mg/l		0	1.7

StreamAnalyzer 2.0 was used to charge balance the composition given in the above table. To simplify the compositions to be used in the experiments, fluoride, silicon, and aluminum were not included.

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The following table lists the results of StreamAnalyzer charge balance recalculations:

SD-6/443.5 (neutral type) pH calc 7.79

	Input	Calculated		% Diff
H2O	55.5082	55.3283	molarity	-0.32423
Na+1	2.85E-03	2.980E-03	molarity	4.58433
K+1	1.02E-04	1.023E-04	molarity	
Mg+2	4.81E-04	4.814E-04	molarity	
Ca+2	1.20E-03	1.203E-03	molarity	
Cl-1	1.33E-03	1.334E-03	molarity	
SO4-2	1.02E-03	1.020E-03	molarity	
NO3-1	1.39E-03	1.387E-03	molarity	
HCO3-1	1.66E-03	1.655E-03	molarity	
CO3-2	1.67E-05	1.666E-05	molarity	

NRG-6/158.2 (Ca-Cl type) pH calc 7.89

	Input	Calculated		% Diff
H2O	55.5082	55.329	molarity	-0.32285
Na+1	1.55E-03	1.549E-03	molarity	
K+1	0	0.000E+00	molarity	
Mg+2	9.59E-04	9.587E-04	molarity	
Ca+2	3.04E-03	3.068E-03	molarity	0.786122
Cl-1	5.22E-03	5.218E-03	molarity	
SO4-2	1.66E-03	1.655E-03	molarity	
NO3-1	5.16E-04	5.161E-04	molarity	
HCO3-1	5.57E-04	5.572E-04	molarity	
CO3-2	0	0.000E+00	molarity	

UZ#16/1343.7 (alkaline type) pH calc 10.02

	Input	Calculated		% Diff
H2O	55.5082	55.3281	molarity	-0.3246
Na+1	4.31E-03	4.306E-03	molarity	
K+1	0	0.000E+00	molarity	
Mg+2	9.87E-05	9.875E-05	molarity	
Ca+2	4.24E-04	4.242E-04	molarity	
Cl-1	1.58E-03	1.580E-03	molarity	
SO4-2	2.39E-04	2.394E-04	molarity	
NO3-1	2.90E-04	2.903E-04	molarity	
HCO3-1	7.80E-04	7.801E-04	molarity	
CO3-2	9.80E-04	1.112E-03	molarity	13.4487

March 7, 2006

Recipes for preparing the solution compositions, listed on page 134, that could be used for the integrated flow and corrosion tests were derived using an Excel spreadsheet. The resulting recipes are the following:

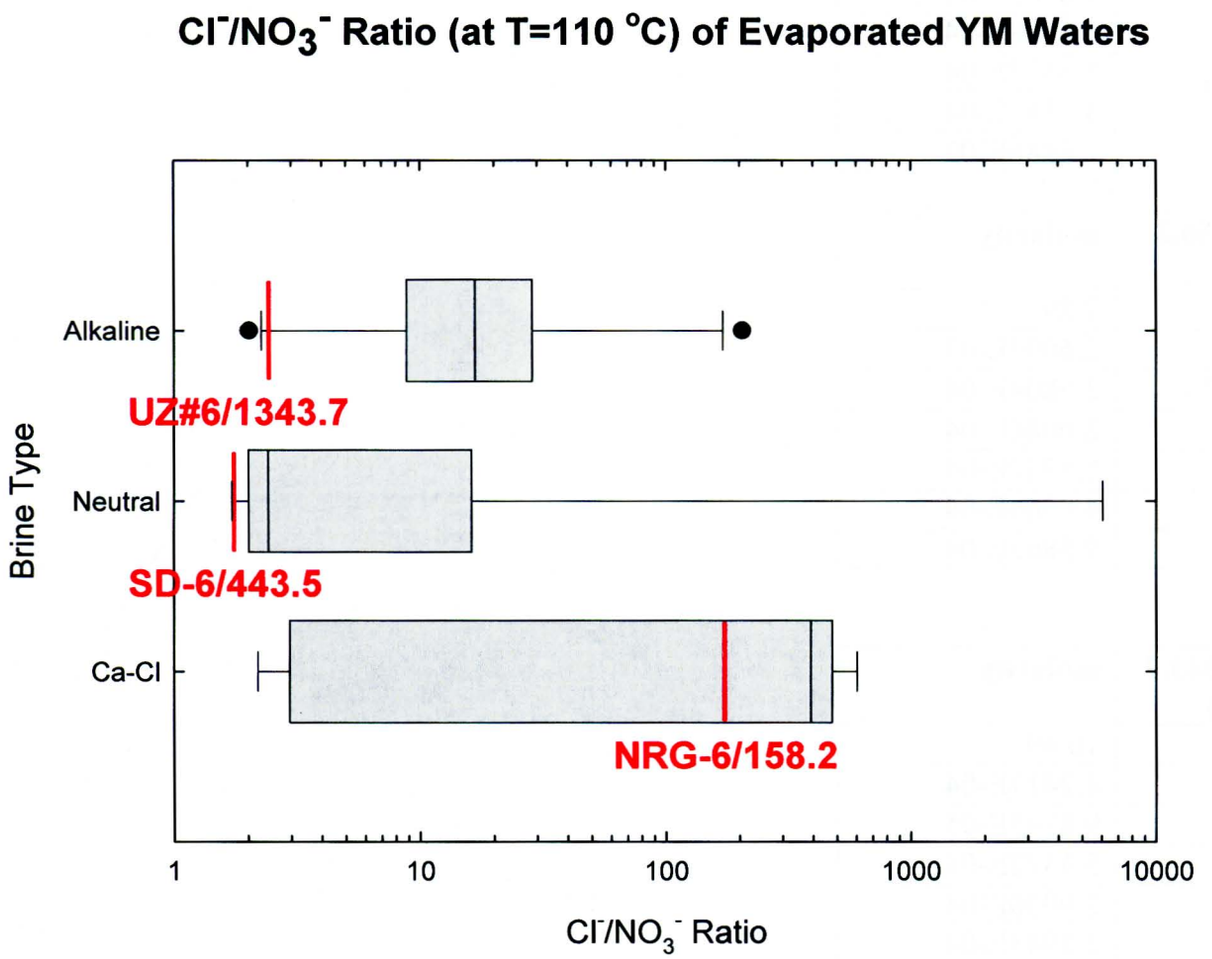
SD-6/443.5 (neutral)	**molarity**
pH calc	7.78
MgSO4	4.8138E-04
K2SO4	5.1153E-05
Na2SO4	4.8763E-04
CaCl2	6.6708E-04
Ca(NO3)2	5.3557E-04
NaNO3	3.1585E-04
NaHCO3	1.6886E-03

NRG-6/158.2 (Ca-Cl)	**molarity**
pH calc	7.89
CaCl2	2.6091E-03
Ca(NO3)2	2.5804E-04
CaSO4	2.0086E-04
NaHCO3	5.5722E-04
Na2SO4	4.9564E-04
MgSO4	9.5865E-04

UZ#16/1343.7 (alkaline)	**molarity**
pH calc	10.49
CaCl2	4.2417E-04
MgCl2	9.8745E-05
NaCl	5.3372E-04
NaNO3	2.9030E-04
Na2SO4	2.3943E-04
Na2CO3	3.0034E-03

May 19, 2006

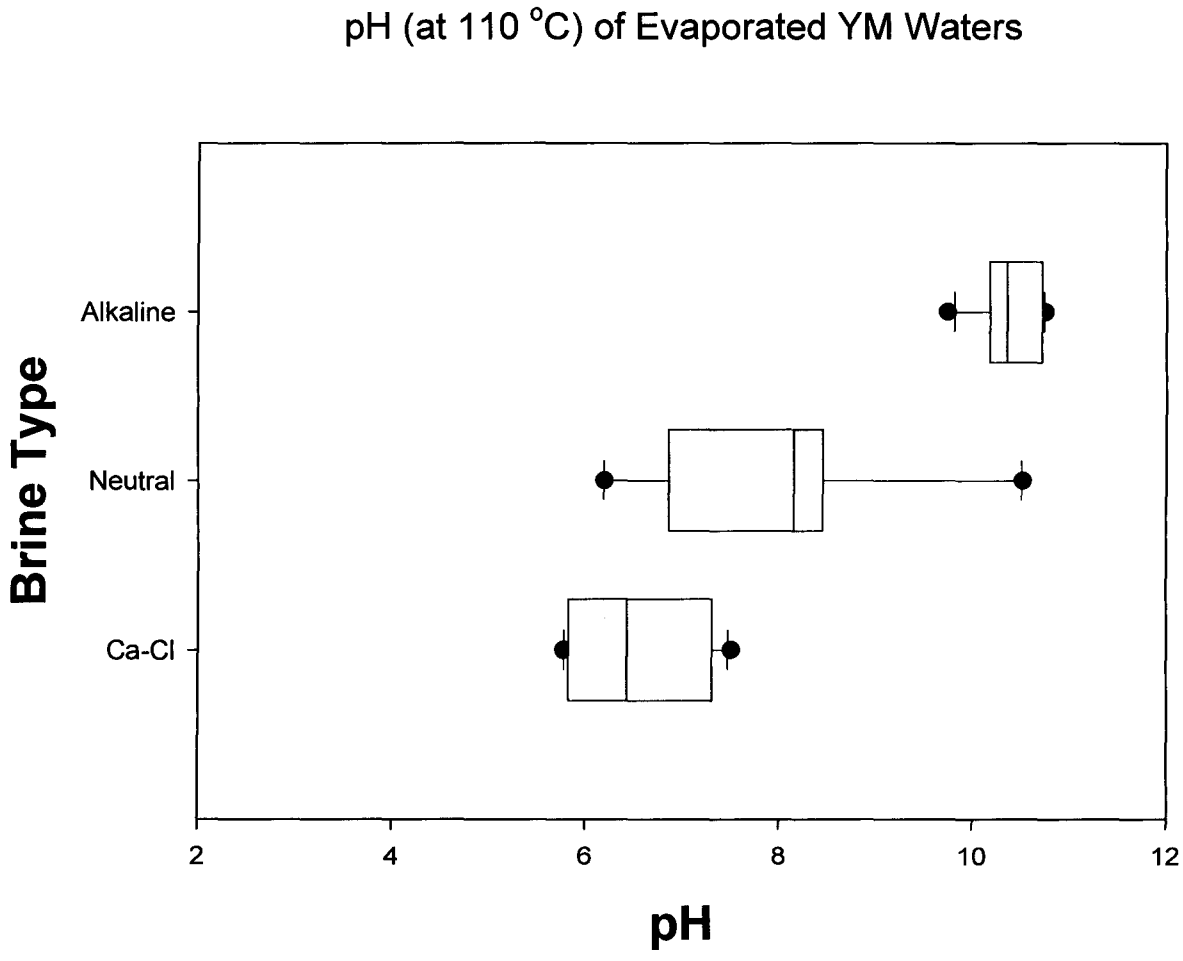
The following figure shows the Cl to NO3 ratio of the three water compositions listed on page 133, after evaporation at 110 °C using StreamAnalyzer 2.0, compared to the ranges of Cl to NO3 ratios of YM porewaters selected from the data of Yang et al. (1996, 1998, 2003) and evaporated using StreamAnalyzer 2.0. The three selected compositions UZ#6/1343.7, SD-6/443.5, and NRG-6/158.2 do not adequately represent the potential range of Cl to NO3 ratios for evaporated YM porewaters. Thus, it would be useful to find additional water compositions for use in the integrated tests.



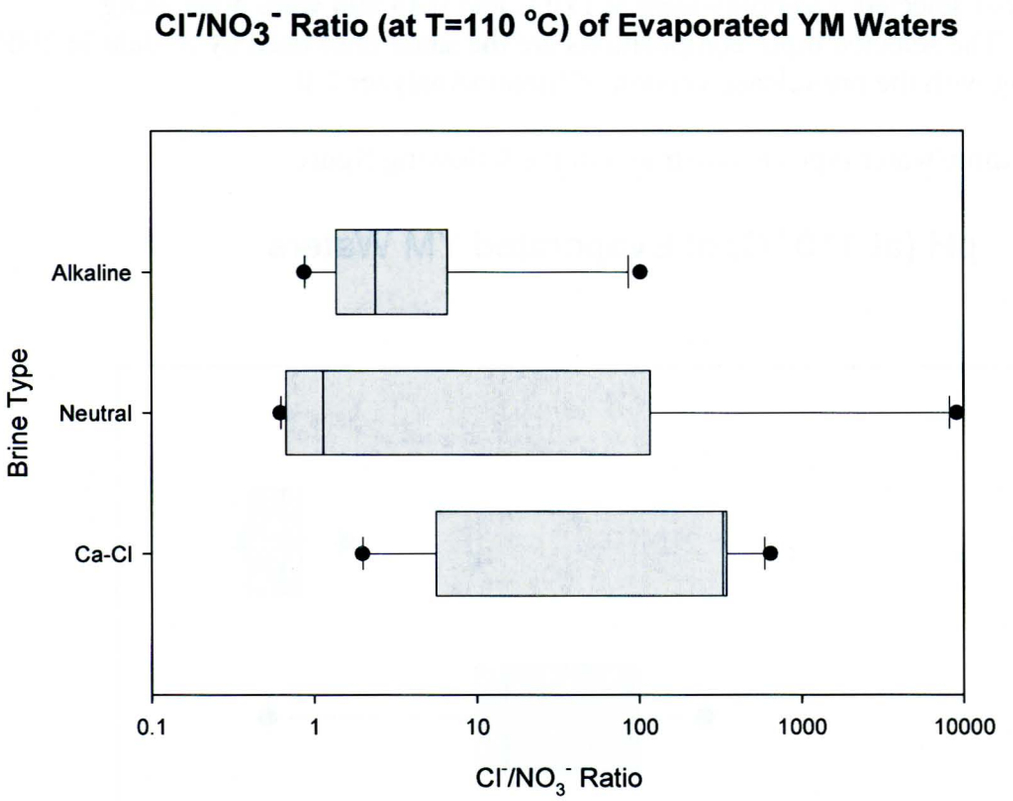
June 2, 2006

Evaporation simulations of selected YM porewaters at 110 C and 0.85 atm were done using StreamAnalyzer 2.0.35. The selected input compositions are the same ones used by A. Jain in 2005 in simulating evaporation with the pre-release version of StreamAnalyzer 2.0.

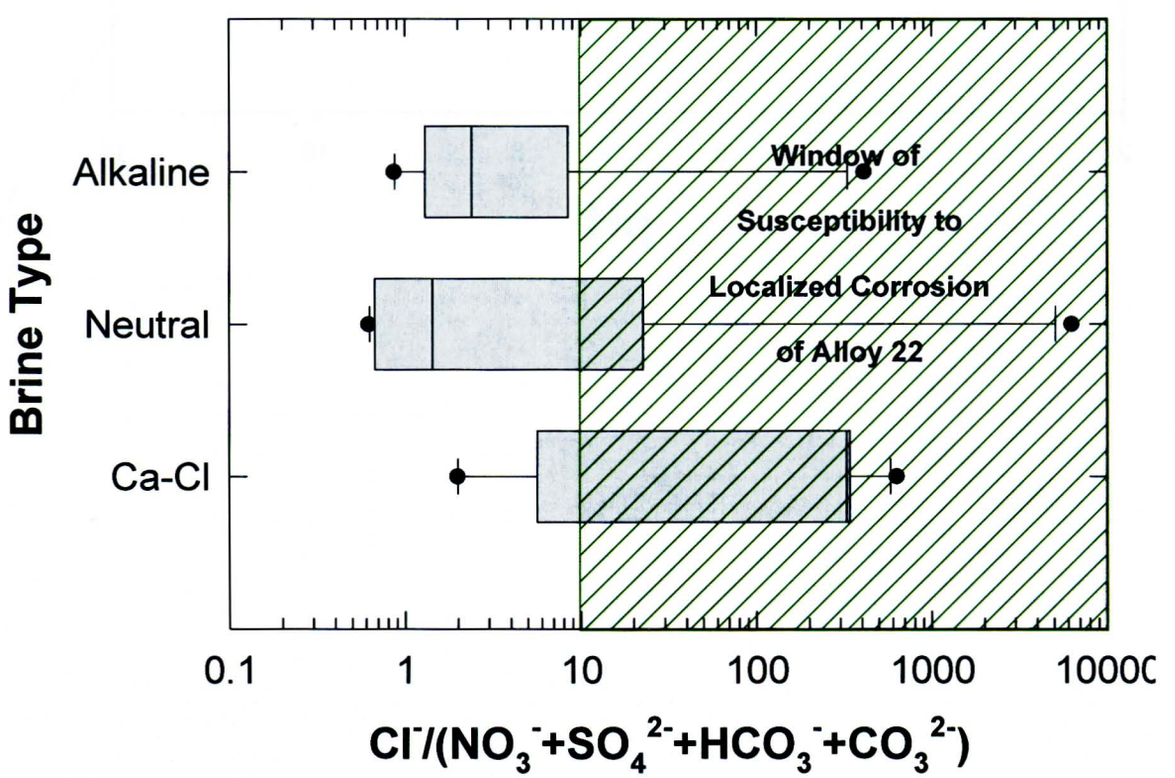
The range of pH for the three water types is illustrated in the following figure:



The range in calculated Cl/NO3 ratio is as follows:



The range in calculated ratio of chloride to corrosion inhibiting species (NO3+SO4+HCO3+CO3) is as follows:



June 6, 2006

Excel spreadsheet calculations were done to develop recipes to simulate three water compositions representing Ca-Cl, neutral, and alkaline-type waters. The selected YM porewater samples are NRG-6/158.2 (Ca-Cl-type), UZ-14/85.2 (Neutral-type), and UZ-14/1542.3 (Alkaline-type). These compositions have ratios of Cl to inhibiting species (NO3+SO4+HCO3+CO3) close to the median of the ranges shown in the figure on page 138. Using the three recipes as input, StreamAnalyzer V.2.0.35 calculations were done to develop recipes that would yield Cl/NO3 ratios close to the median, 25th percentile, and 75th percentile of the Cl/inhibitor ratios of the three water types. The relative amounts of CaCl2 and Ca(NO3)2 were changed in the input file iteratively to yield the target Cl/NO3 ratios. This iterative calculation was successful for the NRG-6/158.2 and UZ-14/85.2 compositions, and recipes were developed that yielded, upon evaporation simulation at 110 C and 1 atm, Cl/NO3 ratios close to the median, 25th and 75th percentiles of Cl/inhibitor ratios shown in the diagram. However, the calculation was not successful for the UZ-14/1542.3 composition because any variation in the input CaCl2 and Ca(NO3)2 ratio always resulted in a Cl/NO3 ratio close to 2.80. The alkaline-type water represented by UZ-14/1542.3 would not be expected to lead to localized corrosion of Alloy 22, as indicated in the figure on page 145. Thus, for purposes of the integrated experiments, it was decided to use the three recipes for NRG-6/158.2, three recipes for UZ-14/85.2, and the median Cl/NO3 recipe for UZ-14/1542.3.

The recipes are listed in the following tables:

NRG-6/158.2 Ca-Cl-type (median Cl/inhibitor; calc'd Cl/NO3 = 324)*	
Component	**Moles/liter solution**
CaCl2	2.777E-03
Ca(NO3)2	9.000E-05
CaSO4	2.009E-04
NaHCO3	5.572E-04
Na2SO4	4.956E-04
MgSO4	9.587E-04

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

NRG-6/158.2 Ca-Cl-type (75th percentile Cl/inhibitor; calc'd Cl/NO3 = 340)*	
Component	**Moles/liter solution**
CaCl2	2.780E-03
Ca(NO3)2	8.600E-05
CaSO4	2.009E-04
NaHCO3	5.572E-04
Na2SO4	4.956E-04
MgSO4	9.587E-04

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

NRG-6/158.2 Ca-Cl-type (25th percentile Cl/inhibitor; calc'd Cl/NO3 = 5.8)*	
Component	**Moles/liter solution**
CaCl2	1.787E-03
Ca(NO3)2	1.080E-03
CaSO4	2.009E-04
NaHCO3	5.572E-04
Na2SO4	4.956E-04
MgSO4	9.587E-04

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

UZ-14/85.2 Neutral-type (median Cl/inhibitor; calc'd Cl/NO3 = 1.36)*	
Component	**Moles/liter solution**
CaCl2	5.236E-04
Ca(NO3)2	5.000E-04
CaSO4	2.713E-04
MgSO4	4.157E-04
MgCO3	1.274E-04
NaHCO3	1.890E-03

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

UZ-14/85.2 Neutral-type (75th percentile Cl/inhibitor; calc'd Cl/NO3 = 22.4)*	
Component	**Moles/liter solution**
CaCl2	9.836E-04
Ca(NO3)2	4.000E-05
CaSO4	2.713E-04
MgSO4	4.157E-04
MgCO3	1.274E-04
NaHCO3	1.890E-03

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

UZ-14/85.2 Neutral-type (25th percentile Cl/inhibitor; calc'd Cl/NO3 = 0.67)*	
Component	**Moles/liter solution**
CaCl2	3.636E-04
Ca(NO3)2	6.600E-04
CaSO4	2.713E-04
MgSO4	4.157E-04
MgCO3	1.274E-04
NaHCO3	1.890E-03

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

UZ-14/1542.3 Alkaline-type (median Cl/inhibitor; calc'd Cl/NO3 = 2.80)*	
Component	**Moles/liter solution**
CaCl2	5.757E-05
Ca(NO3)2	3.226E-05
MgCl2	2.057E-05
NaCl	4.078E-04
Na2SO4	2.915E-04
NaHCO3	6.480E-03
Na2CO3	7.670E-04

*Evaporation simulation, StreamAnalyzer V.2.0.35, T=110 C, P=1 atm

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June 7, 2006

Three samples taken from the Drift Scale Test (Alcove 5) were received today from the DOE. The following is a copy of the sample custody receipt:

BSC

SMF Specimen Custody Receipt

QA:QA

Requestor's Name:	Ship To (Recipient Name):	
Kevin Smart (ID#808) **Southwest Research Institute** **6220 Culebra Road** **San Antonio, TX 78238-0000** **(210) 522-5859**	**Kevin Smart (ID#808)** **Southwest Research Institute** **6220 Culebra Road** **San Antonio, TX 78238-0000** **(210) 522-5859**	Date Received: June 7, 2006 Shipment ID: 01000856 Shipping Date: 05-jun-2006 SMF Staff Michael Pitkale Date 6-01-06

Container ID: 01006947 Type: NonBorehole Specimens in this container: 3

Condition	Specimen ID	Specimen Type	Site Type	Collected For	Date Collected	Collector's Sample ID
	02042399	N/A	Other	Smart	18-apr-2006	
	02042413	N/A	Other	Smart	18-apr-2006	
	02042436	N/A	Other	Smart	18-apr-2006	

Please Sign this form and return to:
Sample Management Facility
Yucca Mountain Site Characterization Project
P.O. Box 617
Mercury, NV 89023-0617
SMF Verified:_____ **Date** _____

Page 1 of 1

I hereby acknowledge the receipt of the Specimens listed above. I will return this form to the SMF within 10 business days of receipt.

Recipient [signature] Date 6/7/06

Roberto T. Rabal

PA-PRO-0809.4-r0

The following are previous emails pertaining to those samples:

From: Kevin Smart [kevin.smart@swri.org]
Sent: Tuesday, May 09, 2006 8:38 AM
To: roberto.pabalan@swri.org; cmanepally@cnwra.swri.edu; jmyers@cnwra.swri.edu; 'Miriam Juckett'
Cc: 'Kevin Smart'
Subject: RE: NRC request for rock samples

The samples that Jack and I had collected all come from the wall rock. The request for samples of the concrete liner was on on-hold until they could bring in a core drill. The concrete cylinders were all catalogued and taken to the sample facility (I think), so you can probably talk to Jack Parrot about acquiring some of those.

As for orientation, we noted where the sample came from (i.e., how far into the drift and where on the wall or ceiling). I also marked the surface of the sample that was facing into the opening. Because of the logistics of getting the pieces, it wasn't possible to truly orient the samples (i.e., put a strike and dip on the rock).

The attached PDF are copies of the three sample collection sheets that YMP personnel completed after the samples were collected.

--Kevin

****
Kevin J. Smart, Ph.D., P.G.
Dept. of Earth, Material, & Planetary Sciences
Geosciences & Engineering Division
Southwest Research Institute
6220 Culebra Road
San Antonio, TX 78238-5166
Phone: 210-522-5859 Fax: 210-522-5155
Email: ksmart@swri.org

> -----Original Message-----
> From: Bobby Pabalan [mailto:rpabalan@swri.edu]
> Sent: Monday, May 08, 2006 10:27 AM
> To: cmanepally@cnwra.swri.edu; jmyers@cnwra.swri.edu; 'Miriam Juckett'
> Cc: 'Kevin Smart'
> Subject: RE: NRC request for rock samples
>
>
> For samples of the rock and cement, I'd like to receive them.
>
> --bobby
>
> Kevin: The rock samples--were these oriented samples?

>
> -----Original Message-----
> From: Chandrika Manepally [mailto:cmanepally@cnwra.swri.edu]
> Sent: Monday, May 08, 2006 9:47 AM
> To: Roberto Pabalan; jmyers@cnwra.swri.edu; Miriam Juckett

> Cc: 'Kevin Smart'
> Subject: FW: NRC request for rock samples
>
>
> FYI
>
> Please let Kevin know the person who should be contacted to
> receive the samples.
>
> -Chandrika
>
>
> -----Original Message-----
> From: Jack Parrott [mailto:JDP1@nrc.gov]
> Sent: Friday, May 05, 2006 3:18 PM
> To: Drew Coleman
> Cc: cmanepally@cnwra.swri.edu; ksmart@cnwra.swri.edu; April
> Gil; Debbie Barr; Neal Hunemuller; Frederick Brown; Jack
> Guttmann; Philip Justus; Robert Latta; Randall Fedors; Vivian Mehrhoff
> Subject: NRC request for rock samples

>
>
> Drew,
>
> On April 18, 2006, personnel from NRC (Jack Parrott) and
> CNWRA (Dr. Kevin
> Smart) participated in an entry of Drift Scale Test (Alcove
> 5). While there, Project personnel collected three loose
> rock samples from locations pointed out by Dr. Smart. This
> is a request to have those samples sent to the Center for
> Nuclear Waste Regulatory Analyses at the Southwest Research
> Institute. The sample numbers are:
>
> SPC02042399
> SPC02042413
> SPC02042437
>
> Please ship the samples to:
>
> Dr. Kevin Smart
> CNWRA
> 6220 Culebra Rd.
> Southwest Research Institute
> San Antonio, TX 78238
> Phone: 210-522-5859
>
> Thanks,
>
> Jack
>

BSC

Sample Collection Report

Complete only applicable items.

QA: QA
Page 1 of 1

Date Collected	Collector's Name	Organization	Phone
4-18-06	John Dinsmoor	TCO	702-295-3727

Address
YMP ESF Pad, Building 7008, Mercury, NV

Recipient Name	Organization	Phone
Kevin Smart	CNWRA	210-522-5859

Address
6220 Culebra Road, Southwest Research Institute, San Antonio, TX, 78238

Planning/Controlling Document Number	Planning/Controlling Document Title
TWP-WIS-MD-000016	Technical Work Plan: Alcove 5 (Drift Scale Test) Post-Test Activities

Type of Sample: (check one)
☒ Rock ☐ Soil ☐ Alluvium ☐ Caliche ☐ Muck
☐ Liquid ☐ Gas ☐ Other _____

Number of Samples Collected

Type of Site: (check one)
☐ Trench ☐ Outcrop ☐ Surface ☐ Spring ☐ Tunnel ☐ Borehole
☒ Other Heated Drift

Describe Sample ☒ Q ☐ Non-Q
SPC02042399
Semi-loose rock from crown of Heated Drift, Post Drift Scale Test
Larger portion of rock that was split in two: other half is SPC02042398

SPC02042399

Describe Site
From Heated Drift of Alcove 5, loose rock pried from crown, 14m inside the bulkhead, 1.7 m off the right rib.

Other Documentation (Field photos, maps, reports, etc.)
SN-SNL-SCI-034-V1

Remarks

FOR SMF USE ONLY

Record Verified By (SMF Staff Printed Name/Signature)	Date

PA-PRO-0804.2-r0

BSC

Sample Collection Report

Complete only applicable items

QA: QA
Page 1 of 1

Date Collected	Collector's Name	Organization	Phone
4-18-06	John Dinsmoor	TCO	702-295-3727

Address: YMP ESF Pad, Building 7008, Mercury, NV

Recipient Name	Organization	Phone
Kevin Smart	CNWRA	210-522-5859

Address: 6220 Culebra Road, Southwest Research Institute, San Antonio, TX, 78238

Planning/Controlling Document Number	Planning/Controlling Document Title
TWP-WIS-MD-000016	Technical Work Plan: Alcove 5 (Drift Scale Test) Post-Test Activities

Type of Sample: (check one)
- ☒ Rock
- ☐ Soil
- ☐ Alluvium
- ☐ Caliche
- ☐ Muck
- ☐ Liquid
- ☐ Gas
- ☐ Other

Number of Samples Collected: 1

Type of Site: (check one)
- ☐ Trench
- ☐ Outcrop
- ☐ Surface
- ☐ Spring
- ☐ Tunnel
- ☐ Borehole
- ☒ Other Heated Drift

Describe Sample ☒ Q ☐ Non-Q

SPC02042413
Semi-loose rock from crown of Heated Drift, Post Drift Scale Test
Larger portion of rock that was split in two: other half is SPC02042414

SPC02042413

Describe Site

From Heated Drift of Alcove 5, loose rock pried from right rib, 29 inside the bulkhead, 1.5m above springline.

Other Documentation (Field photos, maps, reports, etc.)

SN-SNL-SCI-034-V1

Remarks

FOR SMF USE ONLY

Record Verified By (SMF Staff Printed Name/Signature)	Date

PA-PRO-08042-r0

BSC

Sample Collection Report

Complete only applicable items.

QA: QA
Page 1 of 1

Date Collected	Collector's Name	Organization	Phone
4-18-06	John Dinsmoor	TCO	702-295-3727

Address
YMP ESF Pad, Building 7008, Mercury, NV

Recipient Name	Organization	Phone
Kevin Smart	CNWRA	210-522-5859

Address
6220 Culebra Road, Southwest Research Institute, San Antonio, TX, 78238

Planning/Controlling Document Number	Planning/Controlling Document Title
TWP-WIS-MD-000016	Technical Work Plan: Alcove 5 (Drift Scale Test) Post-Test Activities

Type of Sample: (check one)
☒ Rock ☐ Soil ☐ Alluvium ☐ Caliche ☐ Muck
☐ Liquid ☐ Gas ☐ Other _____

Number of Samples Collected: 1

Type of Site: (check one)
☐ Trench ☐ Outcrop ☐ Surface ☐ Spring ☐ Tunnel ☐ Borehole
☒ Other Heated Drift

Describe Sample ☒ Q ☐ Non-Q
SPC02042436
Semi-loose rock from crown of Heated Drift, Post Drift Scale Test
Larger portion of rock that was split in two: other half is SPC02042437

SPC02042436

Describe Site
From Heated Drift of Alcove 5, loose rock pried from left rib, 15.5 inside the bulkhead, 1.5m above floor.

Other Documentation (Field photos, maps, reports, etc.)
SN-SNL-SCI-034-V1

Remarks

FOR SMF USE ONLY

Record Verified By (SMF Staff Printed Name/Signature)	Date

July 31, 2006

Previous analyses and abstractions of the chemistry of evaporated seepage waters were reported in the following references:

> Pabalan, R.T., Yang, Y., and Browning, L. (2002) Effects of Salt Formation on the Chemical Environment of Drip Shields and Waste Packages at the Proposed Nuclear Waste Repository at Yucca Mountain, Nevada. CNWRA 2002-03. Center for Nuclear Waste Regulatory Analyses, San Antonio, TX.
>
> Pabalan, R.T., Yang, L., and Browning, L. (2002) Deliquescence behavior of multicomponent salts: Effects on the drip shield and waste package chemical environment of the proposed nuclear waste repository at Yucca Mountain, Nevada. In P. McGrail, and G.A. Cragnolino, Eds. Scientific Basis for Nuclear Waste Management XXV, 713, p. 37-44. Materials Research Society, Warrendale, PA.
>
> Dunn, D.S., Pensado, O., Pan, Y.-M., Pabalan, R.T., Yang, L., He, X., and Chiang, K.T. (2005) Passive and Localized Corrosion of Alloy 22 - Modeling and Experiments. CNWRA 2005-02. Center for Nuclear Waste Regulatory Analyses, San Antonio, TX.
>
> Pensado, O., Pabalan, R.T., Dunn, D.S., and Chiang, K.-T. (2006) Use of Alloy 22 as a long-term radioactive waste containment material. In P. Marcus, and V. Maurice, Eds. Passivation of Metals and Semiconductors, and Properties of Thin Oxide Layers —A Selection of Papers from the 9th International Symposium, p. 53-57. Elsevier, The Netherlands.

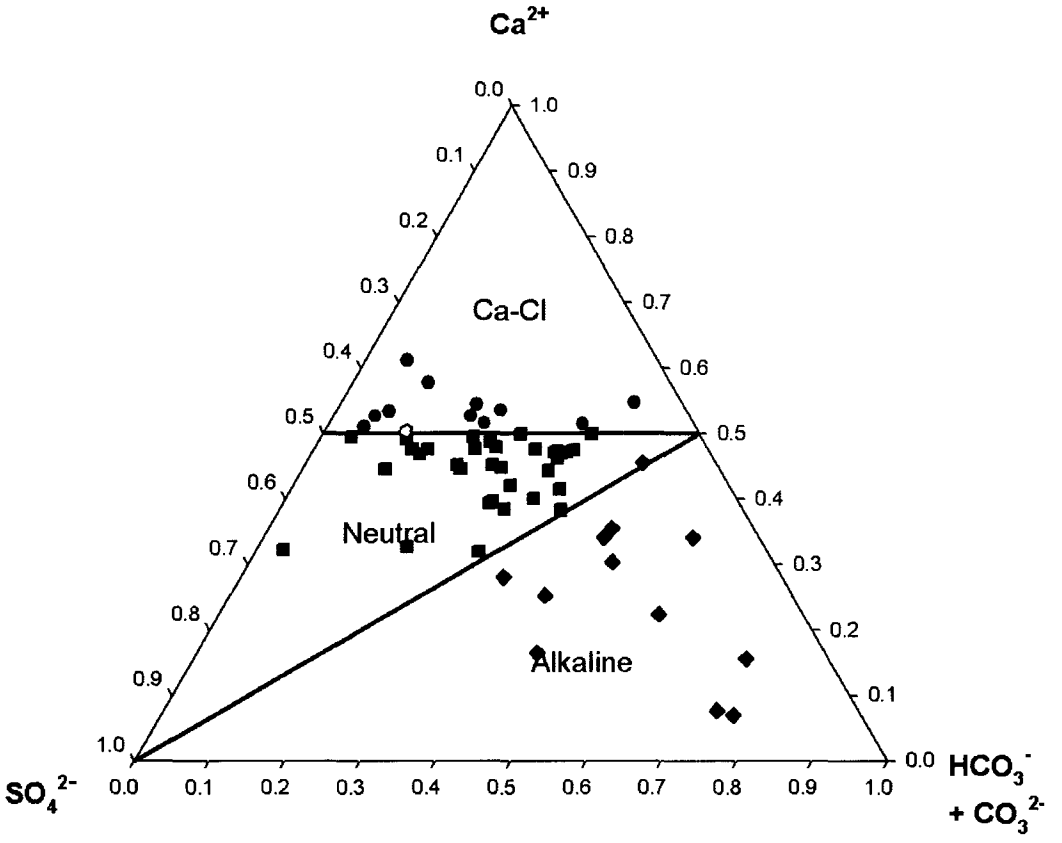
Those analyses and abstractions were based on the assumption that the chemistry of water entering the repository drift will have similar characteristics as YM unsaturated zone pore waters sampled by the USGS (reported in Yang et al., 1996, 1998, 2003). Changes in the composition of seepage waters due to their interaction with the rocks or with engineered materials, such as rock bolts and grout, were neglected. In addition, the USGS data were used in the analyses without consideration of the location of the samples. Many of the USGS samples were taken at elevations below the repository horizon and their compositions might be unlikely to be similar to those of seepage waters.

The focus the analysis to compositions that are more likely to be similar to those of seepage waters, the USGS data set was culled to include only those samples that are above the repository horizon. For purpose of the analysis, the elevation of the repository horizon was assumed equal to 1,070 meters above sea level, based on a map showing the tunnel boring machine progress as of 10/13/98 (3:30 pm PST) at the Exploratory Studies Facility Cross-Drift (figure numbered YMP-98-089.6). Thus, any USGS sample with MSL greater than 1,070 was included in the analysis. The following table lists the USGS samples that were included in the analysis (56 out of the original 208), the borehole elevation, the reported depth of sampling, and the calculated elevation (MSL) of the sample.

Sample Code	Borehole elev	Sampling depth	**Calc elev of sample**
	(m)	(m)	**(m)**
SD-6/411.8 – 412.2/U	1496	125.6	1370.4
SD-6/412.2 – 412.6/U	1496	125.7	1370.3
SD-6/421.6 – 422.1/U	1496	128.6	1367.4
SD-6/430.3 – 430.6/U	1496	131.2	1364.8
SD-6/430.6 – 431.0/U	1496	131.3	1364.7
SD-6/443.2 – 443.5/U	1496	135.2	1360.8
SD-6/443.5 – 443.8/U	1496	135.2	1360.8
SD-6/471.3 – 471.7/U	1496	143.7	1352.3
SD-6/491.2 – 491.5/U	1496	149.8	1346.2
SD-6/507.5 – 507.8/U	1496	154.8	1341.2
SD-6/522.5 – 522.6/U	1496	159.3	1336.7
UE-25 NRG-6/158.2-15	1247	48.28	1198.7
UE-25 NRG-6/160.8	1247	49.07	1197.9
UE-25 NRG-6/171.0	1247	52.18	1194.8
UE-25 NRG-6/175.6	1247	53.58	1193.4
UE-25 NRG-6/219.9	1247	67.09	1179.9
UE-25 NRG-6/244.6	1247	74.62	1172.4
UE-25 NRG-6/255.9	1247	78.03	1169.0
UE-25 NRG-7a/165.8	1282	50.57	1231.4
UE-25 NRG-7a/258.0	1282	78.7	1203.3
UE-25 UZ#16/163.5-16	1219	49.9	1169.1
UE-25 UZ#16/180.9-18	1219	55.2	1163.8
UE-25 UZ-N2 gw	1203	15.8	1187.2
UE-25 UZ-N2 gw	1203	15.8	1187.2
UE-25 UZ-N2 gw	1203	15.8	1187.2
UE-25 UZ-N2 gw	1203	15.8	1187.2
UE-25 UZ-N2 gw	1203	30.1	1172.9
UE-25 UZ-N2 precip	1203	0	1203.0
USW SD-12/265.8	1324	81.08	1242.6
USW SD-12/278.6	1324	84.95	1238.7
USW SD-12/296.1	1324	90.34	1233.4
USW SD-7/339.7	1363	103.63	1259.4
USW SD-7/370.3	1363	112.93	1250.1
USW SD-9/114.1	1302	34.81	1267.5
USW SD-9/135.1	1302	41.21	1261.1
USW SD-9/154.0	1302	46.97	1255.3
USW SD-9/176.2	1302	53.74	1248.6
USW SD-9/251.8	1302	76.78	1225.5
USW SD-9/94.2-94.4	1302	28.7	1273.6
USW UZ-14/100.4	1349	30.66	1318.2
USW UZ-14/114.8	1349	35.02	1313.8
USW UZ-14/135.5	1349	41.36	1307.5
USW UZ-14/144.8	1349	44.2	1304.7
USW UZ-14/147.7	1349	45.08	1303.8
USW UZ-14/177.6	1349	54.19	1294.7

USW UZ-14/178.1	1349	54.35	1294.5
USW UZ-14/215.7	1349	65.81	1283.1
USW UZ-14/225.9	1349	68.92	1279.9
USW UZ-14/235.1	1349	71.72	1277.1
USW UZ-14/240.8	1349	73.46	1275.4
USW UZ-14/245.5	1349	74.89	1274.0
USW UZ-14/45.0-45.4	1349	13.78	1335.1
USW UZ-14/85.2-85.6	1349	26.03	1322.8
USW UZ-14/91.0-91.3	1349	27.8	1321.1
USW UZ-14/95.5-95.9	1349	29.17	1319.7
USW UZ-14/96.2-96.6	1349	29.38	1319.5

The following is the Ca-SO4-carbonate ternary plot showing the distribution of the above samples in terms of brine type (Alkaline, neutral, or Ca-Cl type). Out of the 56 samples, 11 belong to the alkaline-type, 11 to the Ca-Cl-type, and 34 to the neutral-type. The percentages are: alkaline – 20%, Ca-Cl – 20 %, and neutral – 60 %.



A study by Bish et al. (American Mineralogist, Volume 88, pages 1889–1902, 2003) indicate that the stratigraphic distribution profiles of Ca and Mg at Yucca Mountain show downward-diminishing concentration gradients of Mg and Ca, and increasing concentration with depth of Na and (to lesser extent) K due to ion-exchange processes. An abstract by Scofield and Stoller (Geological Society of America Annual Meeting, Nov. 2-3, 2003, Paper No. 134-14) stated the chemistry at Yucca Mountain evolves with increasing depth from the calcium-sulfate-chloride type in the overlying Paintbrush Tuff nonwelded hydrogeologic unit (PTn), to the sodium-bicarbonate type in the underlying Calico Hills nonwelded hydrogeologic unit (CHn). Thus, compared to our earlier analyses that used USGS porewater chemistry data, irrespective of the sample elevation, the analysis using only those samples taken above an elevation of 1,070 MSL resulted in a higher percentage of Ca-Cl-type waters, which are more deleterious than the neutral- and alkaline-type waters to the Alloy 22 waste package material due to the higher ratio of chloride to corrosion inhibitors.

The green symbol represents the mean composition of TSw pore water reported by Peterman and Oliver in a draft manuscript "Geochemistry of Natural Components of the Near-field Environment, Yucca Mountain, Nevada" (Table III), and the yellow symbol is the mean composition of SD-9 PTn pore water reported in the same reference. The following values were taken from that reference:

Mean Concentrations and Standard Deviations of USW SD-9 PTn Pore Water and TSw Pore Water [Data are from Peterman and Oliver, unpub. data. Dashes (---) mean that analyses were not done for these constituents.]

PARAMETER	USW SD-9 PTn Pore Water			TSw Pore Water		
	mg/L		n	mg/L		n
	Mean	Stdev		Mean	Stdev	
pH	7.1	0.2	10	7.6	0.1	42
Na^+	52	18	11	83	32	60
K^+	8	4	5	11	5	60
Mg^{2+}	19	10	11	15	12	59
Ca^{2+}	99	15	11	108	68	60
Cl^-	128	69	11	47	30	58
SO_4^{2-}	183	99	11	56	36	58
HCO_3^-	65	37	8	323	176	51
NO_3^-	11	5	11	13	15	57
F^-	1.2	0.7	5	2.5	2.0	58
SiO_2	68	11	11	52	7	60
Li^+	---		---	0.09	0.05	16
Mn^{2+}	---		---	0.13	0.16	56
TDS	601.2			546.8		

Entries into Scientific Notebook No. 679 for the period October 1, 2005, through September 30, 2006, have been made by

2/6/2008

Roberto T. Pabalan / Date

No original entry into this Scientific Notebook has been removed.

2/6/2008

Roberto T. Pabalan / Date

ELECTRONIC NOTEBOOK #679E

October 1, 2006 through September 30, 2007

20.06002.01.212

Roberto T. Pabalan

The entries in this electronic scientific notebook #679E document activities conducted during the period October 1, 2006, through September 30, 2007, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.06002.01.212).

December 4, 2006

Activity to be Conducted:

Thermodynamic Simulation of Evaporation of Yucca Mountain Porewaters

Conducted by: R. Pabalan

Objective: Determine the range in chemistry of waters that could contact the drip shields and waste packages at the potential repository at Yucca Mountain.

Technical Approach: Use the composition of selected samples collected and analyzed by the U.S. Geological Survey from the unsaturated zone of Yucca Mountain [reported in Yang et al. (1996, 1998, 2003).[1]] as input to thermodynamic calculations. Use the computer code StreamAnalyzer Version 2.0 (validated November 2005) to simulate the evaporation of the selected waters (invoke the standard chemistry option of the code) at fixed temperature.

Personnel qualification requirement: Geochemistry or chemistry background; familiarity in the use of thermodynamic simulation codes.

Input Compositions:

The tables below list the compositions of the USGS samples reported by Yang et al. (1996, 1998, 2003) and used in the evaporation simulation. Most of the samples are porewater samples; a few are perched water samples, which were included to expand the range in water chemistry considered in the analysis. The water compositions given in the table are plotted in a ternary Ca-SO4-(HCO3+CO3) diagram in a later page in order to aid evaluation of the simulation results using a chemical divide approach of Hardie and Eugster (1970).[2,3]

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[1]References:
Yang, I.C., Z.E. Peterman, and K.M. Scofield. 2003. Chemical analyses of pore water from boreholes USW SD-6 and USW WT-24, Yucca Mountain, Nevada. Journal of Contaminant Hydrology 1878, 1–20.
Yang, I.C., G.W. Rattray, and P. Yu. 1996. Interpretation of Chemical and Isotopic Data from Boreholes in the Unsaturated Zone at Yucca Mountain, Nevada. Water-Resources Investigations Report 96-4058. U.S. Geological Survey, Denver, Colorado.
Yang, I.C., P. Yu, G.W. Rattray, J.S. Ferarese, and J.N. Ryan. 1998. Hydrochemical Investigations in Characterizing the Unsaturated Zone at Yucca Mountain, Nevada. Water-Resources Investigations Report 98-4132. U.S. Geological Survey, Denver, Colorado.
[2] Hardie, L.A., and Eugster, H.P. (1970) Evolution of closed-basin brines. 273-290 p.
[3] Spencer, R.J. (2000) Sulfate minerals in evaporite deposits. Reviews in Mineralogy and Geochemistry, 40, 173-192.

Email

p. 154 a, b, c, d, and e

154a

rbrient

From: Yong Kim [Yong.Kim@nrc.gov]
Sent: Friday, April 04, 2008 9:36 AM
To: James Rubenstone
Cc: Bret Leslie; Sheena Whaley; King Stablein; David Misenhimer; Mohanty', 'Sitakanta; Robert Brient
Subject: RE: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

Jim,

Considering the factors including your Branch's continuous involvement with R-IV in QA/Inspection beyond the review of Construction Authorization, I am proposing a following Team structure:

Chapter 2.5.5 - R. Brient (Lead Author) and M. Simpson from CNWRA and F. Jacobs from NRC, and

Chapter 2.5.6 - R. Brient (Lead Author) and M. Simpson from CNWRA and F. Jacobs from NRC.

My name is out from the Team as I am busy with the Preclosure project. However, if the management (including Sheena) requests me to stay in after the Vol. 4 Kickoff meeting on 4/8/08, I shall be ready for that.

Bob already developed draft SER outlines for both Chapters, and I reviewed them. They are well prepared, and will be good foundations for final SER outlines. They are placed in the shared drive under the directory, **SER Vol 4**.

Please let me know if you need my further assistance.

Cheers,

Yong

From: Bret Leslie
Sent: Thursday, April 03, 2008 11:39 AM
To: Sheena Whaley; Yong Kim; James Rubenstone
Cc: Bret Leslie
Subject: RE: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

please keep Jim Rubenstone in the loop for staffing concerning Volume 4 as he is on the line for ensuring that necessary staff are assigned to the teams for Volume 4
bret

From: Sheena Whaley
Sent: Thursday, April 03, 2008 10:18 AM
To: Yong Kim; Bret Leslie
Subject: FW: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

Yong/Bret,

We are still finalizing the resource loading for Volume 2, but it looks like Yong will be overloaded even

without being involved in Volume 4. I think one of the solutions may be to have a Center person be the LA for this chapter.

Sheena

154b

From: Yong Kim
Sent: Thursday, April 03, 2008 10:09 AM
To: Robert Brient
Cc: King Stablein; Sheena Whaley; Mohanty', 'Sitakanta; James Rubenstone; Bret Leslie
Subject: RE: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

Good morning, Bob:

Thank you for the update. Even though you are not officially on the 2.5.5 and 2.5.6 Teams now (but, you were in **before**), please continue working on draft SER outlines for Chapters 2.5.5 and 2.5.6. I believe the management will make a final Team structure after the Vol. 4 meeting on 4/8/2008.

Cheers,
Yong

From: rbrient [mailto:rbrient@cnwra.swri.edu]
Sent: Wednesday, April 02, 2008 2:48 PM
To: Yong Kim
Subject: RE: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

Yong:

I've started on the outlines for 2.5.5 and 2.5.6 using the YMRP as the primary source of input. I also looked at the chapter assignments on the shared drive\project plan\org charts and found that the teams have been slimmed down since the 2/21/2008 version of the Vol 4 org chart (I'm not listed on either chapter, and no CNWRA staff are assigned as EM or TR). You may want to discuss this with Dave Misenhimer to see if he thinks these assignments should be made.

Like several other chapters in Volume IV, these two preface the review plan with the statement that NRC does not expect DOE to provide (detailed) plans in the LA for construction authorization, but before the license amendment to receive and possess HLW, the plans must be in place. I believe the expectation is that the review will just make sure that DOE has described an approach to developing plans that will likely be acceptable at the later stage licensing steps. This limited scope review also justifies having smaller teams. I would also anticipate a very limited role of technical experts – there probably won't be much of technical substance in DOE's "plans to develop plans."

Even though I'm not officially on the 2.5.5 and 2.5.6 teams, I'll go ahead and work on these outlines a bit more and I'll attend the 4/8/2008 meeting and give you feedback regarding these chapters. I expect that the draft outlines will be ready for you to look at before the end of this week.

Bob Brient
Director, Quality Assurance
Geosciences and Engineering Division
Southwest Research Institute
(210) 522-5537

From: Yong Kim [mailto:Yong.Kim@nrc.gov]
Sent: Tuesday, April 01, 2008 10:24 AM
To: Robert Brient
Cc: Bret Leslie; James Rubenstone; King Stablein; George Adams; Ali Simpkins; Patrick Mackin; Mohanty', 'Sitakanta; Jacqueline Simpson; Michael Simpson; Frank Jacobs; Christopher Ryder; David Misenhimer; Brian Benney

Subject: RE: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM

154c

Bob,

It was nice to talk to you. As we discussed, please plan to attend the subject kickoff meeting, and get detailed information from Bret about his plan for Volume 4. My guess is that he will discuss about a schedule for Vol. 4 SER outline development.

I am glad to hear that you have already started to prepare draft SER outlines for Chapters 2.5.4 and 2.5.5. If you need assistance/supports from other members (because of their technical strength), please let them know and interact with them. In our SER outlines, we may eventually need to identify them as Technical Reviewers (TRs) with resource loadings. The NRC organization chart shows that these are our TRs:

Chapter 2.5.5 - Plans for Startup Activities and Testing

Kim (LA) and Ryder at NRC
Brient (my counterpart at Center?), G. Adams, Simpkins, Simpson, Mackin, and Mohanty at CNWRA.

Chapter 2.5.6 - Plans for Conduct of Normal Activities Including Maintenance, surveillance, and Periodic Testing

Kim (LA), Jacobs, and Ryder at NRC
Brient (my counterpart at Center?), G. Adams, Simpkins, Mackin, Mohanty, and Simpson at CNWRA

In addition, I believe that our TRs should start to review the DOE's documents available in LSN, and, if we have any serious concerns about their plans, we should consider to have an Appendix 7 meeting with DOE soon before the LA submission.

As I informed you and Bret, I won't be able to attend our kickoff meeting because I must participate in the Preclosure Tabletop Exercise. Please inform me the outcome of the kickoff meeting.

Thanks,
Yong

Yong S. Kim, Ph.D., P.E.
Senior Structural Engineer
Mail Stop EBB 2B-02
NMSS/DHLWRS/EB
U.S. Nuclear Regulatory Commission
Washington, DC 20555

Phone: (301) 492-3567

-----Original Appointment-----
From: Bret Leslie
Sent: Wednesday, March 26, 2008 12:25 PM
To: Patrick Mackin; Christine Pineda; David Misenhimer; Frank Jacobs; Jeffrey Pohle; Janet Kotra; James Rubenstone; Kien Chang; Thomas Matula; Yong Kim
Cc: Budhi Sagar; Gordon Wittmeyer; Roland Benke; Robert Brient; Wesley Patrick; Xihua He; Eugene Peters; Peters-2
Subject: Volume 4 Kickoff Meeting for Tech. Coords, Lead Authors, SPA, BC, PM, EM
When: Tuesday, April 08, 2008 10:00 AM-11:30 AM (GMT-05:00) Eastern Time (US & Canada).
Where: EBB 2C19 (War Room) 301-492-3561 and Center?

Folks,
I used busy search for the Lead Authors (LA), Technical Coordinators (TC), Project Manager (PM), Branch Chief (BC), Senior Primary Advisor (SPA) to find this available slot. Pat Mackin has been coordinating with the BC,

154d

SPA, and PM with Volume 4 development, and we are using him to help set up this meeting at the Center (Pat, can you get a room, notify me with contact info, and let center staff know as well). Once the Center has identified the Element Manager for Volume 4 (Administrative and Programmatic), the EM should attend as well.

Note the attached marked up organization chart (use your mouse to touch the note boxes to read the notes) identifies some changes in NRC lead authors, the need for the Center EM to be identified, and some missing previously identified expertise for one team.

Those on the cc list (other than Gene P) have been identified by Center management as the Center leads for the team [this is denoted in the attached file by the (strikethrough "EM")]. Your attendance is not required, but if you can make it, that would be great.

The POP (purpose, outcome, process) is below and I will send out a detailed agenda closer to the meeting. Comments or suggestions for other topics to address in the meeting would be welcomed and should be sent to me.

Purpose: We will present and discuss topics that affect all teams in Volume 4 (e.g., when your SER outlines are due (May/June; make sure you know your roles and responsibilities). We will obtain initial feedback from lead authors and technical coordinators on any potential issues affecting their teams (appropriate resources and expertise is available (e.g., any need for Center-consultant support or Technical Assistance Request from other Divisions or Offices?), their understanding of the scope of their team's review, and other areas of concern, including integration across volumes.

Outcome: A common understanding of the upcoming products or events that the teams will need to complete. A list of any issues from each team that need to be resolved prior to submission of the license application. A general understanding of the preparedness of each of the teams.

Process: Prior to this meeting it is expected that either the individual teams have met and discussed and identified any potential issues affecting their teams (described above in the purpose) or that the lead author has developed their list of potential issues. Bret will facilitate and present on upcoming products or events that the teams will need to complete. Each of the lead authors will briefly present (5 minutes) the status of their team's preparations and issues. Dave Misenhimer will capture notes and action items.

nks for your participation and preparatory activities,
, Senior Primary Advisor for Volume 4 << File: Org Chart-Volume 4_markup.pdf >>

154e

Path Forward for NRC-Facilitated, Center Self-Study Program on Regulatory Topics
10:00 – 11:30 AM (EST) 4/8/08 in EBB 2C19, Rockville and Building 61 VTC (210-522-4940)

Purpose: We will present and discuss topics that affect all teams in Volume 4 (e.g., when your SER outlines are due (draft by end of April, final by May 15th; make sure you know your roles and responsibilities). We will obtain initial feedback from lead authors and technical coordinators on any potential issues affecting their teams (appropriate resources and expertise is available (e.g., any need for Center-consultant support or Technical Assistance Request from other Divisions or Offices?), their understanding of the scope of their team's review, and other areas of concern, including integration across volumes.

Outcome: A common understanding of the upcoming products or events that the teams will need to complete. A list of any issues from each team that need to be resolved prior to submission of the license application. A general understanding of the preparedness of each of the teams.

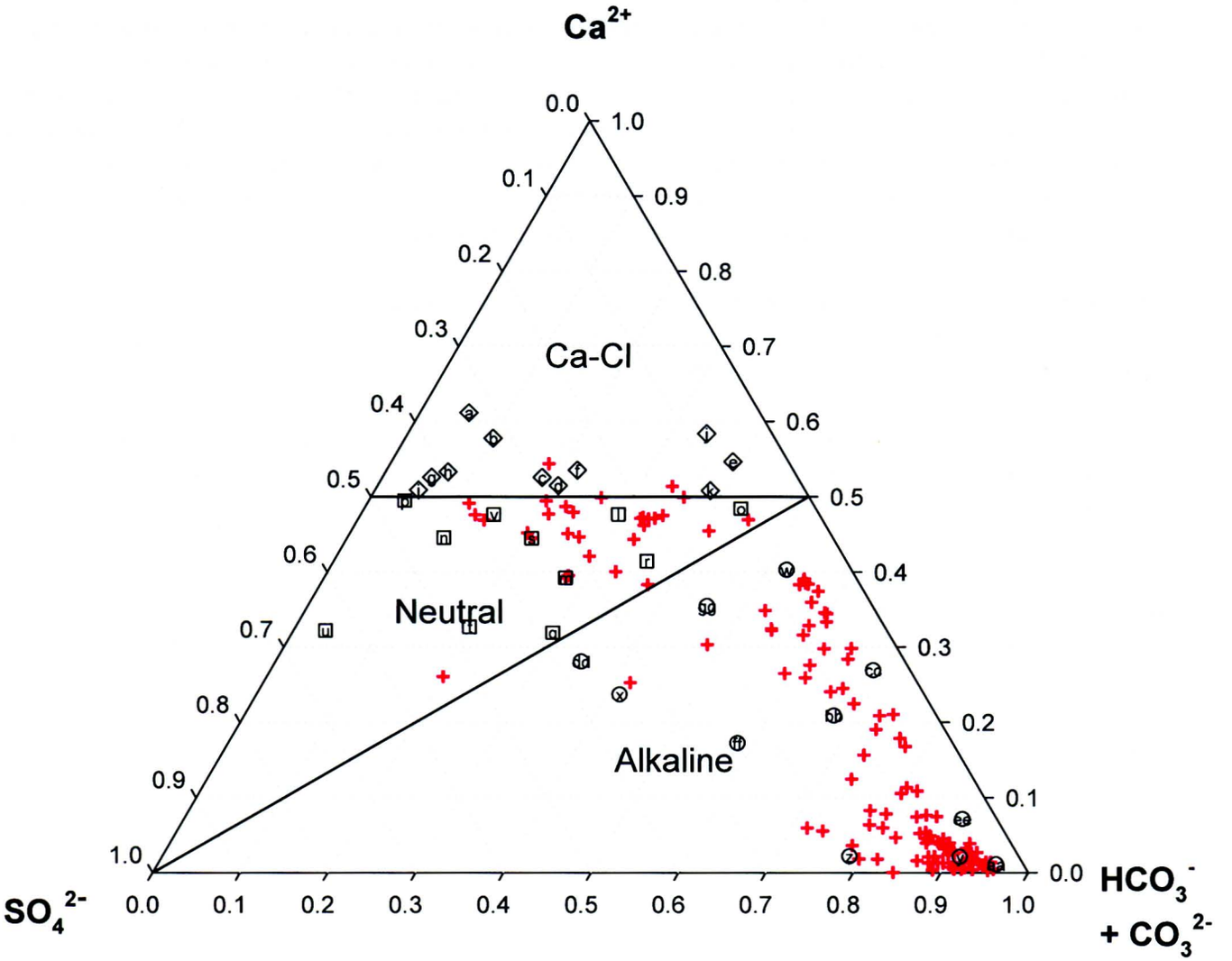
Process: Prior to this meeting it is expected that either the individual teams have met and discussed and identified any potential issues affecting their teams (described above in the purpose) or that the lead author has developed their list of potential issues. Bret will facilitate and present on upcoming products or events that the teams will need to complete. Each of the lead authors will briefly present (5 minutes) the status of their team's preparations and issues. Dave Misenhimer will capture notes and action items.

Agenda

Time	Topic	Details
10:00 - 10:05 AM	Introductions of attendees and agenda	Bret will lead
10:05 - 10:15 AM	Upcoming events and products	Bret to present and respond to questions
10:15 - 11:20 AM	Team status reports for 13 teams	Each team (lead author or their representative) will provide a < 5 minute status of their preparations and of any issues they need to address or where they need assistance. The following items should be addressed: status of staffing (everyone knows who is on their teams and what their responsibilities are; any need for TAR or consultant?); status of outline development; any issues we need to resolve now (e.g., position on groundwater access or rights).
11:20 - 11:30 AM	Summarize meeting	Bret and Dave M. to summarize any action items and outline next steps

Sample ID	Symbol in fig.	Brine type	SIO2	NAION	KION	MGION	CAION
			mg/L				
NRG-6/158.2-15 w/ Br,F	a	Ca-Cl	97.40	35.60	0.00	23.30	122.00
NRG-6/160.8 w/ Br,F	b	Ca-Cl	84.00	35.00	0.00	18.00	104.00
NRG-6/171.0 w/ Br,F	c	Ca-Cl	79.39	29.20	0.00	11.50	70.50
NRG-6/175.6 w/ Br,F	d	Ca-Cl	78.10	29.40	0.00	8.60	49.20
SD-12/296.1 w/ Br,F	e	Ca-Cl	72.20	21.00	0.00	8.00	75.00
SD-6/471.3 w/ Br	f	Ca-Cl	58.50	44.90	2.60	12.30	61.40
SD-9/114.1 w/ Br,F	g	Ca-Cl	62.20	55.00	0.00	18.00	95.00
SD-9/135.1 w/ Br,F	h	Ca-Cl	60.00	66.00	0.00	15.00	91.00
SD-9/94.2 w/ Br & F	i	Ca-Cl	74.00	43.00	0.00	24.00	125.00
UZ-16/1643.4 w/ Br,F	j	Ca-Cl	69.99	34.00	0.00	12.00	91.00
UZ-14/1277.7 w/ Br,F	k	Ca-Cl	38.00	45.00	0.00	5.10	74.00
SD-6/412.2 w/ Br	l	Neutral	41.60	58.70	6.50	11.30	45.80
SD-6/443.5 w/ Br	m	Neutral	84.40	65.50	4.00	11.70	48.20
SD-6/507.5 w/ Br	n	Neutral	64.00	48.30	2.40	24.60	125.00
SD-6/1509.9 w/ Br	o	Neutral	54.50	98.90	8.30	2.60	65.80
SD-7/370.3 w/ Br,F	p	Neutral	25.90	39.00	0.00	0.20	289.00
SD-9/176.2 w/ Br,F	q	Neutral	58.50	95.00	0.00	9.50	43.00
UZ-14/85.2-85.6 w/ Br,F	r	Neutral	89.80	43.50	0.00	13.20	49.90
UZ-14/147.7 w Br,F	s	Neutral	77.3	51.6	0.00	11.5	54.8
NRG-6/244.6 w/ Br,F	t	Neutral	51.00	72.00	0.00	4.90	33.00
NRG-6/255.9 w/ Br,F	u	Neutral	68.00	215.00	0.00	19.00	176.00
UZ-14/178.1 w/ Br,F	v	Neutral	93.10	49.10	0.00	10.60	64.00
UZ-14/1258.5 w/ Br,F	w	Alkaline	35.00	67.00	0.00	3.70	43.00
UZ-14/1409.4 w/ Br,F	x	Alkaline	57.00	88.00	0.00	0.70	30.00
UZ-14/1542.3 w/ Br,F	y	Alkaline	143.00	207.00	0.00	0.50	3.60
UZ-14/1825.8 w/ Br,F	z	Alkaline	47.90	137.00	0.00	0.10	0.60
UZ-14/2014.7 w/ Br,F	aa	Alkaline	37.70	392.00	0.00	0.20	3.20
UZ-16/1343.7 w/ Br,F	bb	Alkaline	62.10	99.00	0.00	2.40	17.00
WT-24/1937.0 w/ Br	cc	Alkaline	45.40	58.00	6.70	0.60	15.90
NRG-6/219.9 w/Br,F	dd	Alkaline	61.40	99.30	0.00	4.20	24.30
NRG-7a/460.25 w/ Br,F	ee	Alkaline	9.00	42.00	6.80	0.00	3.00
SD-12/1495.5 w/ Br,F	ff	Alkaline	87.30	108.00	0.00	0.20	16.00
SD-6/522.5 w/ Br	gg	Alkaline	63.70	59.00	6.00	9.90	43.70

Sample ID	FION	CLION	SO4ION	NO3ION	HCO3ION	CO3ION	BRION
NRG-6/158.2-15 w/ Br,F	2.18	185.00	159.00	32.00	34.00	0.00	13.00
NRG-6/160.8 w/ Br,F	2.18	148.00	139.00	35.00	55.00	0.00	13.00
NRG-6/171.0 w/ Br,F	2.18	58.00	94.01	43.00	48.01	13.00	13.00
NRG-6/175.6 w/ Br,F	2.18	47.00	64.00	42.00	60.00	0.00	13.00
SD-12/296.1 w/ Br,F	2.18	60.00	21.00	18.00	163.00	0.00	13.00
SD-6/471.3 w/ Br	8.60	66.80	68.00	67.30	74.00	1.00	13.00
SD-9/114.1 w/ Br,F	2.18	138.00	181.00	10.90	31.00	0.00	13.00
SD-9/135.1 w/ Br,F	2.18	144.00	162.00	12.00	37.00	0.00	13.00
SD-9/94.2 w/ Br & F	2.18	170.00	260.00	11.00	37.00	0.00	13.00
UZ-16/1643.4 w/ Br,F	2.18	70.00	28.00	8.00	162.02	0.00	13.00
UZ-14/1277.7 w/ Br,F	2.18	130.00	38.00	15.00	170.00	0.00	13.00
SD-6/412.2 w/ Br	11.30	47.20	53.00	78.20	84.00	1.00	13.00
SD-6/443.5 w/ Br	6.30	47.30	98.00	86.00	101.00	1.00	13.00
SD-6/507.5 w/ Br	3.10	20.30	299.00	25.70	92.00	1.00	13.00
SD-6/1509.9 w/ Br	14.70	98.70	28.00	1.80	178.00	0.00	13.00
SD-7/370.3 w/ Br,F	2.18	133.00	650.00	0.60	73.00	0.00	13.00
SD-9/176.2 w/ Br,F	2.18	64.00	124.00	1.90	122.00	0.00	13.00
UZ-14/85.2-85.6 w/ Br,F	2.18	60.00	66.00	22.00	131.00	0.00	13.00
UZ-14/147.7 w Br,F	2.18	83.00	102.00	22.00	79.00	0.00	13.00
NRG-6/244.6 w/ Br,F	2.18	49.00	115.00	40.00	61.00	0.00	13.00
NRG-6/255.9 w/ Br,F	2.18	115.00	840.00	35.00	61.00	0.00	13.00
UZ-14/178.1 w/ Br,F	2.18	97.00	120.00	21.00	62.00	0.00	13.00
UZ-14/1258.5 w/ Br,F	2.18	88.00	19.00	16.00	170.00	0.00	13.00
UZ-14/1409.4 w/ Br,F	2.18	75.00	106.00	5.00	160.00	0.00	13.00
UZ-14/1542.3 w/ Br,F	2.18	20.00	28.00	4.00	384.00	46.00	13.00
UZ-14/1825.8 w/ Br,F	2.18	23.50	12.90	11.80	42.00	12.00	13.00
UZ-14/2014.7 w/ Br,F	2.18	32.10	22.20	1.80	409.00	219.00	13.00
UZ-16/1343.7 w/ Br,F	2.18	56.00	23.00	18.00	47.60	58.80	13.00
WT-24/1937.0 w/ Br	4.20	35.80	6.00	0.50	124.00	0.00	13.00
NRG-6/219.9 w/Br,F	2.18	77.00	77.00	47.00	92.00	0.00	13.00
NRG-7a/460.25 w/ Br,F	2.18	7.00	4.00	1.00	114.00	0.00	13.00
SD-12/1495.5 w/ Br,F	2.18	57.00	55.00	8.10	49.00	57.00	13.00
SD-6/522.5 w/ Br	7.70	26.30	56.00	34.50	167.00	2.00	13.00



- Chemistry data (+) on Yucca Mountain unsaturated zone pore waters published by USGS (Yang, et al., 1996, 1998, 2003)
- Data on selected samples (diamonds, squares, and circles, with letters cross-referenced to sample names listed in the table above, column-2) used as input to thermodynamic simulations of evaporation

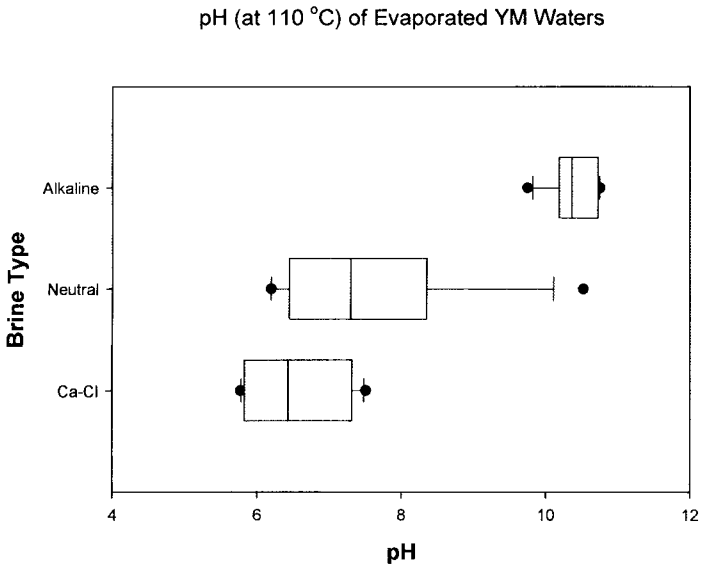
Most the chemical analysis reported by USGS did not include values for fluoride ion concentration, and none included bromide concentration data. To allow evaluation of the effects of evaporation on the evolution of fluoride and bromide concentrations, a bromide concentration equal to 13 mg/L was added to all input compositions and fluoride concentration of 2.18 mg/L was added to compositions of samples that did not include a value for fluoride. The value of 2.18 mg/L for fluoride is a mean value for J-13 well water analyses reported by Harrar et al. (1990)[4]. The value of 13 mg/L for bromide is arbitrary. The sample IDs were taken (and truncated in some cases) from the sample IDs used by Yang et al. (1996, 1998, 2003) and modified to indicate whether Br and/or F concentrations were added for the thermodynamic simulations.

The evaporation simulations were done using StreamAnalyzer 2.0. The simulation temperature was set to 110 C and a total pressure of 0.85 atm. In one case, the run did not converge and the total pressure had to be set to 0.90 atm to achieve convergence.

The StreamAnalyzer 2.0 file is in a CD accompanying this notebook, filename: "StreamAnalyzer YM Waters with Br&F". The results of the calculations are summarized in Excel file "YM Waters with Br&F.xls".

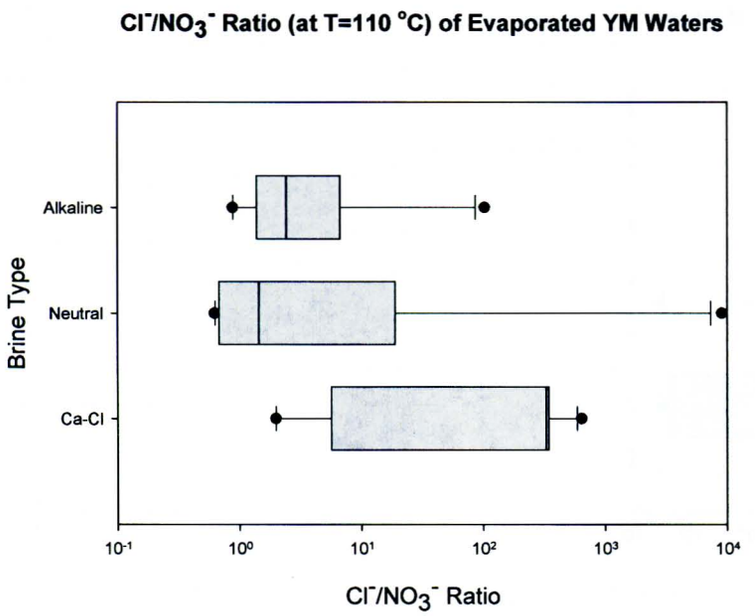
The range in composition of the brines that result from evaporation of the initially dilute YM porewaters are illustrated in the following box plots, grouped according to the water-type (alkaline-, neutral-, or calcium-chloride-type). The figures were generated using the software Sigmaplot.

The ranges in pH for the three water types are illustrated in the following figure:

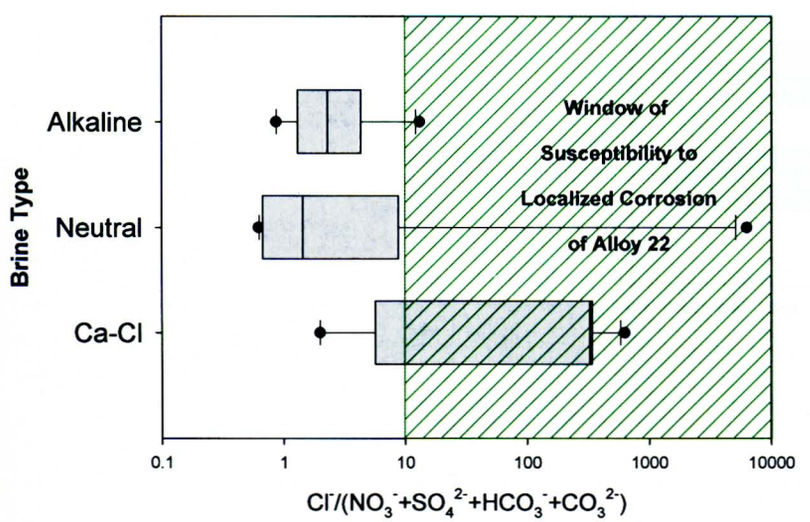


[4] Harrar, J.E., Carley, J.F., Isherwood, W.F., and Raber, E. (1990) Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations.UCID-21867. Lawrence Livermore National Laboratory, Livermore, CA.

The range in calculated Cl/NO3 ratio is as follows:

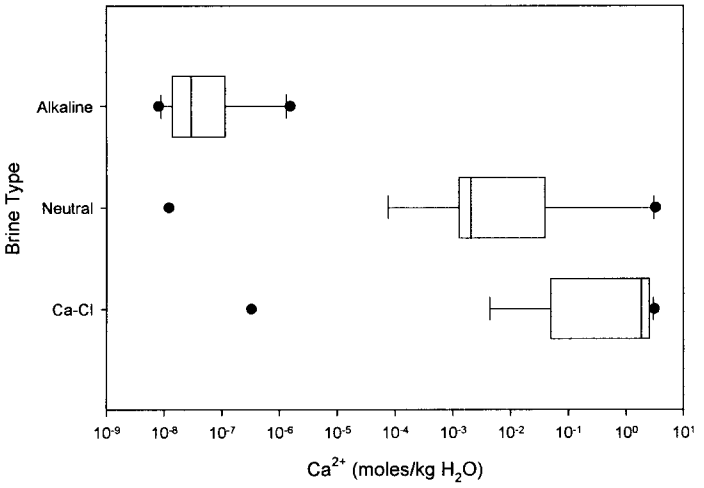


The range in calculated ratio of chloride to corrosion inhibiting species (NO3+SO4+HCO3+CO3) is as follows. The green hatched area indicates the Cl to inhibitor molar ratio (≥10) under which Alloy 22, the proposed waste package outer barrier material, is susceptible to localized corrosion.

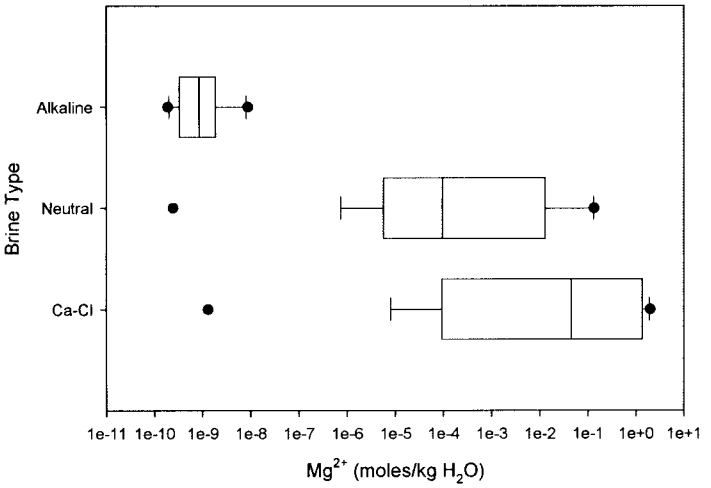


Other results are plotted in the following diagrams:

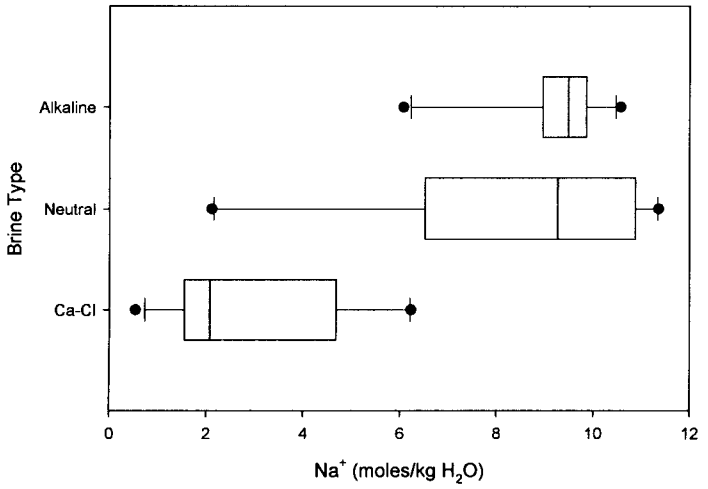
Calcium Conc. (at T=110 °C) of Evaporated YM Waters



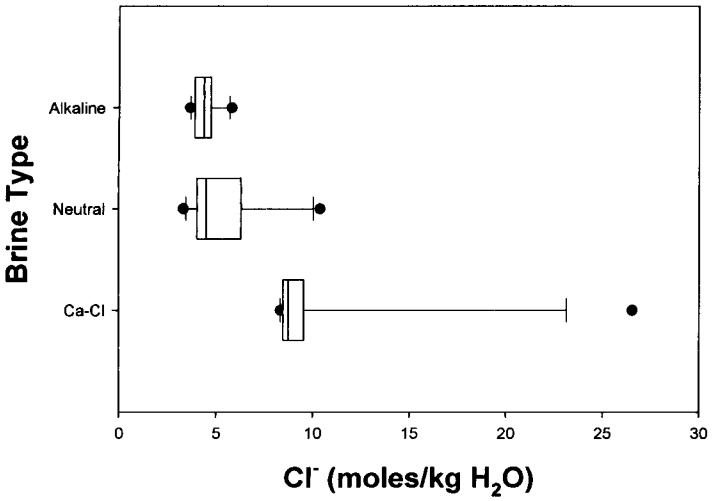
Magnesium Conc. (at T=110 °C) of Evaporated YM Waters



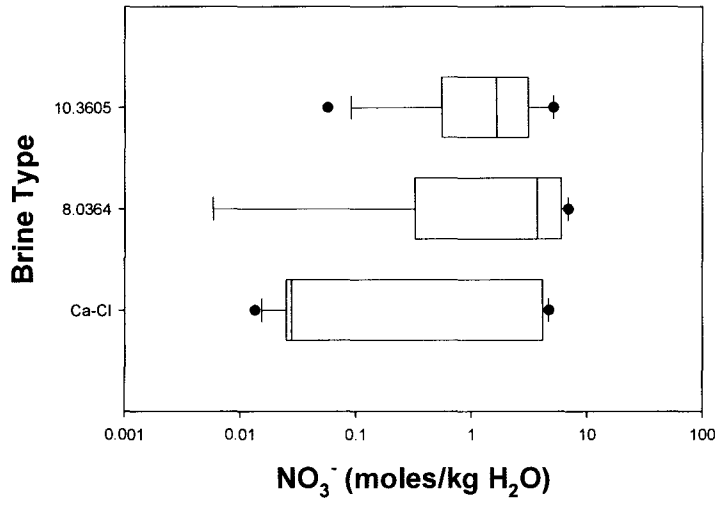
Sodium Conc. (at T=110 °C) of Evaporated YM Waters



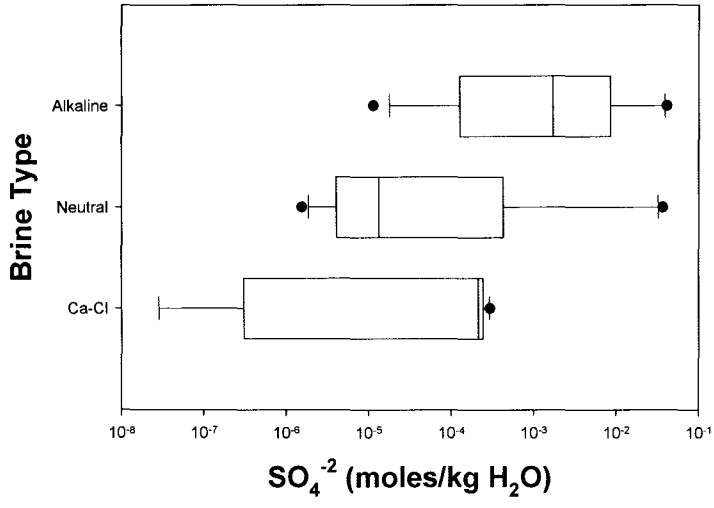
Chloride Conc. (at T=110 °C) of Evaporated YM Waters



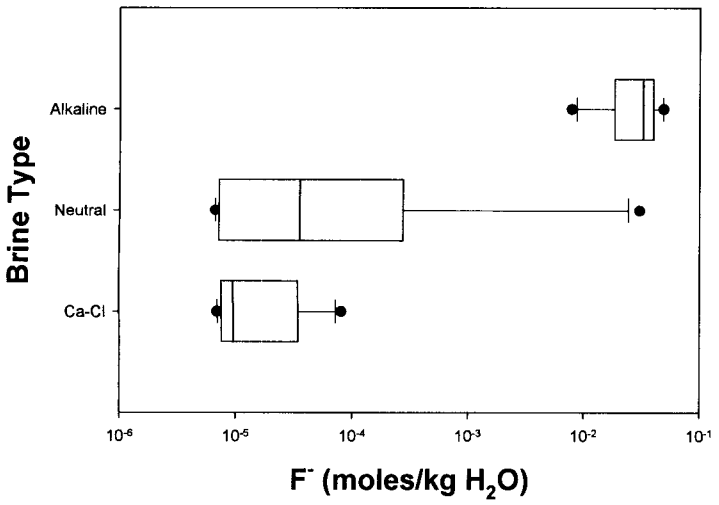
Nitrate Conc. (at T=110 °C) of Evaporated YM Waters



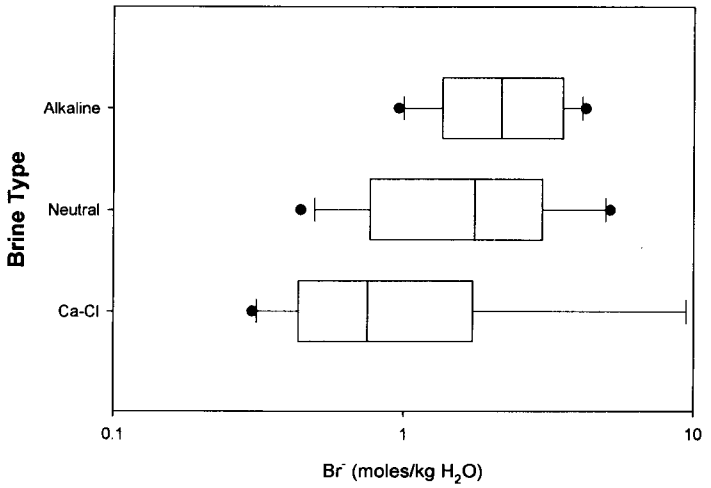
SO_4^{-2} Conc. (at T=110 °C) of Evap. YM Waters



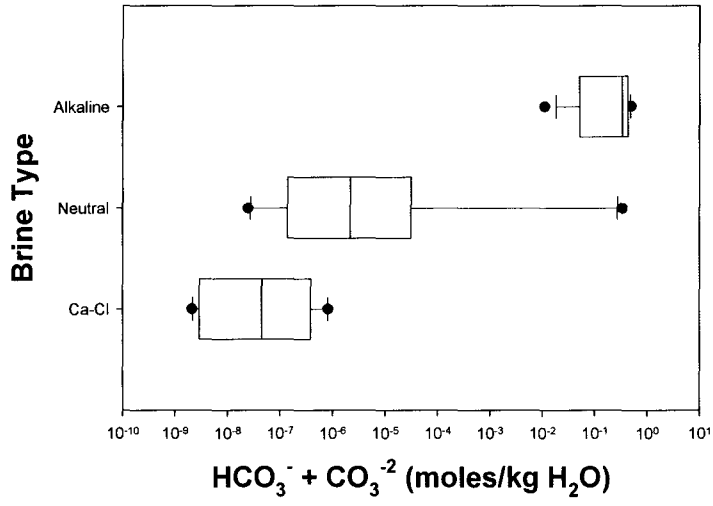
Fluoride Conc. (at T=110 °C) of Evaporated YM Waters



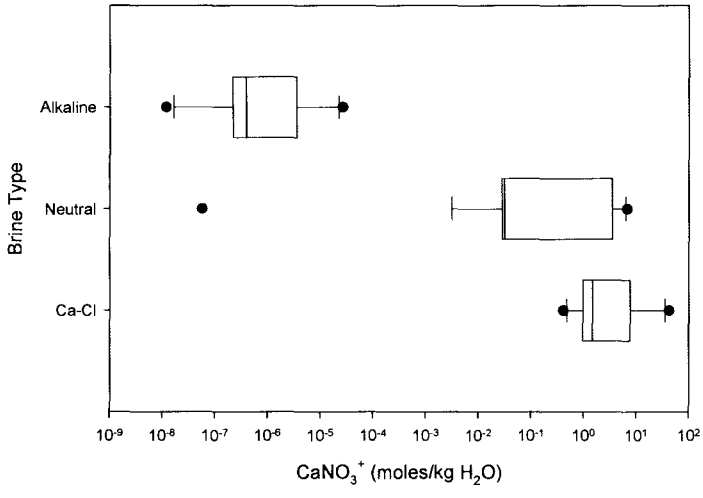
Bromide Conc. (at T=110 °C) of Evaporated YM Waters



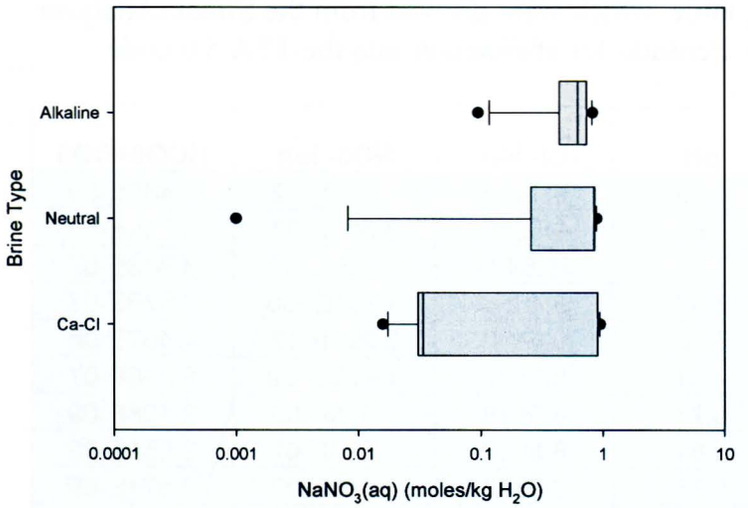
Carbonate Conc. (at T=110 °C) of Evaporated YM Waters

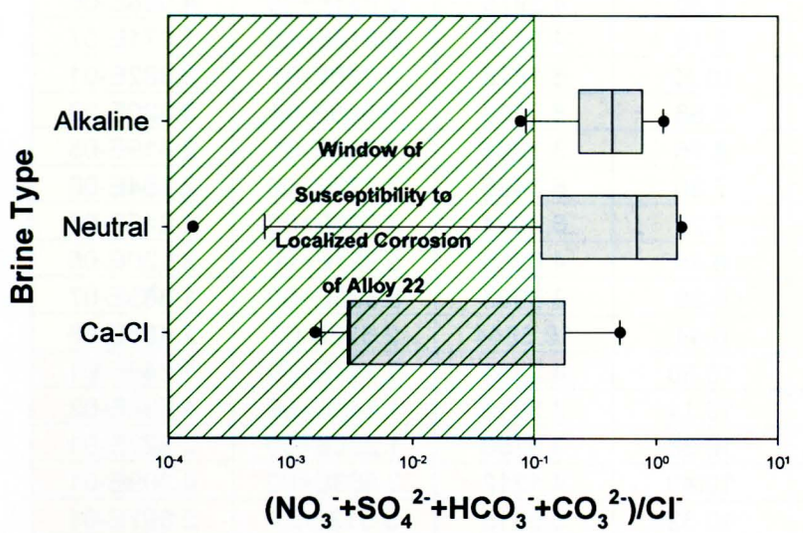


$CaNO_3^+$ Conc. (at T=110 °C) of Evap. YM Waters



$NaNO_3$(aq) Conc. (at T=110 °C) of Evaporated YM Waters





January 5, 2007

The water chemistries listed in the following table, which were derived from the StreamAnalyzer evaporation simulations, were provided to O. Pensado for abstraction into the TPA 5.0 code.

Sample Name	Brine type	pH	Cl- ion	NO3- ion	HCO3+CO3
NRG-6/158.2-15 w/ Br,F	Ca-Cl	5.83	9.1475	2.781E-02	2.435E-09
NRG-6/160.8 w/ Br,F	Ca-Cl	5.89	9.5907	3.338E-02	4.739E-09
NRG-6/171.0 w/ Br,F	Ca-Cl	7.50	26.5429	4.708E+00	3.846E-07
NRG-6/175.6 w/ Br,F	Ca-Cl	7.37	8.4656	4.131E+00	7.576E-07
SD-12/296.1 w/ Br,F	Ca-Cl	6.46	9.5446	3.226E-02	4.497E-08
SD-6/471.3 w/ Br	Ca-Cl	7.31	8.7427	4.416E+00	8.216E-07
SD-9/114.1 w/ Br,F	Ca-Cl	5.77	8.3679	2.538E-02	2.108E-09
SD-9/135.1 w/ Br,F	Ca-Cl	5.81	8.5930	2.500E-02	2.951E-09
SD-9/94.2 w/ Br & F	Ca-Cl	5.85	8.6243	1.348E-02	2.871E-09
UZ-16/1643.4 w/ Br,F	Ca-Cl	6.43	8.3365	2.543E-02	7.844E-08
UZ-14/1277.7 w/ Br,F	Ca-Cl	6.60	9.1436	2.300E-02	5.267E-08
SD-6/412.2 w/ Br	Neutral	8.04	4.5225	6.709E+00	1.706E-05
SD-6/443.5 w/ Br	Neutral	8.35	4.2975	6.931E+00	4.058E-05
SD-6/507.5 w/ Br	Neutral	6.19	4.2715	5.014E+00	1.971E-07
SD-6/1509.9 w/ Br	Neutral	10.52	6.1475	3.256E-01	3.382E-01
SD-7/370.3 w/ Br,F	Neutral	6.86	8.6653	9.588E-04	3.820E-08
SD-9/176.2 w/ Br,F	Neutral	8.16	3.3294	7.785E-01	2.419E-05
UZ-14/85.2-85.6 w/ Br,F	Neutral	7.30	5.3486	3.722E+00	2.164E-06
UZ-14/147.7 w Br,F	Neutral	7.29	6.3094	3.396E+00	1.245E-06
NRG-6/244.6 w/ Br,F	Neutral	8.46	4.0266	5.991E+00	3.120E-05
NRG-6/255.9 w/ Br,F	Neutral	6.20	3.9993	5.636E+00	1.385E-07
UZ-14/178.1 w/ Br,F	Neutral	6.44	10.3844	2.532E-02	2.496E-08
UZ-14/1258.5 w/ Br,F	Alkaline	10.36	4.2891	3.117E+00	1.744E-01
UZ-14/1409.4 w/ Br,F	Alkaline	10.11	3.9015	1.649E+00	4.535E-02
UZ-14/1542.3 w/ Br,F	Alkaline	10.36	3.8150	1.254E+00	3.322E-01
UZ-14/1825.8 w/ Br,F	Alkaline	10.49	4.1212	2.563E+00	4.299E-01
UZ-14/2014.7 w/ Br,F	Alkaline	10.32	3.6615	5.513E-01	2.897E-01
UZ-16/1343.7 w/ Br,F	Alkaline	10.73	4.6959	1.950E+00	4.888E-01
WT-24/1937.0 w/ Br	Alkaline	10.65	5.8126	5.702E-02	3.487E-01
NRG-6/219.9 w/Br,F	Alkaline	10.18	4.3817	5.008E+00	5.122E-02
NRG-7a/460.25 w/ Br,F	Alkaline	10.73	5.1938	2.259E-01	3.553E-01
SD-12/1495.5 w/ Br,F	Alkaline	10.75	4.7476	1.015E+00	4.465E-01
SD-6/522.5 w/ Br	Alkaline	9.74	4.7451	5.149E+00	1.089E-02

Based on data on chemistry of UZ porewater samples from Yang et al. (1996, 1998, 2003)

Occurrence of Ca-Cl brine type = 8 %; Neutral brine type = 24%; Alkaline brine type = 68 %

February 14, 2007

```
MessageFrom: Osvaldo Pensado [opensado@cnwra.swri.edu]
Sent: Wednesday, February 14, 2007 4:51 PM
To: Roberto Pabalan
Cc: James Myers
Subject: Relative humidity range

Find attached the relative humidity range, as a function of WP temperature, to
support speciation computations.

================================
Osvaldo Pensado, Ph.D.
Senior Research Scientist, SwRI
6220 Culebra Road. San Antonio TX 78238
(210) 522 6084
Fax: (210) 522 6081
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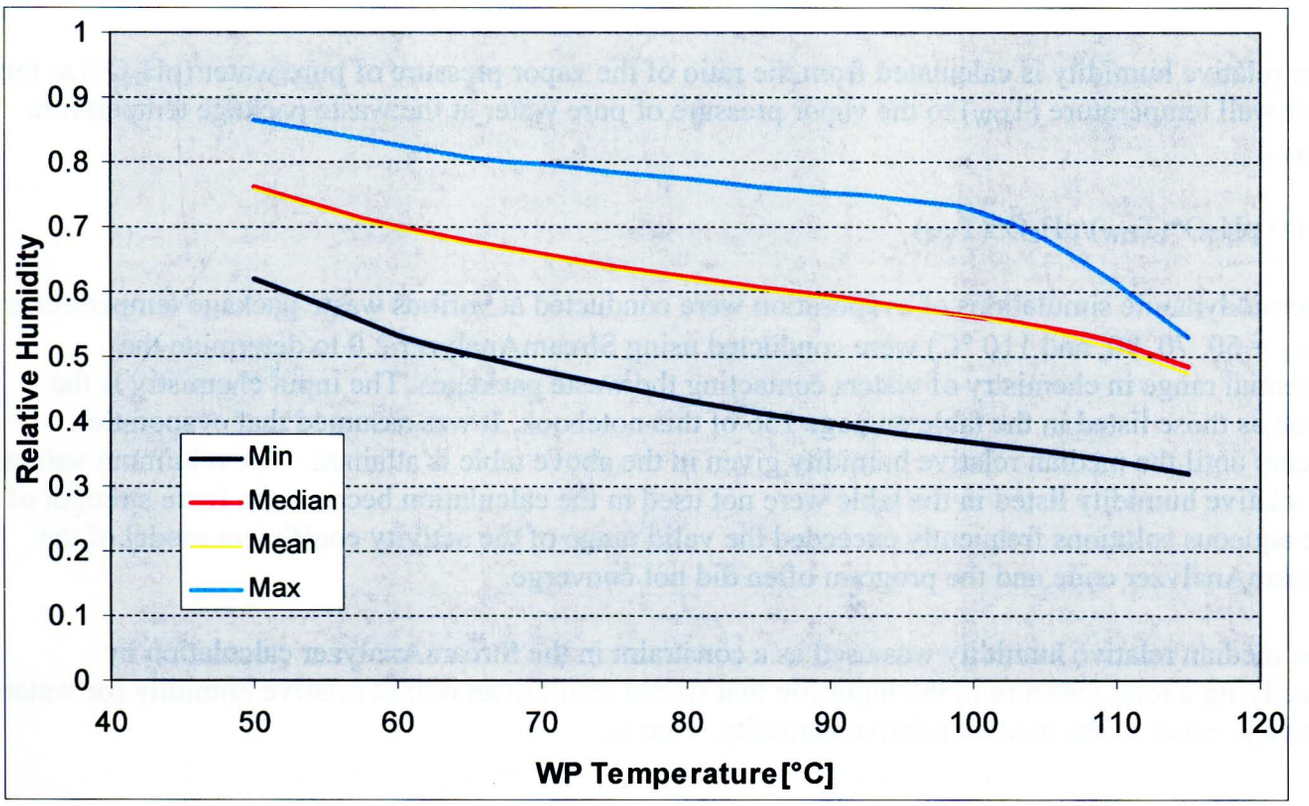


Relative humidity range derived with TPA 5.1 betaF, nominal case (i.e., includes drift degradation), 600 realizations.
The plot represents the relative humidity range for fixed values of the waste package temperature.

T[°C]	Relative Humidity				
	Min	Median	Mean	Max	SDev
50	0.620649	0.762094	0.75871	0.863537	0.053797
55	0.576193	0.729053	0.726945	0.845013	0.059228
60	0.53284	0.70024	0.697771	0.82645	0.064609
65	0.502686	0.67685	0.673351	0.807784	0.069505
70	0.476544	0.656696	0.653231	0.795367	0.073192
75	0.453925	0.638221	0.63553	0.783978	0.07601
80	0.432806	0.621742	0.619162	0.773571	0.07832
85	0.413775	0.606645	0.60378	0.762867	0.080336
90	0.396549	0.59223	0.589239	0.752453	0.082087
95	0.380907	0.578578	0.575403	0.742252	0.083497
100	0.366626	0.56263	0.561086	0.725288	0.083855
105	0.353765	0.546456	0.542317	0.680133	0.079122
110	0.33923	0.523311	0.513355	0.613476	0.065958
115	0.319488	0.485339	0.472949	0.529713	0.047837

The relative humidity is calculated from the ratio of the vapor pressure of pure water ($pH_2O°$) at the drift wall temperature (T_{DW}) to the vapor pressure of pure water at the waste package temperature (T_{WP}):

$$RH = pH_2O°(T_{DW})/pH_2O°(T_{WP})$$

Thermodynamic simulations of evaporation were conducted at various waste package temperatures (T_{WP} = 50, 70, 90, and 110 °C) were conducted using StreamAnalyzer 2.0 to determine the potential range in chemistry of waters contacting the waste packages. The input chemistry is the same as those listed in the table on page 156 of this notebook. It was assumed that evaporation occurs until the median relative humidity given in the above table is attained. The minimum values of relative humidity listed in the table were not used in the calculation because the ionic strength of the aqueous solutions frequently exceeded the valid range of the activity coefficient model of the StreamAnalyzer code and the program often did not converge.

The median relative humidity was used as a constraint in the StreamAnalyzer 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,

$$P_{Total} = Median_RH \times pH_2O°(T_{WP})$$

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)
50	0.762094452	0.12207	0.093029
55	0.729053299	0.15571	0.113521
60	0.700239677	0.196965	0.137923
65	0.676850287	0.247171	0.167298
70	0.656695885	0.307827	0.202149
75	0.638220581	0.380599	0.242906
80	0.621741631	0.467334	0.290561
85	0.606644858	0.570063	0.345826
90	0.592229762	0.69101	0.409237
95	0.578578318	0.832599	0.481724
100	0.562630197	0.997457	0.561199
105	0.546455612	1.18842	0.649419
110	0.523311368	1.40854	0.737105
115	0.485339356	1.66108	0.806187

The StreamAnalyzer files that have the input and output information are included in a CD that accompanies this notebook. The filenames are:

1. StreamAnalyzer YM Waters with Br&F temp=110 C P=0.737105 atm Median RH.sta
2. StreamAnalyzer YM Waters with Br&F temp=90 C P=.409237 atm Median RH.sta
3. StreamAnalyzer YM Waters with Br&F temp=70 C P=.202149 atm Median RH.sta
4. StreamAnalyzer YM Waters with Br&F temp=50 C P=.093029 atm Median RH.sta
5. YM Pore Waters with Br&F Temp=110C_P=0.737105 atm Median RH.xls
6. YM Pore Waters with Br&F Temp=90C_P=0.409237 atm Median RH.xls
7. YM Pore Waters with Br&F Temp=70C_P=0.202149 atm Median RH.xls
8. YM Pore Waters with Br&F Temp=50C_P=0.093029 atm Median RH.xls

For the TPA 5.0 abstraction, the following chemistry information was provided to O. Pensado in the file "Brine chemistry for TPA 5.0 abstraction.xls". The information in that file is given in the following four tables:

(the rest of this page is left blank)

Temperature = 110 °C						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2-15 w/ Br,F	Ca-Cl	6.64111	3.97E+01	6.35E-01	1.11E-09	0.00E+00
NRG-6/160.8 w/ Br,F	Ca-Cl	6.63709	4.00E+01	6.32E-01	1.77E-09	0.00E+00
NRG-6/171.0 w/ Br,F	Ca-Cl	7.86695	2.78E+01	1.05E+01	4.76E-07	0.00E+00
NRG-6/175.6 w/ Br,F	Ca-Cl	7.4771	9.10361565	6.49569571	7.24E-07	0.00E+00
SD-12/296.1 w/ Br,F	Ca-Cl	7.41087	37.8477742	0.87792716	1.08E-07	0.00E+00
SD-6/471.3 w/ Br	Ca-Cl	7.40034	9.64759234	7.01521356	7.14E-07	0.00E+00
SD-9/114.1 w/ Br,F	Ca-Cl	5.55867	13.2781128	0	2.29E-10	2.89872171
SD-9/135.1 w/ Br,F	Ca-Cl	5.6509	9.92543345	0.01239598	9.51E-10	0.00010066
SD-9/94.2 w/ Br & F	Ca-Cl	6.7031	36.3289926	0.64948852	1.58E-09	0.00E+00
UZ-16/1643.4 w/ Br,F	Ca-Cl	7.32205	35.0934367	0.63009848	1.03E-07	0.00E+00
UZ-14/1277.7 w/ Br,F	Ca-Cl	7.37809	3.75E+01	6.54E-01	8.73E-08	0.00E+00
SD-6/412.2 w/ Br	Neutral	8.00715	3.22244738	12.7018953	1.95E-05	0
SD-6/443.5 w/ Br	Neutral	8.36668	2.93572785	13.0290492	5.13E-05	0
SD-6/507.5 w/ Br	Neutral	6.18036	3.01962969	9.24947975	2.48E-07	1.6843E-09
SD-6/1509.9 w/ Br	Neutral	10.4947	5.32300038	0.97110741	1.78E-01	0.00694562
SD-7/370.3 w/ Br,F	Neutral	6.74764	9.99789565	0.00057333	1.36E-08	0.00023746
SD-9/176.2 w/ Br,F	Neutral	8.21384	2.20203772	6.91513545	3.13E-05	5.0887E-07
UZ-14/85.2-85.6 w/ Br,F	Neutral	7.35273	4.5719518	6.15540705	2.39E-06	4.3016E-09
UZ-14/147.7 w Br,F	Neutral	7.38592	5.92378094	5.52648353	1.36E-06	4.1711E-12
NRG-6/244.6 w/ Br,F	Neutral	8.46146	2.67E+00	1.08E+01	3.61E-05	2.02E-11
NRG-6/255.9 w/ Br,F	Neutral	6.18621	2.6763953	10.255875	1.82E-07	2.0986E-10
UZ-14/178.1 w/ Br,F	Neutral	8.04871	39.5508837	1.0991E-27	1.15E-06	0.5280225
UZ-14/1258.5 w/ Br,F	Alkaline	10.5502	2.42471418	7.55117303	3.35E-01	7.4732E-09
UZ-14/1409.4 w/ Br,F	Alkaline	10.5041	2.37E+00	4.11E+00	2.16E-01	2.48E-05
UZ-14/1542.3 w/ Br,F	Alkaline	10.3455	2.26592248	5.51222344	2.53E-01	1.3703E-06
UZ-14/1825.8 w/ Br,F	Alkaline	10.4674	2.71653637	5.5129891	3.24E-01	3.1554E-06
UZ-14/2014.7 w/ Br,F	Alkaline	10.295	2.50093492	2.74851093	2.19E-01	0.00019233
UZ-16/1343.7 w/ Br,F	Alkaline	10.7807	3.16942659	5.45679415	4.00E-01	5.5233E-06
WT-24/1937.0 w/ Br	Alkaline	10.659	5.69542964	0.19903926	1.78E-01	0.02078851
NRG-6/219.9 w/Br,F	Alkaline	10.5138	2.96E+00	9.54E+00	2.05E-01	4.25E-10
NRG-7a/460.25 w/ Br,F	Alkaline	10.6966	5.76810807	0.45535351	1.79E-01	0.0126878
SD-12/1495.5 w/ Br,F	Alkaline	10.784	2.75811284	4.03650229	2.83E-01	3.6605E-05
SD-6/522.5 w/ Br	Alkaline	9.7496	3.74336711	0.00748011	9.44E-03	0.86938392

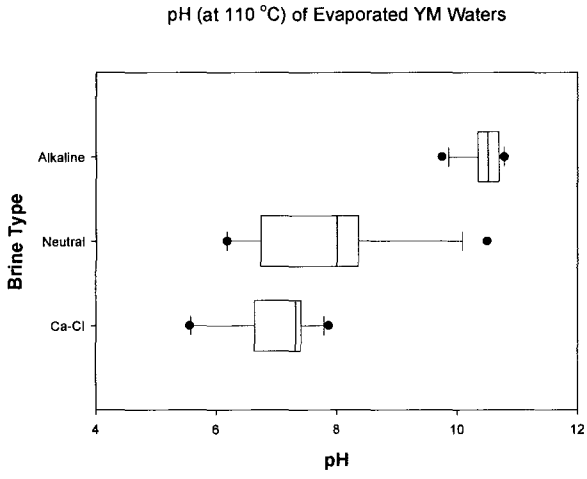
Temperature = 90 °C						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2-15 w/ Br,F	Ca-Cl	6.18744	9.25E+00	2.39E-02	5.83E-09	2.20E-04
NRG-6/160.8 w/ Br,F	Ca-Cl	6.24534	9.69E+00	2.82E-02	1.15E-08	1.77E-04
NRG-6/171.0 w/ Br,F	Ca-Cl	9.57917	1.37E+01	1.03E+00	2.37E-03	2.00E-04
NRG-6/175.6 w/ Br,F	Ca-Cl	7.54927	8.172662	4.811359	1.18E-06	1.51E-07
SD-12/296.1 w/ Br,F	Ca-Cl	6.56823	9.58E+00	2.57E-02	5.74E-08	9.70E-05
SD-6/471.3 w/ Br	Ca-Cl	7.48352	8.54E+00	5.17E+00	1.27E-06	3.56E-07
SD-9/114.1 w/ Br,F	Ca-Cl	6.13439	8.44E+00	2.18E-02	4.84E-09	2.31E-04
SD-9/135.1 w/ Br,F	Ca-Cl	6.17663	8.65E+00	2.14E-02	6.81E-09	1.96E-04
SD-9/94.2 w/ Br & F	Ca-Cl	6.21361	8.70E+00	1.19E-02	6.77E-09	2.58E-04
UZ-16/1643.4 w/ Br,F	Ca-Cl	7.26895	3.25E+01	7.19E-01	1.18E-07	0.00E+00
UZ-14/1277.7 w/ Br,F	Ca-Cl	6.72074	9.17E+00	2.03E-02	6.90E-08	2.16E-04
SD-6/412.2 w/ Br	Neutral	8.19343	3.807495	2.05E-06	2.31E-05	2.49E-12
SD-6/443.5 w/ Br	Neutral	8.47053	3.580219	8.71371	4.82E-05	5.18E-06
SD-6/507.5 w/ Br	Neutral	6.35063	3.710476	5.649634	2.24E-07	0.000132
SD-6/1509.9 w/ Br	Neutral	10.7568	5.700423	0.022076	5.23E-01	0.178909
SD-7/370.3 w/ Br,F	Neutral	6.98632	8.675025	0.000896	4.94E-08	0.000317
SD-9/176.2 w/ Br,F	Neutral	8.25226	2.765687	0.999545	2.45E-05	0.015131
UZ-14/85.2-85.6 w/ Br,F	Neutral	7.4601	4.782382	4.496022	2.94E-06	8.15E-06
UZ-14/147.7 w Br,F	Neutral	7.46609	5.792164	4.036291	1.79E-06	4.09E-06
NRG-6/244.6 w/ Br,F	Neutral	8.57218	3.332362	7.381276	3.53E-05	1.97E-05
NRG-6/255.9 w/ Br,F	Neutral	6.35839	3.426562	6.290701	1.52E-07	5.52E-05
UZ-14/178.1 w/ Br,F	Neutral	6.5299	10.45002	0.01831	3.20E-08	4.26E-05
UZ-14/1258.5 w/ Br,F	Alkaline	10.5446	3.62E+00	3.93E+00	2.39E-01	2.03E-04
UZ-14/1409.4 w/ Br,F	Alkaline	10.3142	3.09E+00	2.27E+00	6.44E-02	1.44E-03
UZ-14/1542.3 w/ Br,F	Alkaline	10.5714	3.12E+00	1.60E+00	5.30E-01	2.53E-03
UZ-14/1825.8 w/ Br,F	Alkaline	10.7067	3.30E+00	3.33E+00	7.08E-01	4.49E-04
UZ-14/2014.7 w/ Br,F	Alkaline	10.5329	3.03E+00	7.39E-01	4.60E-01	7.51E-03
UZ-16/1343.7 w/ Br,F	Alkaline	10.9629	3.84E+00	2.80E+00	8.55E-01	1.07E-03
WT-24/1937.0 w/ Br	Alkaline	10.8887	5.38E+00	9.90E-02	5.66E-01	2.91E-02
NRG-6/219.9 w/Br,F	Alkaline	10.3782	3.71E+00	6.27E+00	7.40E-02	1.85E-05
NRG-7a/460.25 w/ Br,F	Alkaline	10.9295	5.31E+00	3.02E-01	4.87E-01	2.07E-02
SD-12/1495.5 w/ Br,F	Alkaline	10.9207	4.73E+00	6.59E-01	8.52E-01	1.97E-02
SD-6/522.5 w/ Br	Alkaline	9.79484	4.06E+00	6.63E+00	7.97E-03	6.41E-05

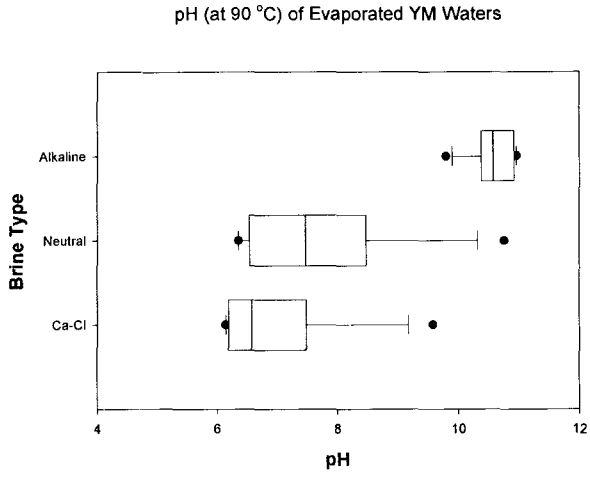
Temperature = 70 °C						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2-15 w/ Br,F	Ca-Cl	6.77652	7.923908647	0.043520341	4.1539E-08	0.00048251
NRG-6/160.8 w/ Br,F	Ca-Cl	6.81505	8.183358132	0.054829589	7.7918E-08	0.000399244
NRG-6/171.0 w/ Br,F	Ca-Cl	7.43934	9.701266961	0.635979803	8.9944E-07	0.000704615
NRG-6/175.6 w/ Br,F	Ca-Cl	7.66142	7.385744463	3.292500127	1.7133E-06	0.000103318
SD-12/296.1 w/ Br,F	Ca-Cl	6.94964	8.047099478	0.05820912	2.299E-07	0.00026374
SD-6/471.3 w/ Br	Ca-Cl	7.61271	7.582994478	3.485647799	1.9739E-06	9.69783E-05
SD-9/114.1 w/ Br,F	Ca-Cl	6.70878	7.363579757	0.039736972	3.1666E-08	0.00054766
SD-9/135.1 w/ Br,F	Ca-Cl	6.76832	7.495073774	0.039991726	4.6847E-08	0.00045623
SD-9/94.2 w/ Br & F	Ca-Cl	6.78581	7.540198592	0.020784736	4.5337E-08	0.000562348
UZ-16/1643.4 w/ Br,F	Ca-Cl	6.9269	7.124706801	0.044373664	3.4645E-07	0.000339498
UZ-14/1277.7 w/ Br,F	Ca-Cl	7.06404	7.776578102	0.036860126	2.5856E-07	0.000450316
SD-6/412.2 w/ Br	Neutral	8.37131	4.593484045	4.961858031	2.5331E-05	0.000227495
SD-6/443.5 w/ Br	Neutral	8.62164	4.421773917	5.124374277	4.8913E-05	0.000493155
SD-6/507.5 w/ Br	Neutral	6.89062	4.535835128	3.13144194	5.271E-07	0.003276274
SD-6/1509.9 w/ Br	Neutral	10.8136	5.584450179	0.210876036	0.55249373	0.092917648
SD-7/370.3 w/ Br,F	Neutral	7.2907	7.46575966	0.001454541	1.7959E-07	0.000604647
SD-9/176.2 w/ Br,F	Neutral	8.46786	3.618936777	0.66211839	3.1216E-05	0.05135482
UZ-14/85.2-85.6 w/ Br,F	Neutral	7.61514	5.105605061	2.931578936	3.5437E-06	0.000104942
UZ-14/147.7 w Br,F	Neutral	7.59142	5.790308677	2.693790646	2.2484E-06	0.000146363
NRG-6/244.6 w/ Br,F	Neutral	8.73287	4.190596192	4.463343235	3.7245E-05	0.000607103
NRG-6/255.9 w/ Br,F	Neutral	6.8989	4.321282729	3.565467596	3.5285E-07	0.00166829
UZ-14/178.1 w/ Br,F	Neutral	6.94665	8.640401546	0.05142809	1.3758E-07	0.000150473
UZ-14/1258.5 w/ Br,F	Alkaline	10.2999	5.079707842	1.532623754	0.0458502	0.013454923
UZ-14/1409.4 w/ Br,F	Alkaline	10.2901	4.229537966	1.205196113	0.03463276	0.022777182
UZ-14/1542.3 w/ Br,F	Alkaline	10.7397	3.98469608	0.839297225	0.69125697	0.019759553
UZ-14/1825.8 w/ Br,F	Alkaline	10.846	4.170886405	1.597932944	0.82240033	0.009934383
UZ-14/2014.7 w/ Br,F	Alkaline	10.715	3.932993691	0.410584769	0.64188282	0.033650584
UZ-16/1343.7 w/ Br,F	Alkaline	11.0509	4.440095452	1.461943778	0.90323104	0.013415832
WT-24/1937.0 w/ Br	Alkaline	10.9829	5.318851177	0.046538608	0.77123723	0.042359401
NRG-6/219.9 w/Br,F	Alkaline	10.2487	4.546197298	3.706550237	0.02319205	0.000600903
NRG-7a/460.25 w/ Br,F	Alkaline	11.1318	3.306054442	0.219835083	1.01061214	0.054384573
SD-12/1495.5 w/ Br,F	Alkaline	10.9274	5.109967589	0.557536128	0.45851187	0.043263584
SD-6/522.5 w/ Br	Alkaline	9.89564	4.809280148	3.708158076	0.00766036	0.001905326

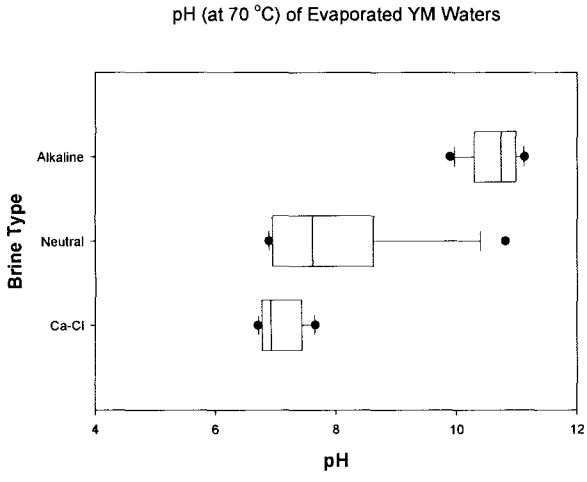
Temperature = 50 °C						
			Concentration (moles per kg H2O)			
Sample Name	Brine Type	pH	Cl-1	NO3-1	HCO3+CO3	SO4-2
NRG-6/158.2-15 w/ Br,F	Ca-Cl	7.53516	5.720138225	0.105883326	3.4276E-07	0.001357634
NRG-6/160.8 w/ Br,F	Ca-Cl	7.63996	5.806620386	0.141787367	8.0213E-07	0.001218489
NRG-6/171.0 w/ Br,F	Ca-Cl	7.80733	5.704713683	0.783850433	1.7955E-06	0.00079643
NRG-6/175.6 w/ Br,F	Ca-Cl	7.91261	5.143959464	1.191438837	2.4814E-06	0.000573233
SD-12/296.1 w/ Br,F	Ca-Cl	7.6005	5.538456813	0.21207298	1.4565E-06	0.001280899
SD-6/471.3 w/ Br	Ca-Cl	7.89264	5.17349807	1.371449397	3.0814E-06	0.000514318
SD-9/114.1 w/ Br,F	Ca-Cl	7.53077	5.609830208	0.089474082	4.1762E-07	0.002788417
SD-9/135.1 w/ Br,F	Ca-Cl	7.62959	5.650293985	0.090085493	7.017E-07	0.002579274
SD-9/94.2 w/ Br & F	Ca-Cl	7.53807	5.5711157	0.047609051	4.0086E-07	0.001793662
UZ-16/1643.4 w/ Br,F	Ca-Cl	7.63683	5.449943128	0.127039073	2.9247E-06	0.00245382
UZ-14/1277.7 w/ Br,F	Ca-Cl	7.62502	5.60927474	0.088875483	1.388E-06	0.00166614
SD-6/412.2 w/ Br	Neutral	8.60223	3.499333329	2.999823146	3.2276E-05	0.000715808
SD-6/443.5 w/ Br	Neutral	8.96264	3.330270233	3.166527389	8.8694E-05	0.002457586
SD-6/507.5 w/ Br	Neutral	7.7164	3.273227929	2.129759651	3.0514E-06	0.013661051
SD-6/1509.9 w/ Br	Neutral	10.3711	4.852456274	0.040224361	0.04587474	0.371988913
SD-7/370.3 w/ Br,F	Neutral	7.73591	5.469694658	0.002931841	7.2208E-07	0.001642894
SD-9/176.2 w/ Br,F	Neutral	8.8653	4.900619973	0.063982873	6.856E-05	0.541845647
UZ-14/85.2-85.6 w/ Br,F	Neutral	7.97502	5.142300356	0.698934594	6.1057E-06	0.002510755
UZ-14/147.7 w Br,F	Neutral	7.9911	5.402182968	0.48541692	4.411E-06	0.002994079
NRG-6/244.6 w/ Br,F	Neutral	9.0434	4.204211291	1.738631944	6.0884E-05	0.018089455
NRG-6/255.9 w/ Br,F	Neutral	7.86157	4.986619068	0.734271514	3.0071E-06	0.134951452
UZ-14/178.1 w/ Br,F	Neutral	7.82064	5.615552832	0.243274789	1.8266E-06	0.001894441
UZ-14/1258.5 w/ Br,F	Alkaline	10.116	4.804166874	0.411871446	0.01014375	0.248189321
UZ-14/1409.4 w/ Br,F	Alkaline	10.5424	4.251020304	0.12709897	0.07240391	0.581770074
UZ-14/1542.3 w/ Br,F	Alkaline	10.9988	2.941196684	0.297397542	1.36329191	0.152849423
UZ-14/1825.8 w/ Br,F	Alkaline	11.0655	3.101748912	0.798724467	1.28764657	0.08567355
UZ-14/2014.7 w/ Br,F	Alkaline	10.9491	3.936744373	0.109346377	1.08811641	0.158864171
UZ-16/1343.7 w/ Br,F	Alkaline	11.057	4.05821159	0.645061795	0.42976757	0.108805957
WT-24/1937.0 w/ Br	Alkaline	11.0904	4.091391498	0.028043999	0.67867295	0.113308968
NRG-6/219.9 w/Br,F	Alkaline	10.2985	4.244327073	1.301927416	0.01490302	0.036846195
NRG-7a/460.25 w/ Br,F	Alkaline	11.3267	2.60611987	0.193862439	1.20659837	0.086400016
SD-12/1495.5 w/ Br,F	Alkaline	10.8059	3.674509292	0.238567932	0.14365339	0.512138047
SD-6/522.5 w/ Br	Alkaline	9.81708	3.484100915	2.379767478	0.00286886	0.008519008

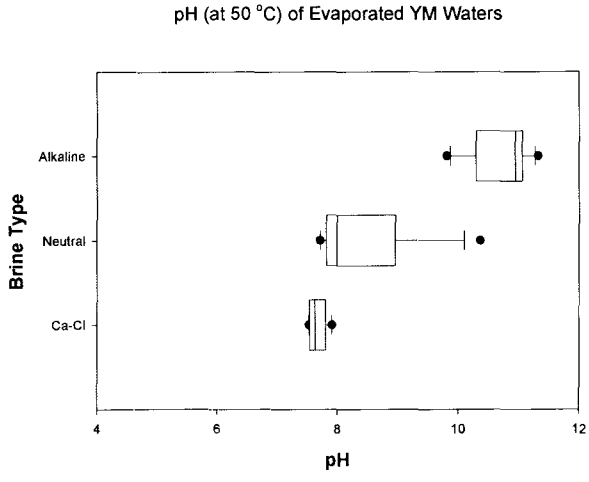
April 5, 2007

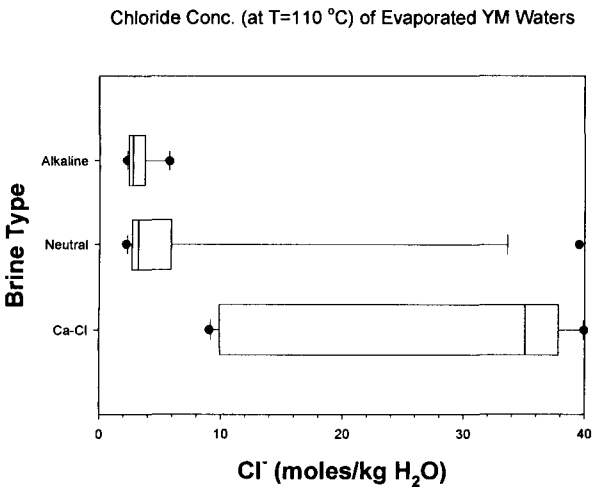
The following figures compare the pH, Cl, and inhibitor/Cl ratio calculated at 110, 90, 70, and 50 C (total pressure corresponding to median RH):

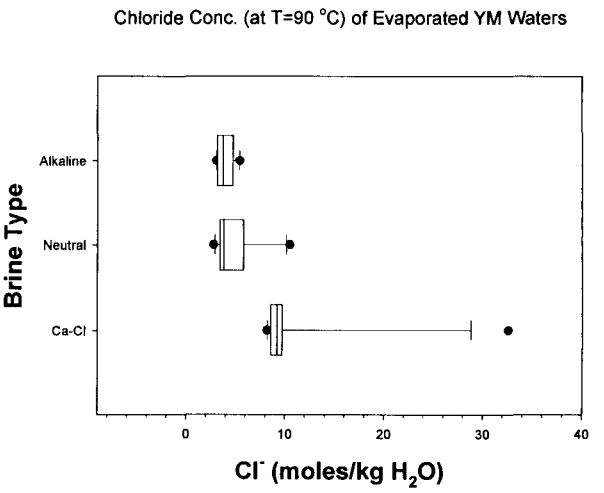


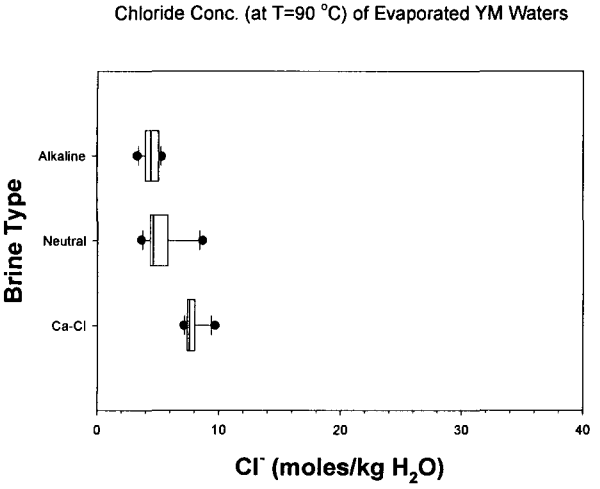


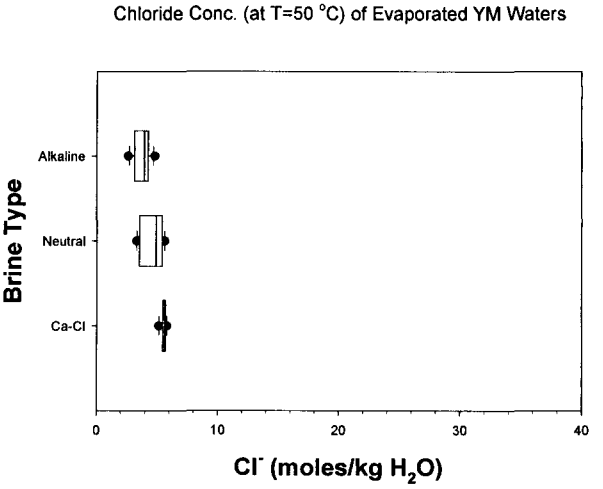


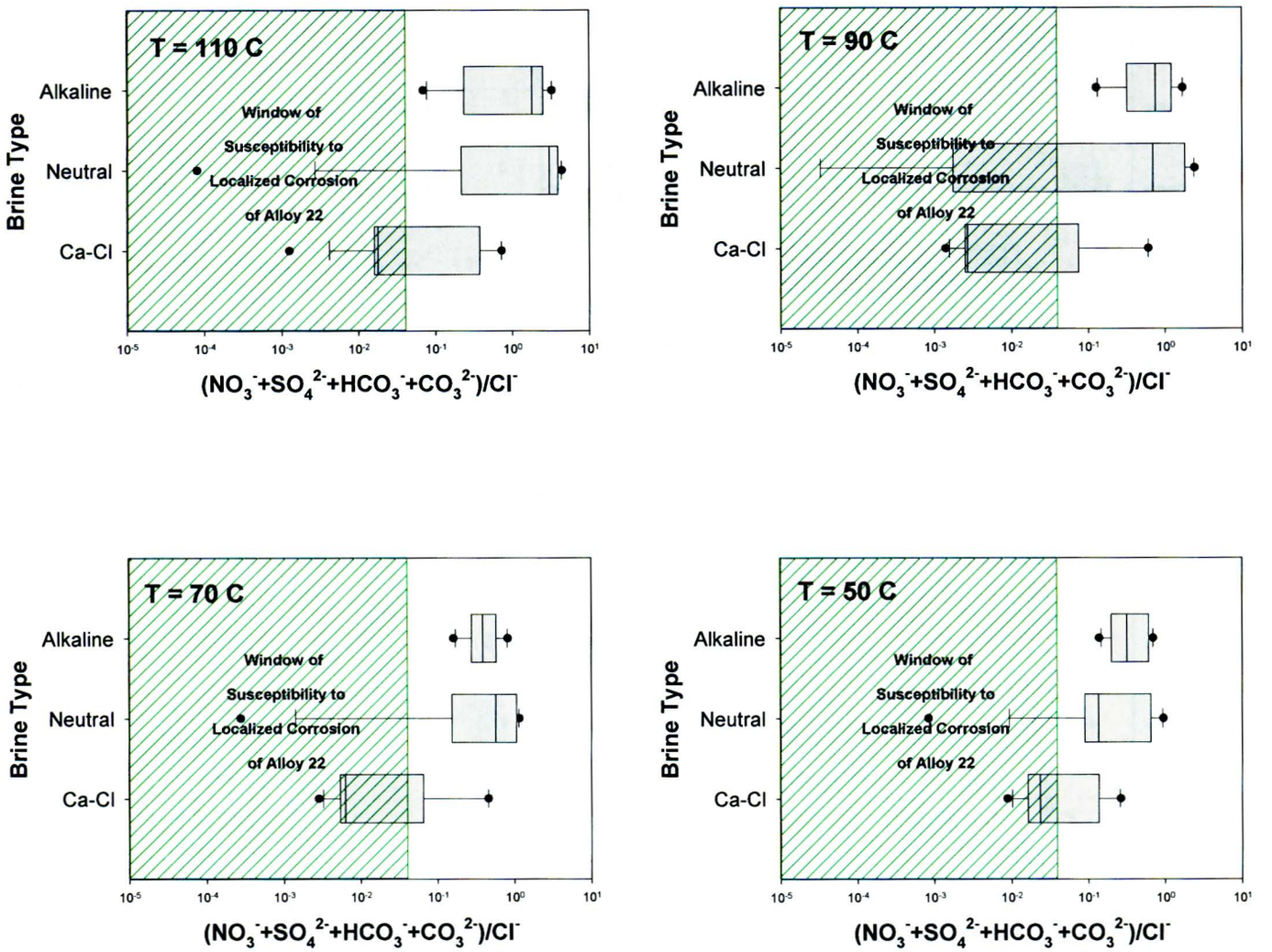



Chloride Conc. (at T=110 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0
10
20
30
40
Cl⁻ (moles/kg H2O)

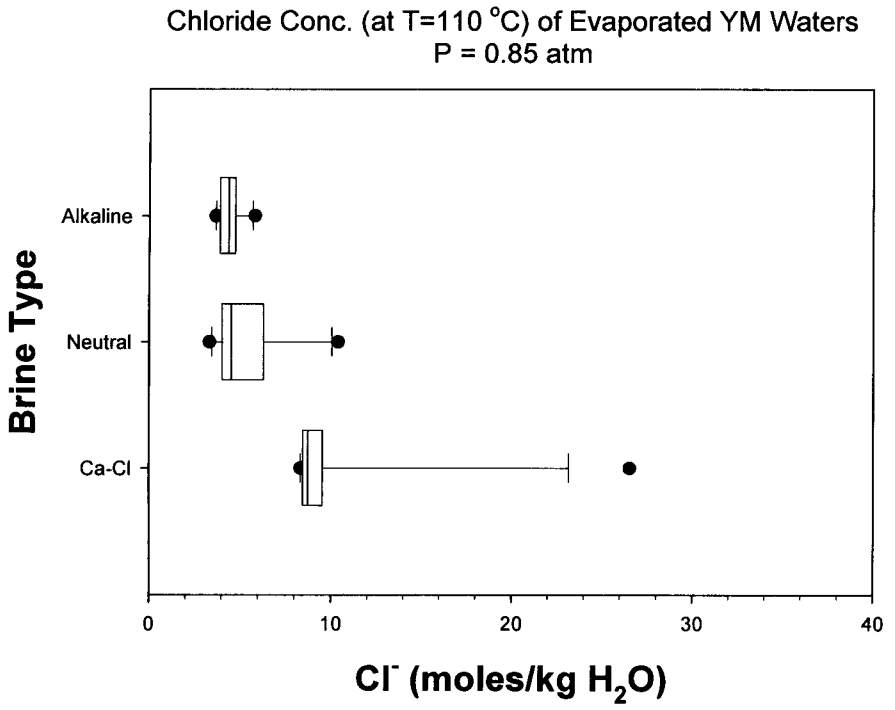

Chloride Conc. (at T=90 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0
10
20
30
40
Cl⁻ (moles/kg H2O)

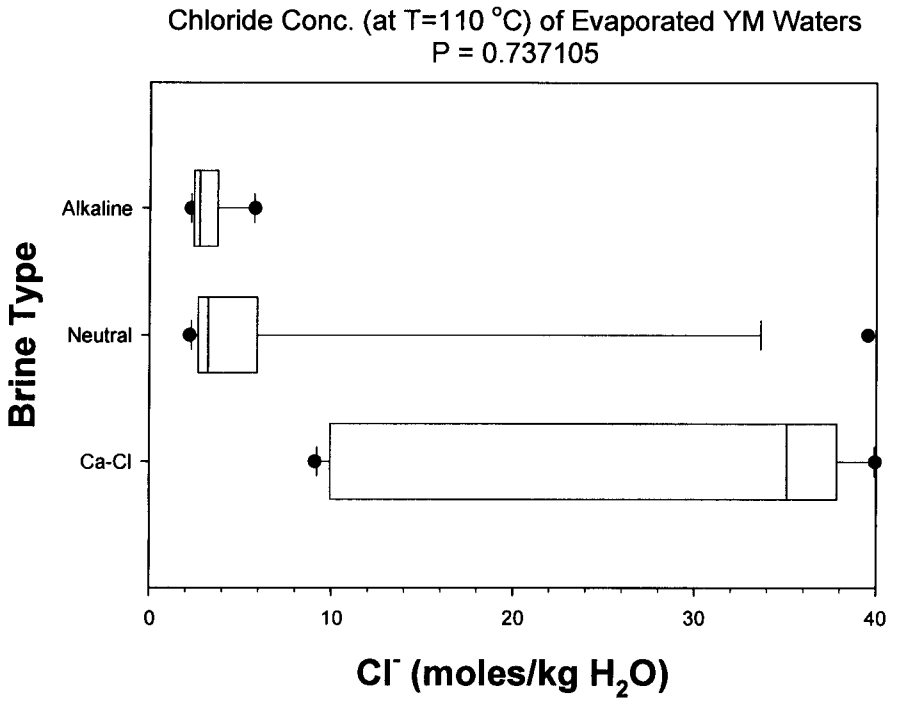

Chloride Conc. (at T=90 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0
10
20
30
40
Cl⁻ (moles/kg H2O)

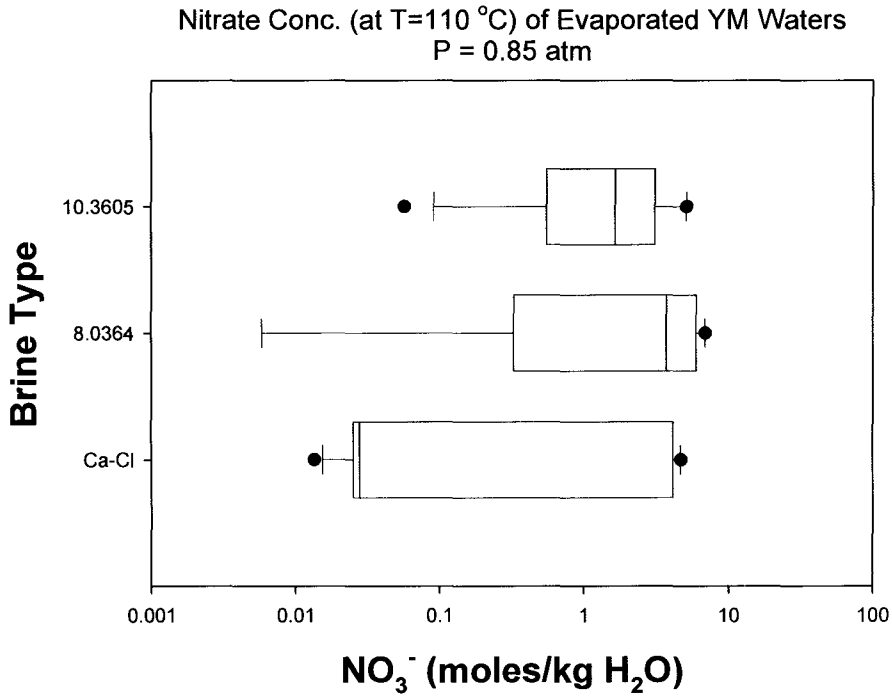

Chloride Conc. (at T=50 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0
10
20
30
40
Cl⁻ (moles/kg H2O)

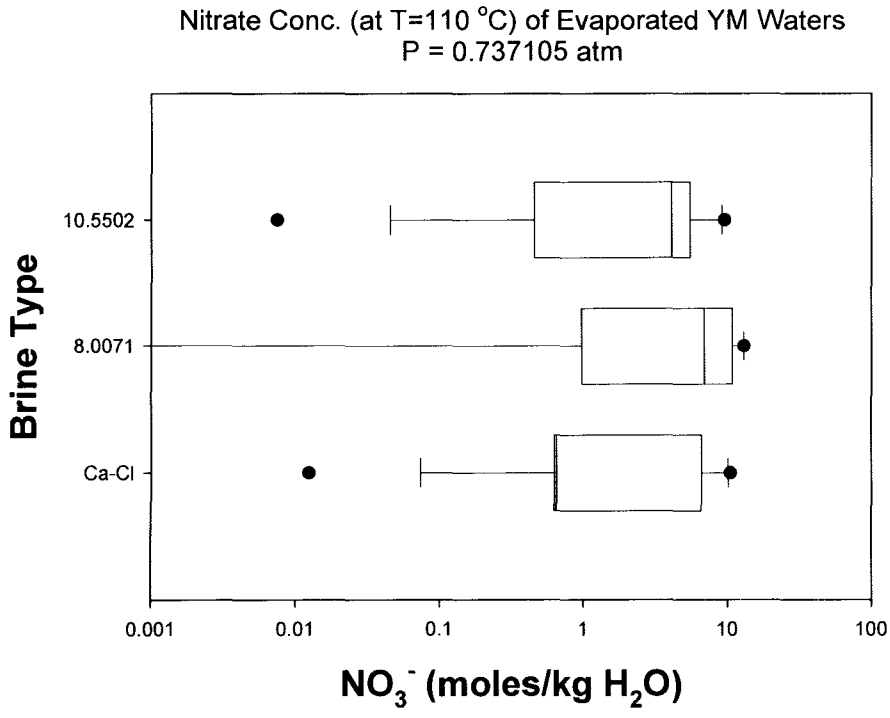

T = 110 C
T = 90 C
T = 70 C
T = 50 C
Brine Type
Alkaline
Neutral
Ca-Cl
Window of
Susceptibility to
Localized Corrosion
of Alloy 22
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1}
$(NO_3^- + SO_4^{2-} + HCO_3^- + CO_3^{2-})/Cl^-$

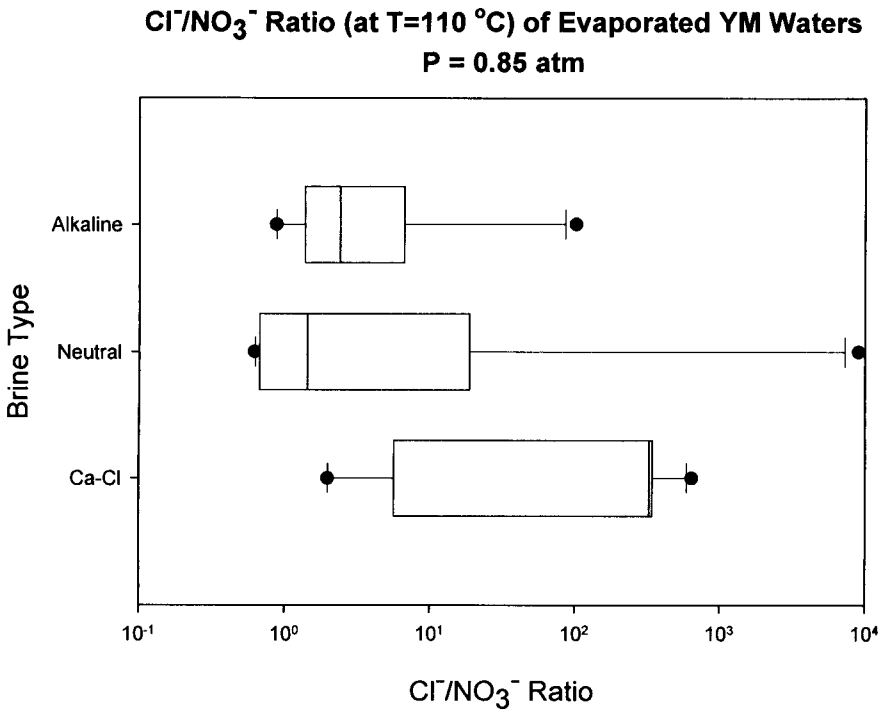
The following is a comparison of the Cl and NO3 concentrations and Cl/NO3 ratio calculated at 110 °C at two values of total pressure: 0.85 and 0.737105 atm, corresponding to relative humidities of 0.61 and 0.53, respectively. The figures show that at the lower total pressure (and lower relative humidity – a drier system), the brine that forms by evaporation is more benign to Alloy 22 (higher NO3 concentration and lower Cl/NO3 ratio), even though the Cl concentration is higher.

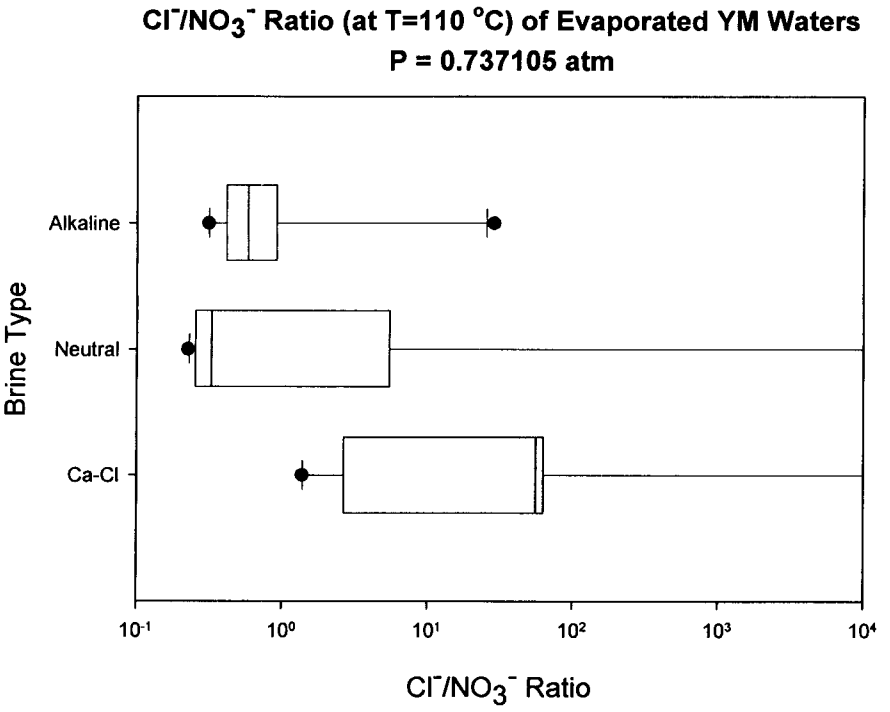




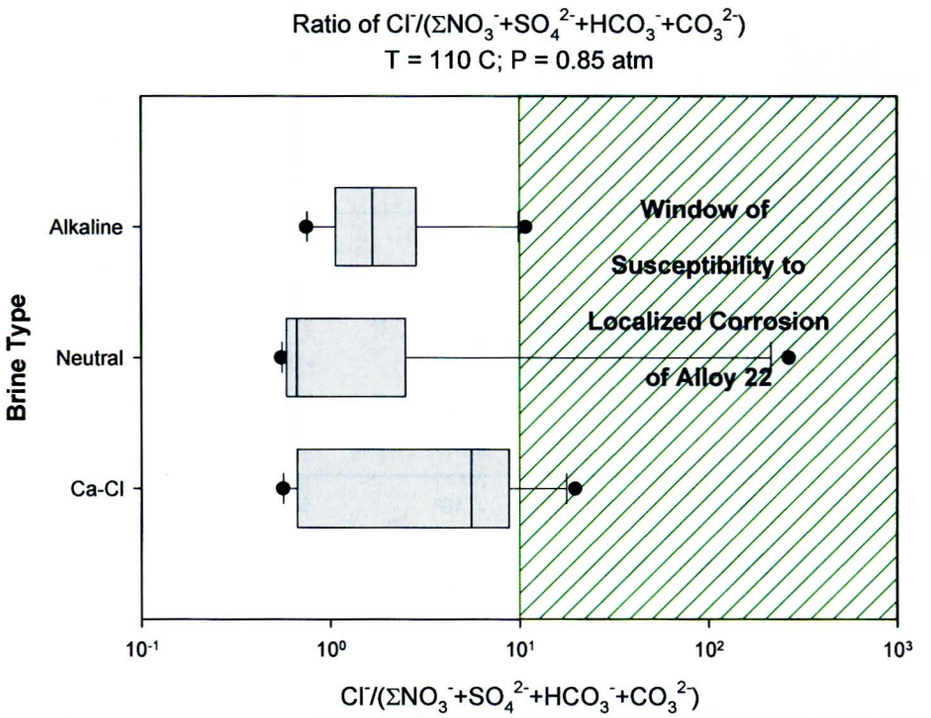

Nitrate Conc. (at T=110 °C) of Evaporated YM Waters
P = 0.85 atm
Brine Type
10.3605
8.0364
Ca-Cl
0.001
0.01
0.1
1
10
100
NO3- (moles/kg H2O)

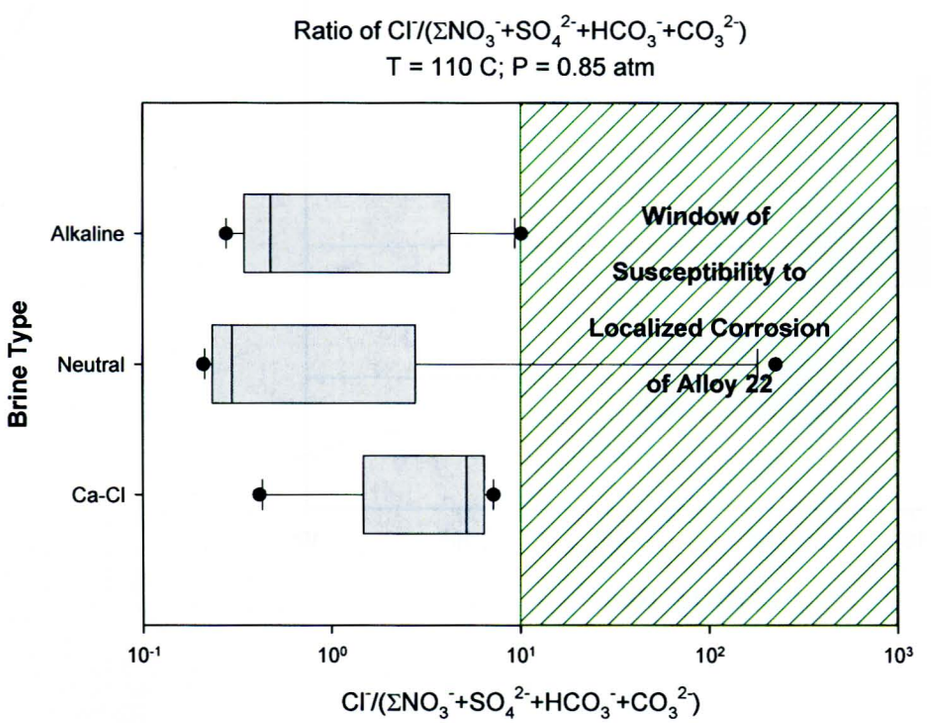

Nitrate Conc. (at T=110 °C) of Evaporated YM Waters
P = 0.737105 atm
Brine Type
10.5502
8.0071
Ca-Cl
0.001
0.01
0.1
1
10
100
NO3- (moles/kg H2O)


Cl⁻/NO3⁻ Ratio (at T=110 °C) of Evaporated YM Waters
P = 0.85 atm
Brine Type
Alkaline
Neutral
Ca-Cl
10-1
100
101
102
103
104
Cl⁻/NO3⁻ Ratio

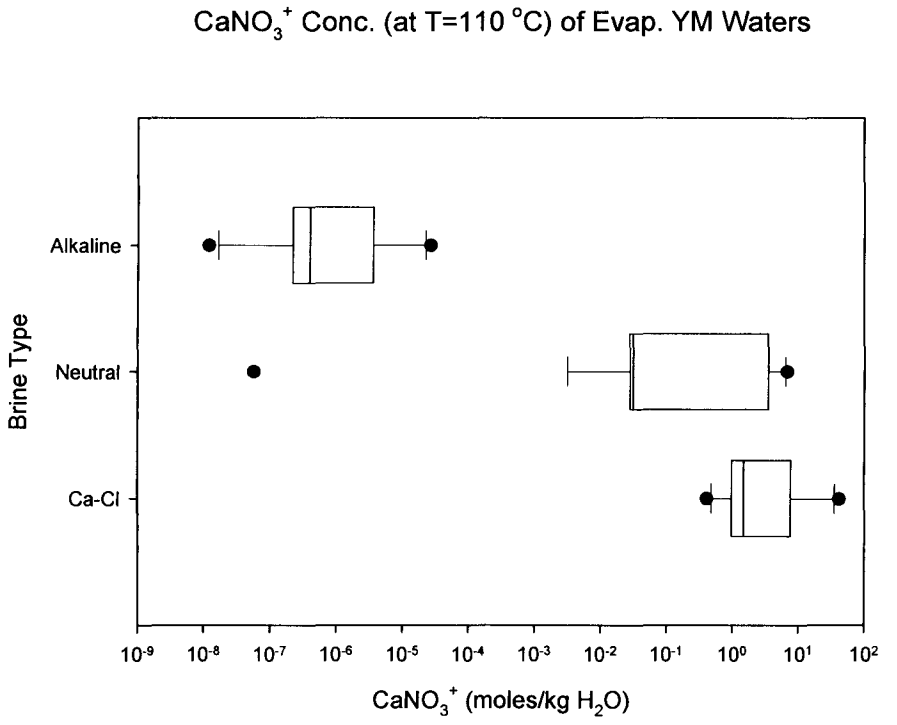

Cl⁻/NO3⁻ Ratio (at T=110 °C) of Evaporated YM Waters
P = 0.737105 atm
Brine Type
Alkaline
Neutral
Ca-Cl
10-1
100
101
102
103
104
Cl⁻/NO3⁻ Ratio

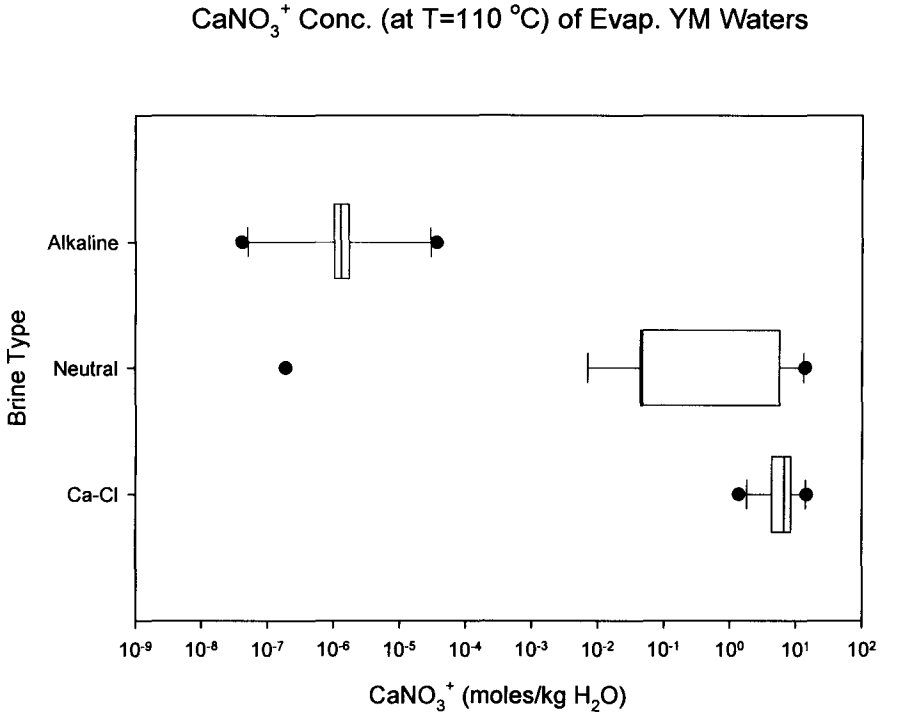
The following is a comparison of the ratio of Cl/(Total NO3+SO4 +HCO3+CO3) calculated at 110 °C at 0.85 and 0.737105 atm. In these cases, total NO3 refers to the sum of all dissolved nitrate-bearing species [NO_3^-, $NaNO_3$(aq), and $CaNO_3^+$].





The following is a comparison of $CaNO3^+$ concentration calculated at 110 °C at 0.85 and 0.737105 atm.





April 18, 2007

MessageFrom: Pavan Shukla [pshukla@cnwra.swri.edu]
Sent: Monday, April 16, 2007 4:48 PM
To: rpabalan@cnwra.swri.edu
Subject: RE: List of potential dust deliquescent brines

Between 120 to 170 degree Celsius.

-----Original Message-----
From: Bobby Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Monday, April 16, 2007 4:47 PM
To: 'Pavan Shukla'
Subject: RE: List of potential dust deliquescent brines

what temperature range?

-----Original Message-----
From: Pavan Shukla [mailto:pshukla@cnwra.swri.edu]
Sent: Monday, April 16, 2007 4:39 PM
To: Roberto Pabalan
Subject: List of potential dust deliquescent brines

Bobby,

Can you please provide me a list of potential dust deliquescence brines

that could form on the waste package surface? If possible, please provide the

of electrolyte conductivity as a function of brine temperature. This information will

be used to determine the cathodic capacity of oxygen reduction reaction.

Sincerely

Pavan K. Shukla
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute
6220 Culebra Road
San Antonio, Texas, 78238-5166
Phone: 210-522-6534
Fax: 210-522-5155

Temp, C	Spec. conductivity, 1/(ohm-cm)	Conc. O2,aq (ppm) at a PO2 of 0.21 atm	DRH (%)	Solids present	NaCl conc (molal)	NaNO3 conc (molal)
120	0.03546	0.334	26.7	NaCl+NaNO3+KNO3	2.53	81.0
130	0.03348	0.347	22.2	NaCl+NaNO3+KNO3	2.91	103.5
140	0.03152	0.365	18.2	NaCl+NaNO3+NaNO3·KNO3	3.53	131.1
150	0.03818	0.386	17.7	NaCl+NaNO3+NaNO3·KNO3	4.07	131.2
160	0.04193	0.412	16.5	NaCl+NaNO3+NaNO3·KNO3	4.80	139.2
170	0.04230	0.443	14.6	NaCl+NaNO3+NaNO3·KNO3	5.88	157.4

*Calculations of specific conductivity, DRH, composition, and saturated solids were done using StreamAnalyzer Version 2.0. The NaCl concentration given in the above table was assumed equal to the chloride ion concentration from the StreamAnalyzer Version 2.0 output. The NaNO3 concentration was assumed equal to the nitrate ion concentration from the StreamAnalyzer output. The NaCl and NaNO3 concentrations in the last two columns were used as input for calculating the oxygen solubility using the equations presented in Tromans (1998, 2000).

May 22, 2007

Pavan Shukla requested that the oxygen diffusivities be calculated for the temperature and composition listed on page 184 of this notebook. StreamAnalyzer 2.0 was used to calculate the values, which are listed below. O2(g) concentration was set to 2.0E-4 moles in the StreamAnalyzer calculation.

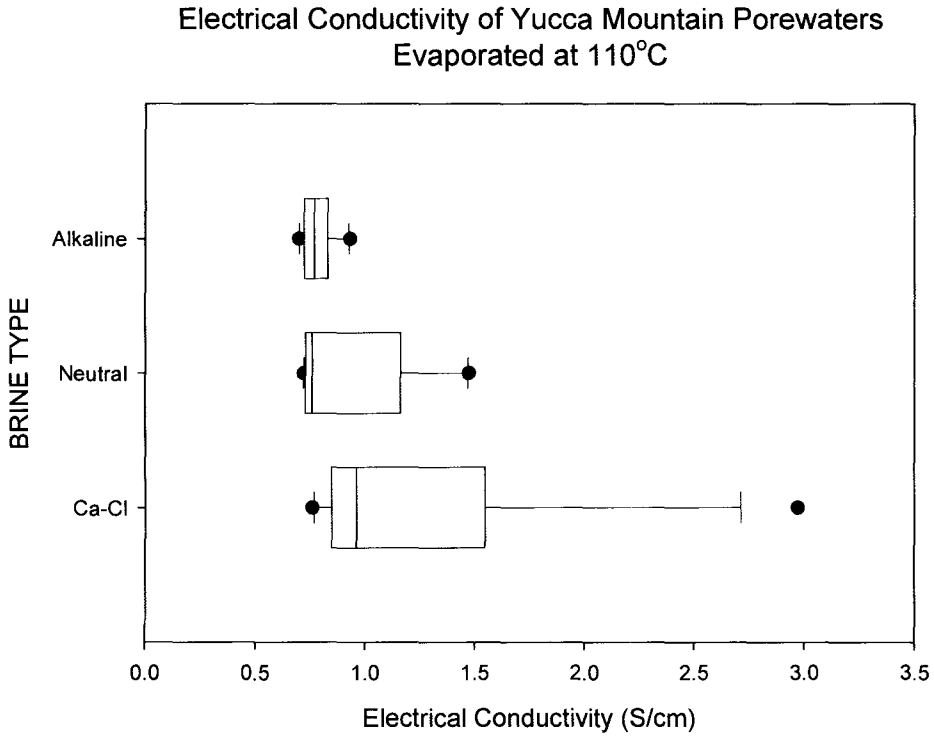
Temp, C	Spec. conductivity, 1/(ohm-cm)	Conc. O2,aq (ppm) at a PO2 of 0.21 atm	DRH (%)	Solids present	Oxygen diffusivity (m2/s)
120	0.03546	0.334	26.7	NaCl+NaNO3+KNO3	1.04e-19
130	0.03348	0.347	22.2	NaCl+NaNO3+KNO3	7.30320e-22
140	0.03152	0.365	18.2	NaCl+NaNO3+NaNO3·KNO3	1.53779e-18
150	0.03818	0.386	17.7	NaCl+NaNO3+NaNO3·KNO3	3.12809e-15
160	0.04193	0.412	16.5	NaCl+NaNO3+NaNO3·KNO3	6.14758e-13
170	0.04230	0.443	14.6	NaCl+NaNO3+NaNO3·KNO3	2.48701e-11

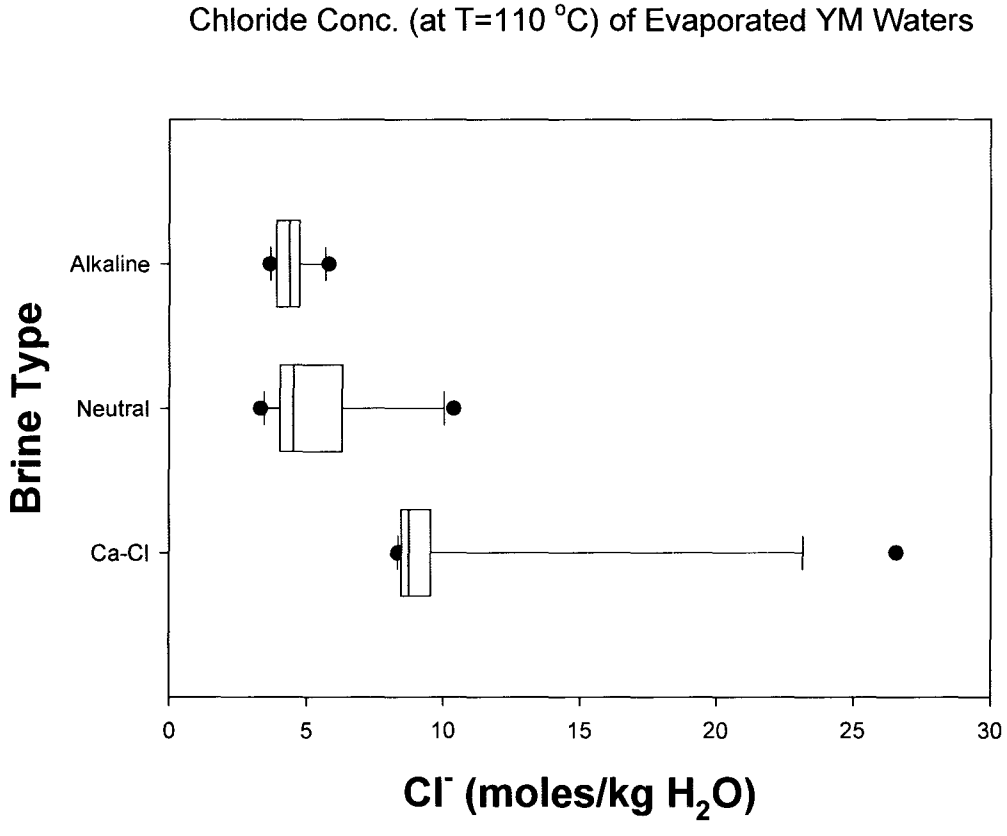
June 8, 2007

P. Shukla requested the electrical conductivity of YM porewaters that were evaporated at 110°C using StreamAnalyzer 2.0, for use in TPA 5.0 abstractions. The values were extracted from the StreamAnalyzer file and copied onto an Excel spreadsheet, then plotted in Sigmaplot. The values are shown below:

Sample Name	Brine type	Electrical Cond, specific (S/cm)	Cl- ion Concentration (moles/kg H2O)
NRG-6/158.2-15 w/ Br,F	Ca-Cl	0.8616	9.1475
NRG-6/160.8 w/ Br,F	Ca-Cl	0.962193	9.59
NRG-6/171.0 w/ Br,F	Ca-Cl	2.97181	26.543
NRG-6/175.6 w/ Br,F	Ca-Cl	1.68245	8.4656
SD-12/296.1 w/ Br,F	Ca-Cl	1.15509	9.5446
SD-6/471.3 w/ Br	Ca-Cl	1.54846	8.74
SD-9/114.1 w/ Br,F	Ca-Cl	0.801567	8.3679
SD-9/135.1 w/ Br,F	Ca-Cl	0.848008	8.59
SD-9/94.2 w/ Br & F	Ca-Cl	0.75965	8.62
UZ-16/1643.4 w/ Br,F	Ca-Cl	0.989974	8.34
UZ-14/1277.7 w/ Br,F	Ca-Cl	0.874263	9.1436
SD-6/412.2 w/ Br	Neutral	0.751349	4.52
SD-6/443.5 w/ Br	Neutral	0.727249	4.30
SD-6/507.5 w/ Br	Neutral	0.758611	4.27
SD-6/1509.9 w/ Br	Neutral	0.918309	6.15
SD-7/370.3 w/ Br,F	Neutral	0.719415	8.67
SD-9/176.2 w/ Br,F	Neutral	0.851722	3.33
UZ-14/85.2-85.6 w/ Br,F	Neutral	1.161	5.35
UZ-14/147.7 w Br,F	Neutral	1.47126	6.31
NRG-6/244.6 w/ Br,F	Neutral	0.734838	4.03
NRG-6/255.9 w/ Br,F	Neutral	0.724563	4.00
UZ-14/178.1 w/ Br,F	Neutral	1.45234	10.384
UZ-14/1258.5 w/ Br,F	Alkaline	0.745829	4.29
UZ-14/1409.4 w/ Br,F	Alkaline	0.799416	3.90
UZ-14/1542.3 w/ Br,F	Alkaline	0.790365	3.815
UZ-14/1825.8 w/ Br,F	Alkaline	0.741522	4.1212
UZ-14/2014.7 w/ Br,F	Alkaline	0.814209	3.66
UZ-16/1343.7 w/ Br,F	Alkaline	0.698596	4.70
WT-24/1937.0 w/ Br	Alkaline	0.877398	5.8126
NRG-6/219.9 w/Br,F	Alkaline	0.726373	4.38

The median values of electrical conductivity and Cl- concentration for the alkaline-type waters, calculated using Excel, are 0.778 S/cm and 0.238 moles/kg H2O, respectively. The pH of evaporated YM porewaters are given on page 173 of this notebook. The median pH for the alkaline-type waters, calculated using Excel, is 10.9.


Electrical Conductivity of Yucca Mountain Porewaters
Evaporated at 110°C
BRINE TYPE
Alkaline
Neutral
Ca-Cl
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
Electrical Conductivity (S/cm)


Chloride Conc. (at T=110 °C) of Evaporated YM Waters
Brine Type
Alkaline
Neutral
Ca-Cl
0
5
10
15
20
25
30
Cl⁻ (moles/kg H2O)

June 22, 2007

P. Shukla requested that the effective conductivity of brine films that form by salt deliquescence be calculated.

Used information from DOE document Analysis of Dust Deliquescence for FEP Screening ANL-EBS-MD-000074 REV 01 August 2005.

Also from C. Bryan presentation to NWTRB:
http://www.nwtrb.gov/meetings/2006/sept/bryan.pdf

- **Estimated amount and composition of dust on WPs**
  - **Atmospheric dust concentration (site-specific): 22 μg/m³ (typical)**
  - **Drift and ventilation design parameters**
  - **Upper-bound particle size (10 and 30 μm)**
  - **Deposition on first waste package in drift**
  - **Ventilation period: 50 years**
  - **Dry particle deposition model (Sehmel 1980)**
- **Estimate brine volume**
  - **Dust soluble salt content (site-specific): 10.5%**
  - **Ammonium minerals volatilize (~1/2 of total salts)**
  - **Thermodynamic modeling with Pitzer database**

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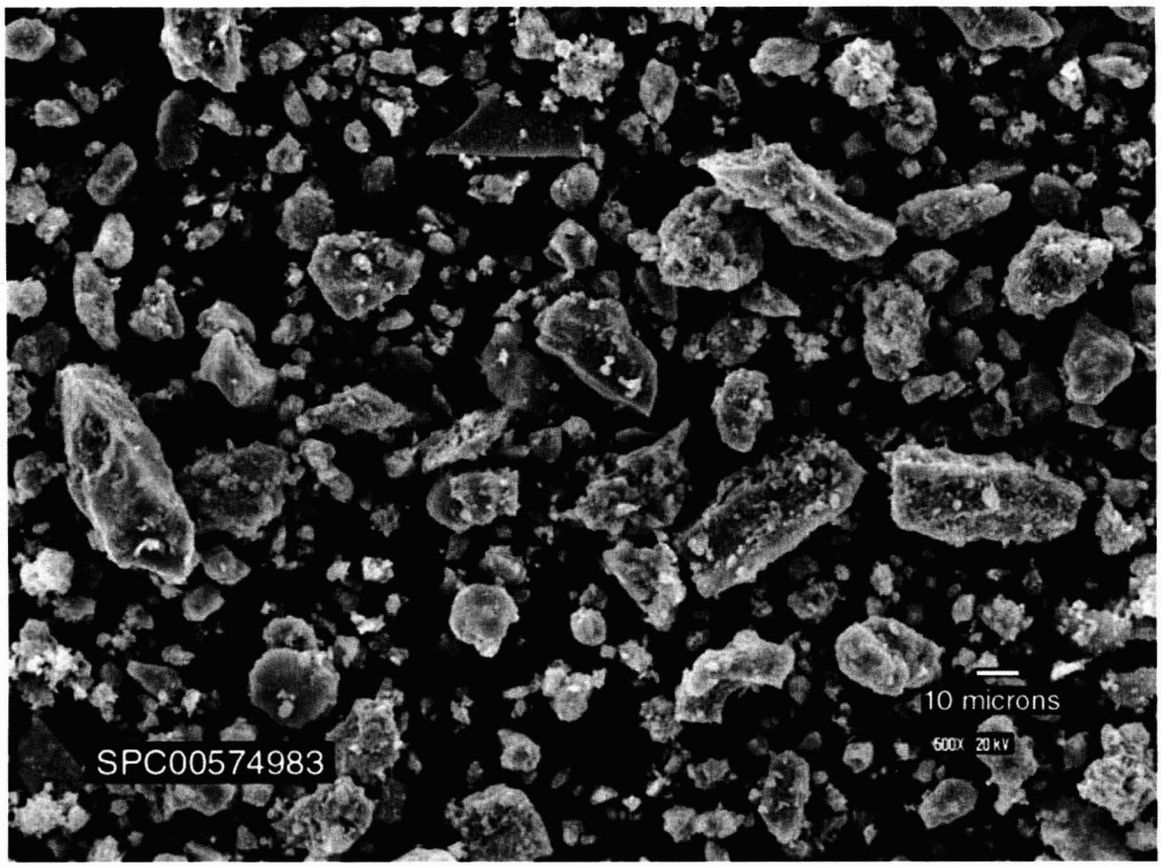
bryan_NWTRB_9/25-26/06.ppt
www.ocrwm.doe.gov
10

- **Upper bound for dust deposited: 26 mg/cm²**
  - **260 μm thick layer for bulk density 1 g/cm³**
  - **Rock dust may add mass, not soluble salts**
- **Upper bound brine volume: 1.8 μL/cm² (18 μm thick layer)**
  - **At 120°C; less volume at higher temperatures**
  - **Assumes all salts are internally mixed (no geometric isolation)**
  - **Average liquid saturation for dust layer ~ 11% for porosity of 60%**
- **Lower bound approx. 1 order of magnitude less at 200°C**

From M.Juckett viewgraphs from Goldschmidt 2006 showing range of dust particle size:

Tunnel Dust



Use 10 and 30 microns as estimated diameters for dust (consistent with M. Juckett samples).
Use 26 mg/cm^2 for amount of dust deposited on waste package.
Use density of 1 gm/cm^3.

Volume of sphere = 4/3 * Pi * r^3
Volume of cube = (2r)^3

1. For a 10 micrometer diameter sphere,
   - The volume of a spherical particle = 5.23E-16 m^3 = 5.23E-10 cm^3.
   - The volume of a cube = 1E-15 m^3 = 1E-9 cm^3

   Mass of one particle = density (gm/cm^3) × volume (cm^3)
   = 1 gm/cm^3 × 5.23E-10 cm^3 = 5.23E-10 gm.

   Assume each particle is in contact with other particles in cubic packing (but not closest packing, i.e., approximate the spherical volume by a cube).
   - Then the area of horizontal (square) surface occupied by each particle = (2r)^2 = (10E-6 m)^2 = 1E-10 m^2 = 1E-6 cm^2

Number of particles in 1 cm^2 of surface (based on 26E-3 gm/cm^2 deposited on waste package surface) = 26E-3 gm ÷ 5.23E-10 gm = **4.97E7 particles**

Assume each particle is in contact with other particles in cubic packing (but not closest packing, i.e., approximate the spherical volume by a cube)

- Then the area that can be covered (in one layer) by 4.97E7 particles is: 4.97E7 × 1E-10 m^2 = 4.97E-3 m^2 = 49.7 cm^2.
- Thus, to fit within a 1-cm^2 area, the number of layers need to be 50.
  (check calculation: area of one layer equals number of particles in one layer multiplied by horizontal area of each particle = (4.97E7 ÷ 49.7 × 1E-6 cm^2 = 1.00 cm^2)
- The volume of the rectangular space = # of layers × particle diameter × 1 cm^2 = 50 layers × 1.0E-3 cm × 1 cm^2 = 5.00E-2 cm^3.
- The volume of the 4.97E7 spherical particles = 4.97E7 × 5.23E-10 cm^3 = 2.60E-2 cm^3
- The volume of the pore space between the particles = 5.0E-2 – 2.60E-2 cm^3 = 2.40E-2 cm^3

Assume 10% of the dust comprises deliquescent salt (NaCl-NaNO3-KNO3 mixture) and that a brine forms by deliquescence of the salt mixture without affecting the volume of the solids previously calculated. What is the volume of the brine that forms on 1 cm^2 area on the waste package at 150°C?

- There are 26E-3 gm of dust in 1 cm^2 area. Ten percent of that is 2.6E-3 gm of NaCl-NaNO3-KNO3 salt mixture.
- The DRH of NaCl-NaNO3-KNO3 is 17.7 percent
- The calculated concentration of salts in solution at 150 C is 69.6 molal KNO3, 4.07 molal NaCl, 61.55 molal NaNO3.
- Assume 2.6E-3 gm salt mixture is placed inside a humidity chamber at 150 C, and the relative humidity in the chamber is raised from low to higher values. Theoretically, the salt will deliquesce at a relative humidity of 17.7 %. At the deliquescence point, a brine will form with 69.6 molal (moles/kgH2O) KNO3, 4.07 molal NaCl, 61.55 molal NaNO3. As the relative humidity is raised further, more salt will dissolve until the 2.6E-3 gm of salt present in the chamber is dissolved completely.
- **How much volume of solution is formed by the deliquescence of the salt?**
- In 1 kg of H2O, the amount of KNO3, NaCl, and NaNO3 would be 69.6, 4.07, and 61.55 moles/kgH2O, respectively. In terms of mass, it would be 7,037 g of KNO3, 238 g of NaCl, and 5,231 g NaNO3 dissolved in solution. The limited mass of the salt placed in the humidity chamber would determine the volume of brine that would form. For an initial total salt mass of 2.6E-3 g, there would be (2.6E-3 g ÷ (7,037+238+5,231) g) × 1000 g H2O = 2.08E-4 g H2O.
- The calculated density of the NaCl+KNO3+NaNO3 aqueous solution at 150 °C is 1.29 g/cm^3. The total weight of the solution is the weight of water plus the weight of solutes = 2.08E-4 g H2O + 2.6E-3 g salt = 2.81E-3 g solution. **The volume of this amount of brine is 2.81E-3 g ÷ 1.29 g/cm^3 <u>= 2.18E-3 cm^3</u>.**

The total pore space in between the spherical dust particles in the whole volume of dust is 2.4E-2 cm^3. There are 50 layers, so each layer has:

2.4E-2 cm^3 ÷ 50 = 4.8E-4 cm^3 of pore space. Therefore, the brine will occupy the pore space in: 2.18E-3 cm^3 ÷ 4.8E-4 cm^3 = 4.54 layers.

The specific conductivity of the brine without particles present is 0.0382 1/(ohm-cm). Using Bruggeman's equation (Agarwal et al., 2006; Modeling the Cathodic Region in Crevice Corrosion under a Thin Electrolyte Film Including Particulates; http://www.ocrwm.doe.gov/science/pdf/papers/46519.pdf:

$$k_{eff} = k(1-\phi_{particles})^{3/2}$$

Where keff is the effective conductivity of the brine, k is the equivalent conductivity of the brine without the dust particles present, and $\phi_{particles}$ is

$$\phi_{particles} = V_{particles}/(V_{solution} + V_{particles}) \text{ and}$$

$$(1-\phi_{particles}) = \phi_{solution} = V_{solution}/(V_{solution} + V_{particles})$$

- The 4.54 layers has a geometric volume of
  4.54 × 10.0E-4 cm × 1 cm^2 = 4.54E-3 cm^3
  and the brine has a volume of 2.18E-3 cm^3.

  Thus, $\phi_{solution}$ = 2.18E-3 cm^3 ÷ 4.54E-3 cm^3 = 0.480, and the effective conductivity of the NaCl-NaNO3-KNO3 brine is:
  0.0382 × 0.480 = 0.01834 1/(ohm-cm).

2. For a 30 micrometer diameter sphere,
   - The volume of a spherical particle = 1.41E-14 m^3 = 1.41E-8 cm^3.
   - The volume of a cube = 2.70E-14 m^3 = 2.70E-8 cm^3

   Mass of one particle = density (gm/cm^3) × volume (cm^3)
   = 1 gm/cm^3 × 1.41E-8 cm^3 = 1.41E-8 gm.

   Assume each particle is in contact with other particles in cubic packing (but not closest packing, i.e., approximate the spherical volume by a cube).
   - Then the area of horizontal (square) surface occupied by each particle = (2r)^2 = (30E-6 m)^2 = 9.00E-10 m^2 = 9.00E-6 cm^2

   Number of particles in 1 cm^2 of surface (based on 26E-3 gm/cm^2 deposited on waste package surface) = 26E-3 gm ÷ 1.41E-8 gm = 1.84E6 particles

   Assume each particle is in contact with other particles in cubic packing (but not closest packing, i.e., approximate the spherical volume by a cube)
   - Then the area that can be covered (in one layer) by 4.97E7 particles is: 1.84E6 × 9E-10 m^2 = 1.656E-3 m^2 = 16.56 cm^2.
   - Thus, to fit within a 1-cm^2 area, the number of layers need to be 16.56.
     (check calculation: area of one layer equals number of particles in one layer multiplied by horizontal area of each particle = (1.84E6 ÷ 16.56 × 9E-6 cm^2 = 1.00 cm^2)
   - The volume of the rectangular space = # of layers × particle diameter × 1 cm^2 = 16.56 layers × 3.0E-3 cm × 1 cm^2 = 4.97E-2 cm^3.
   - The volume of the 1.84E6 spherical particles = 1.84E6 × 1.41E-8 cm^3 =

2.59E-2 cm^3

- The volume of the pore space between the particles =
  4.97E-2 – 2.59E-2 cm^3 = 2.38E-2 cm^3

Assume 10% of the dust comprises deliquescent salt (NaCl-NaNO3-KNO3 mixture) and that a brine forms by deliquescence of the salt mixture without affecting the volume of the solids previously calculated. What is the volume of the brine that forms on 1 cm^2 area on the waste package at 150°C?

- There are 26E-3 gm of dust in 1 cm^2 area. Ten percent of that is 2.6E-3 gm of NaCl-NaNO3-KNO3 salt mixture.
- The DRH of NaCl-NaNO3-KNO3 is 17.7 percent
- The calculated concentration of salts in solution at 150 C is 69.6 molal KNO3, 4.07 molal NaCl, 61.55 molal NaNO3.
- Assume 2.6E-3 gm salt mixture is placed inside a humidity chamber at 150 C, and the relative humidity in the chamber is raised from low to higher values. Theoretically, the salt will deliquesce at a relative humidity of 17.7 %. At the deliquescence point, a brine will form with 69.6 molal (moles/kgH2O) KNO3, 4.07 molal NaCl, 61.55 molal NaNO3. As the relative humidity is raised further, more salt will dissolve until the 2.6E-3 gm of salt present in the chamber is dissolved completely.
- **How much volume of solution is formed by the deliquescence of the salt?**
- In 1 kg of H2O, the amount of KNO3, NaCl, and NaNO3 would be 69.6, 4.07, and 61.55 moles/kgH2O, respectively. In terms of mass, it would be 7,037 g of KNO3, 238 g of NaCl, and 5,231 g NaNO3 dissolved in solution. The limited mass of the salt placed in the humidity chamber would determine the volume of brine that would form. For an initial total salt mass of 2.6E-3 g, there would be (2.6E-3 g ÷ (7,037+238+5,231) g) × 1000 g H2O = 2.08E-4 g H2O.
- The calculated density of the NaCl+KNO3+NaNO3 aqueous solution at 150 °C is 1.29 g/cm^3. The total weight of the solution is the weight of water plus the weight of solutes = 2.08E-4 g H2O + 2.6E-3 g salt = 2.81E-3 g solution. **The volume of this amount of brine is 2.81E-3 g ÷ 1.29 g/cm^3 <u>= 2.18E-3 cm^3</u>.**

The total pore space in between the spherical dust particles in the whole volume of dust is 2.38E-2 cm^3. There are 16.56 layers, so each layer has:

2.38E-2 cm^3 ÷ 16.56 = 1.437E-3 cm^3 of pore space. Therefore, the brine will occupy the pore space in: 2.18E-3 cm^3 ÷ 1.437E-3 cm^3 = 1.52 layers.

The specific conductivity of the brine without particles present is 0.0382 1/(ohm-cm). Using Bruggeman's equation (Agarwal et al., 2006; Modeling the Cathodic Region in Crevice Corrosion under a Thin Electrolyte Film Including Particulates; http://www.ocrwm.doe.gov/science/pdf/papers/46519.pdf:

$$k_{eff} = k(1-\phi_{particles})^{3/2}$$

Where keff is the effective conductivity of the brine, k is the equivalent conductivity of the brine without the dust particles present, and $\phi_{particles}$ is

$$\phi_{particles} = V_{particles}/(V_{solution} + V_{particles})$$ **and**

$(1-\phi_{particles}) = \phi_{solution} = V_{solution}/(V_{solution} + V_{particles})$

- The 1.52 layers has a geometric volume of
  1.52 × 30.0E-4 cm × 1 cm^2 = 4.56E-3 cm^3
  and the brine has a volume of 2.18E-3 cm^3.

  Thus, $\phi_{solution}$ = 2.18E-3 cm^3 ÷ 4.56E-3 cm^3 = 0.478, and the effective conductivity of the NaCl-NaNO3-KNO3 brine is:
  0.0382 × 0.478 = 0.01826 1/(ohm-cm).

Summary:

Particle size (cm)	Dust layer thickness (cm)	Brine film thickness (cm)	Specific conductivity of NaCl-KNO3-NaNO3 brine (1/ohm-cm)	Effective conductivity of brine (1/ohm-cm)*
0.001	0.05 (50 dust layers)	0.00454 (4.54 dust layers)	0.0382	0.01834
0.003	1.34 (448 dust layers)	0.00456 (1.52 dust layers)	0.0382	0.01826
Temp = 150 °C; Relative humidity = 17.7 % Brine composition at the deliquescence point of the NaCl–KNO3–NaNO3 salt mixture: 69.6 molal (moles/kgH2O) KNO3, 4.07 molal NaCl, 61.55 molal NaNO3 *Calculated using Bruggeman's equation				

Entries into Scientific Notebook No. 679 for the period October 1, 2006, through September 30, 2007, have been made by

Roberto T. Pabalan / Date 7/6/2008

No original entry into this Scientific Notebook has been removed.

Roberto T. Pabalan / Date 7/6/2008

ELECTRONIC NOTEBOOK #679E

October 1, 2007 through February 29, 2008

20.14002.01.071

Roberto T. Pabalan

The entries in this electronic scientific notebook #679E document activities conducted during the period October 1, 2007, through September 30, 2008, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.14002.01.071).

October 16, 2007

Table taken and revised from page 183 of ESN#679E. The oxygen solubility values were recalculated because an error was found in the Excel spreadsheet provided by A.Jung.

Temp, C	Spec. conductivity, 1/(ohm-cm)	Conc. O2,aq (ppm) at a PO2 of 0.21 atm	DRH (%)	Solids present	NaCl conc (molal)	NaNO3 conc (molal)
120	0.03546	0.121	26.7	NaCl+NaNO3+KNO3	2.53	81.0
130	0.03348	0.092	22.2	NaCl+NaNO3+KNO3	2.91	103.5
140	0.03152	0.068	18.2	NaCl+NaNO3+NaNO3·KNO3	3.53	131.1
150	0.03818	0.065	17.7	NaCl+NaNO3+NaNO3·KNO3	4.07	131.2
160	0.04193	0.057	16.5	NaCl+NaNO3+NaNO3·KNO3	4.80	139.2
170	0.04230	0.044	14.6	NaCl+NaNO3+NaNO3·KNO3	5.88	157.4

*Calculations of specific conductivity, DRH, composition, and saturated solids were done using StreamAnalyzer Version 2.0 (Mixed-Solvent Electrolyte Model). The NaCl concentration given in the above table was assumed equal to the chloride ion concentration from the StreamAnalyzer Version 2.0 output. The NaNO3 concentration was assumed equal to the nitrate ion concentration from the StreamAnalyzer output. The NaCl and NaNO3 concentrations in the last two columns were used as input for calculating the oxygen solubility using the equations presented in Tromans (1998, 2000).

October 22, 2007

The following are comparisons of oxygen solubility in water and in NaCl solutions from various sources or codes.

Temp, C	*Tromans (2000)* *mol O2/kgH2O*	Tromans (2000) ppm O2 in pure H2O	Compare GWB 6.0 calc'n ppm O2 in pure H2O
273	*0.00046*	14.62	14.81
298	*0.00027*	8.59	8.49
333	*0.00018*	5.83	5.81
368	*0.00016*	5.24	5.18
373	*0.00016*	5.25	5.25
393	*0.00017*	5.46	5.41
433	*0.00021*	6.74	6.63
473	*0.00029*	9.35	8.98
493	*0.00035*	11.35	10.88
525	*0.00050*	15.96	15.31

Temp, C	*Millero et al. (2002)* *mol O2/kgH2O*	Millero et al. (2002) ppm O2 in pure water	Compare Tromans (2000) ppm O2 in pure water	Compare GWB 6.0 calc'n ppm O2 in pure water
5.12	*0.0003969*	12.70	12.79	12.92
15.14	*0.0003144*	10.06	10.25	10.35
25.12	*0.0002589*	8.28	8.56	8.61
35.17	*0.0002182*	6.98	7.39	7.4
45.11	*0.0001894*	6.06	6.58	6.57

Temp, C	Cramer (1982) ppm O2 in H2O	Compare Tromans (2000) ppm O2 in H2O	Compare GWB 6.0 calc'n ppm O2 in H2O
0	14.29	14.62	14.81
10	11.23	11.42	11.54
25	8.29	8.59	8.49
40	6.41	6.96	6.96
50	5.45	6.28	6.26
60	4.58	5.83	5.81
70	3.71	5.51	5.47
80	2.73	5.33	5.28
90	1.54	5.25	5.19
100	0	5.25	5.25

Temp, C	Cramer (1982) ppm O2 in 5.69 m NaCl	Compare Tromans (2000) ppm O2 in 5.69 m NaCl	Compare GWB 6.0 calc'n ppm O2 in 5.69 m NaCl
0	1.7	3.13	11.12
10	1.53	2.46	8.66
25	1.35	1.84	6.37
40	1.22	1.49	5.22
50	1.14	1.35	4.7
60	1.06	1.25	4.36
70	0.95	1.18	4.1
80	0.8	1.14	3.96
90	0.59	1.12	3.9
100	0.28	1.12	3.94

T=25C NaCl (m)	*Millero et al. (2002) mol O2/kgH2O*	Millero et al. (2002) ppm O2	Compare Tromans (2000) ppm O2	Compare GWB 6.0 calc'n ppm O2	Compare StreamAnal V2.0 ppm O2
0	*0.0002584*	8.27	8.57	8.49	8.24
0.2541	*0.0002351*	7.52	7.92	8.37	7.98
0.5066	*0.0002174*	6.96	7.32	8.25	7.49
1.0231	*0.0001857*	5.94	6.25	8.01	6.58
1.5561	*0.000159*	5.09	5.34	7.79	5.75
2.065	*0.0001387*	4.44	4.61	7.58	5.08
3.2116	*0.0000994*	3.18	3.38	7.15	3.83
3.9745	*0.0000809*	2.59	2.77	6.89	3.19
4.9832	*0.0000624*	2.00	2.17	6.58	2.5
5.8885	*0.0000497*	1.59	1.76	6.32	2.02

November 20, 2007
The following information could be used in evaluating the potential composition of brines that form by deliquescence of salts present in dusts at Yucca Mountain.

From (ANL-EBS-MD-000001 REV 01; 2004)"
"4.1.14 Geochemical Composition of Dust Samples
Dust samples were collected from the Exploratory Studies Facility in two separate phases. The samples were analyzed by leaching with water, and chemical analysis of the leachate. The results are reported by chemical element and some common chemical compounds. Only leachable components are used in this report, to represent soluble salts present in the dust. The Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier ANL-EBS-MD-000001 REV 01 4-18 November 2004 leachate data for Phase I samples (DTN: MO0207EBSDUSTS.020 [DIRS 162556]) are given in Table 4.1-19; those for Phase II samples (DTN: MO0209EBSDUST2.030 [DIRS 162557]) are given in Table 4.1-20. Of particular interest here are the data for soluble nitrate and chloride. The leachate data are thought to reflect the actual salt mineral content of the dust. Mineralogical data on the dust, or its salt components, are not available. Section 6.7.2.10 describes EQ3/6 calculations that estimate the original salt component mineralogy by simulating evaporation to dryness (or near dryness) of the leachate solutions."

Table 4.1-19. Dust Leachate Compositions, Phase I (ANL-EBS-MD-000001 REV 01; 2004)

Lab No.	Field No.	Meters	Ca	Mg	Na	K	Si	Cl	F	NO3	SO4	Br	P	As	Pb
			ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppb	ppb
C-186098	SPC00573629	202	268	26.7	346	126	34.5	184	10	240	360	38	9.6	92	1.2
C-186091	SPC00573622	558	980	83.6	358	183	43.5	182	6	800	1,120	10	1.8	43	0.88
C-186099	SPC00573630	669	392	42	344	149	27.9	196	8	280	480	28	4.6	74	2.5
C-186092	SPC00573623	901	638	79.7	431	193	46.6	180	6	580	980	22	3.5	69	1.3
C-186093	SPC00573624	901	332	35.7	386	128	14.9	240	10	280	340	54	0.8	116	3.1
C-186100	SPC00573631	1,100	630	31.4	389	150	82.5	220	40	260	640	64	4.6	158	1.8
C-186094	SPC00573625	1,272	974	79.1	617	260	58.7	300	8	680	1,340	26	3.2	100	1.1
C-186101	SPC00573632	1,510	229	18.9	262	101	42.3	220	8	114	300	28	5	74	3
C-186102	SPC00573633	1,720	543	9.76	158	80	97.5	114	18	62	320	22	2.2	63	1.4
C-186095	SPC00573626	1,808	575	34.3	415	206	94.9	200	14	400	660	26	5.7	99	1.5
C-186096	SPC00573627	2,273	394	53.4	511	237	65	260	32	420	1,020	34	196	152	0.91
C-186097	SPC00573628	2,708	480	34.8	287	142	61.2	160	8	380	620	18	40.2	86	1.1
C-186090	SPC00573620	3,109	226	10.6	157	101	79.1	56	4	82	162	6	3.6	34	0.8
C-186089	SPC00573619	3,514	635	43.6	397	214	100	200	24	420	720	22	10.9	108	1.4
C-186088	SPC00573618	3,900	439	13.7	345	479	120	114	12	300	400	16	5.5	67	0.81

C-186087	SPC00573617	4,300	919	32.8	332	221	96.4	140	18	440	1,180	20	6.1	81	0.94
C-186086	SPC00573616	4,721	893	35.7	374	248	107	130	12	400	1,480	26	5.6	97	0.8
C-186085	SPC00573615	5,040	863	25.9	369	220	134	162	12	380	740	22	6.5	97	0.54
C-186084	SPC00573614	5,300	939	27.1	343	219	121	130	12	380	1,160	24	5.6	103	0.85
C-186082	SPC00573612	6,297	630	28.3	388	231	95.1	154	10	340	1,060	50	5.5	132	0.75
C-186081	SPC00573611	6,700	941	6.32	378	242	213	200	30	340	840	56	3.1	186	0.3
C-186080	SPC00573610	6,895	430	19.4	304	221	89.2	162	24	220	640	34	4.4	102	0.4
C-186077	SPC00573607	7,798	2,490	12.8	455	350	173	260	8	1,820	2,200	14	4.2	81	1.1
Mean		—	607	34.2	363	204	81.7	181	14.5	418	816	28.7	6.5	96.2	1.24
Median		—	630	31.4	369	214	89.2	182	12	380	720	26	5	96.5	1.1
Std. Dev.		—	258	21.9	98	87	49.2	56	9.4	351	472	14.9	7.9	35.6	0.74
Min		—	226	6	157	80	14.9	56	4	62	162	6	0.8	33.5	0.3
Max		—	2,490	84	617	479	213	300	40	1,820	2,200	64	196	186	3.1
% Soluble		—	5.3	1.8	1.5	0.6	—	15.1	2.1	—	43.4	56.7	3.7	1.2	0.004
Micromoles/g		—	15.14	1.41	15.78	5.23	—	5.11	0.76	6.74	8.49	0.36	—	—	—

Source: DTN: MO0207EBSDUSTS.020 [DIRS 162556].
NOTES: (1) SPC in the field number denotes specimen.
(2) "Meters" denotes distance inside the tunnel from the North Portal

Table 4.1-20. Dust Leachate Compositions, Phase II

Lab No.	Sample No.	Ca	Mg	K	Na	Si	Cl	Br	F	NO3	SO4	PO4	Pb	As
		ppm	ppm	ppm	Ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppb	ppb
C-203112	00574979A	147	16.3	159	55.4	161	<24	<1.6	8	<7	<32	7.67	3.7	41.6
C-203113	00574979B	91.7	9.47	127	46.4	96.5	<24	<1.6	4	10	<32	14.1	3.4	26.4
C-203114	00574979C	119	12.6	174	66	144	<24	<1.6	8	24	<32	19	3.9	43.2
C-203115	00574980A	270	34.3	193	115	169	76	<1.6	18	220	220	11.7	1.7	28.1
C-203116	00574980B	466	49.3	181	124	76.6	98	4	4	400	360	6.75	4.1	24.2
C-203117	00574980C	1,080	80.1	206	195	176	154	8	12	640	840	7.05	1.2	56.2
C-203118	00574981A	772	44.1	280	188	33.4	74	4	8	116	3,800	3160	2	94.6
C-203119	00574981B	1,060	39.5	389	471	287	280	44	22	360	1,000	15	2.7	126
C-203120	00574981C	2,340	130	389	392	42.8	320	6	8	1,760	4,600	4,380	1.6	166
C-203121	00574982A	246	39.6	196	262	164	86	4	20	240	320	17.2	4	36
C-203122	00574982B	458	64.1	244	339	51.6	118	6	4	520	520	14.4	3.6	30.6

C-203123	00574982C	1,010	99.6	345	556	99.2	170	12	6	1,000	1,060	14.1	2.7	42.4
C-203124	00574983A	262	23.7	281	296	94.9	114	8	12	198	380	17.8	3.6	46.6
C-203125	00574983B	770	50.8	303	425	57.3	260	10	4	540	720	11	5.3	39.6
C-203126	00574983C	1,240	85.9	369	666	62.7	360	10	10	980	1,200	10.7	3	45.3
C-203127	00574984A	335	49.4	339	265	87.3	128	10	10	220	440	166	4.8	57.4
C-203128	00574984B	—	—	—	—	—	—	—	—	—	—	—	—	—
C-203129	00574984C	—	—	—	—	—	220	18	10	500	1,040	—	—	—
C-203130	00574985A	994	65.4	303	349	248	170	20	18	340	880	15.9	1.6	97.8
C-203131	00574985B	1,260	52.4	333	461	181	168	14	22	480	1,180	24.8	1.5	83.1
C-203132	00574985C	1,030	54.7	275	480	130	166	16	22	500	1,220	22.1	1.8	90.3
C-203133	00574986A	248	23.4	234	222	75.4	96	6	6	146	320	5.21	3.5	39
C-203134	00574986B	806	38	220	292	131	170	10	12	300	740	9.51	1.8	52.6
C-203135	00574986C	1,190	51.4	260	408	159	220	14	18	440	1,140	12.9	1.9	70.4
C-203136	00574987A	1,290	84.6	257	201	21.8	188	2	8	600	5,800	12,700	2.5	266
C-203137	00574987B	1,180	64.1	313	564	135	360	42	22	540	1,400	19.3	2.9	117
C-203138	00574987C	1,280	70.5	288	570	143	320	32	24	520	1,480	19	1.6	110
C-203139	00574990A	274	19.8	186	149	44.7	88	10	8	170	500	3.99	1.4	31.1
C-203140	00574990B	434	25.9	151	186	38.9	102	16	6	220	760	7.05	2	39.1
C-203141	00574990C	689	34.7	251	370	82.2	136	22	14	300	940	12.9	1.9	69.8
C-203142	00574991A	281	55.4	139	128	161	88	12	22	122	440	4.91	1.6	39.6
C-203143	00574991B	319	56.8	114	121	79.4	76	10	4	156	520	7.05	4.7	29.7
C-203144	00574991C	622	53.6	177	196	215	82	12	10	164	700	7.97	1.2	51
C-203145	00574992A	122	10.3	155	171	57.4	98	6	8	70	116	5.52	3.2	44.2
C-203146	00574992B	110	9.48	121	126	12.3	82	<1.6	2	68	124	6.44	2.1	13.1
C-203147	00574992C	305	19.8	173	187	60.2	166	2	6	150	280	10.1	2.3	33.1

Source: DTN: MO0209EBSDUST2.030 [DIRS 162557], Table 4.

NOTE: The terminal letters of the sample numbers designate sample particle size range: A = 60 to 200 mesh (74 to 200 microns), B = 200 to 325 mesh (44 to 74 microns), and C = <325 mesh (<44 microns).

November 21, 2007

Use the following composition as input to GWB React and StreamAnalyzer calculations:

Lab No.	Ca	Mg	Na	K	Si	Cl	F	NO3	SO4	Br
	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
C-186098	268	26.7	346	126	34.5	184	10	240	360	38

34.5 ppm Si is equivalent to 73.7 ppm SiO2.

No carbonate concentration is given. For React calculation, log fCO2 was fixed at –3.5. For StreamAnalyzer calculation, the input concentrations were input as water analysis concentrations and charge balance was specified to use HCO3– as the balancing species.

The following is the React script:

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
Ca++ 268 mg/l
Mg++ 26.7 mg/l
K+ 126 mg/l
Na+ 346 mg/l
SiO2(aq) 73.7 mg/l
Cl- 184 mg/l
F- 10 mg/l
NO3- (swapped for NH3(aq)) 240 mg/l
SO4-- 360 mg/l
Br- 38 mg/l
H+ charge balance
O2(g) (swapped for O2(aq)) -.7 log fugacity
CO2(g) (swapped for HCO3-) -3.5 log fugacity
No reactants specified.

The following is the output from React:

Step # 0 Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 9.178 log fO2 = -0.700
Eh = 0.6758 volts pe = 11.4239
Ionic strength = 0.035866
Activity of water = 0.999818
Solvent mass = 1.000000 kg
Solution mass = 1.002453 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.005190 molal
Dissolved solids = 2447 mg/kg sol'n

Rock mass = 0.000000 kg
Carbonate alkalinity= 629.12 mg/kg as CaCO3

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.01466	336.1	0.8393	-1.9100
HCO3-	0.008709	530.1	0.8393	-2.1361
Cl-	0.005177	183.1	0.8315	-2.3660
Ca++	0.003848	153.8	0.5241	-2.6953
NO3-	0.003832	237.0	0.8315	-2.4967
K+	0.003187	124.3	0.8315	-2.5768
SO4--	0.003029	290.3	0.4913	-2.8274
CaCO3(aq)	0.002210	220.7	1.0000	-2.6556
CO3--	0.001032	61.79	0.4999	-3.2874
SiO2(aq)	0.0009491	56.89	1.0000	-3.0227
Mg++	0.0007110	17.24	0.5532	-3.4053
F-	0.0005163	9.785	0.8355	-3.3652
Br-	0.0004753	37.89	0.8315	-3.4031
CaSO4(aq)	0.0003876	52.64	1.0000	-3.4116
O2(aq)	0.0002522	8.050	1.0000	-3.5983
CaHCO3+	0.0001956	19.72	0.8393	-3.7848
MgCO3(aq)	0.0001933	16.26	1.0000	-3.7137
HSiO3-	0.0001898	14.60	0.8393	-3.7977
MgSO4(aq)	0.0001510	18.14	1.0000	-3.8209
NaSO4-	0.0001441	17.11	0.8393	-3.9174
NaHCO3(aq)	0.0001282	10.74	1.0000	-3.8921
NaHSiO3(aq)	8.725e-005	8.711	1.0000	-4.0592
CaNO3+	3.837e-005	3.908	0.8393	-4.4920
MgHCO3+	3.719e-005	3.165	0.8393	-4.5057
KSO4-	3.560e-005	4.801	0.8393	-4.5246
NaCO3-	2.472e-005	2.047	0.8393	-4.6830
OH-	1.821e-005	0.3090	0.8355	-4.8176
CO2(aq)	1.074e-005	0.4716	1.0000	-4.9689
NaCl(aq)	8.849e-006	0.5159	1.0000	-5.0531
CaF+	4.980e-006	0.2935	0.8393	-5.3788
MgF+	4.550e-006	0.1966	0.8393	-5.4180
CaCl+	2.085e-006	0.1571	0.8393	-5.7570
MgCl+	1.479e-006	0.08814	0.8393	-5.9062
NaF(aq)	5.336e-007	0.02235	1.0000	-6.2728
CaOH+	5.107e-007	0.02908	0.8393	-6.3679
KCl(aq)	3.652e-007	0.02716	1.0000	-6.4374
NaBr(aq)	2.138e-007	0.02195	1.0000	-6.6700
H6(H2SiO4)4--	8.560e-008	0.03266	0.4913	-7.3762
H2SiO4--	4.797e-008	0.004503	0.4913	-7.6277
NaOH(aq)	2.969e-008	0.001185	1.0000	-7.5274
KBr(aq)	1.918e-008	0.002277	1.0000	-7.7171
KOH(aq)	1.383e-008	0.0007738	1.0000	-7.8593

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	137.6215s/sat	Coesite	0.1666s/sat
Tremolite	20.6501s/sat	Cristobalite(bet	-0.0174

Anthophyllite	13.6705s/sat	Ice	-0.1388
Talc	11.6203s/sat	SiO2(am)	-0.3091
Sepiolite	11.2186s/sat	Gyrolite	-0.6587
Chrysotile	7.6784s/sat	Sellaite	-0.7513
Dolomite	5.4688s/sat	Okenite	-0.7674
Dolomite-ord	5.4688s/sat	Forsterite	-0.9857
Huntite	4.9536s/sat	Gypsum	-1.0406
Dolomite-dis	3.9244s/sat	Artinite	-1.0704
Diopside	3.5998s/sat	Wollastonite	-1.1235
Calcite	2.4974s/sat	Lansfordite	-1.2051
Aragonite	2.3530s/sat	Anhydrite	-1.2163
Monohydrocalcite	1.6636s/sat	Brucite	-1.3483
Magnesite	1.3426s/sat	Nesquehonite	-1.3596
Quartz	0.9766s/sat	Hydromagnesite	-1.3598
Tridymite	0.8051s/sat	Pseudowollastoni	-1.3627
Chalcedony	0.7054s/sat	Bassanite	-1.8612
Fluorite	0.6114s/sat	Monticellite	-1.9984
Enstatite	0.6002s/sat	CaSO4:0.5H2O(bet	-2.0293
Cristobalite(alp	0.4261s/sat		

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

Gases	fugacity	log fug.
O2(g)	0.1995	-0.700
H2O(g)	0.02597	-1.585
CO2(g)	0.0003162	-3.500
HF(g)	2.212e-014	-13.655
HCl(g)	1.415e-018	-17.849
N2(g)	1.243e-019	-18.906
NO2(g)	7.212e-020	-19.142
Br2(g)	1.090e-021	-20.963
HBr(g)	3.450e-022	-21.462
NO(g)	1.082e-025	-24.966
Cl2(g)	1.298e-028	-27.887
SiF4(g)	9.994e-039	-38.000
H2(g)	6.273e-042	-41.203
CO(g)	6.197e-049	-48.208
SO2(g)	7.726e-058	-57.112
NH3(g)	4.223e-069	-68.374
Na(g)	2.009e-073	-72.697
K(g)	8.295e-075	-74.081
F2(g)	2.488e-083	-82.604
Mg(g)	3.159e-126	-125.500
H2S(g)	4.711e-145	-144.327
CH4(g)	3.907e-146	-145.408
Ca(g)	2.405e-148	-147.619
C(g)	3.254e-190	-189.488
Si(g)	4.214e-220	-219.375
S2(g)	1.258e-232	-231.900
C2H4(g)	7.655e-239	-238.116

		In fluid	Sorbed	Kd	
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Br-	0.000476	0.000476	37.9			
Ca++	0.00669	0.00669	267.			

Cl-	0.00519	0.00519	184.
F-	0.000526	0.000526	9.98
H+	-0.00762	-0.00762	-7.66
H2O	55.5	55.5	9.97e+005
HCO3-	0.0125	0.0125	763.
K+	0.00322	0.00322	126.
Mg++	0.00110	0.00110	26.6
NH3(aq)	0.00387	0.00387	65.8
Na+	0.0151	0.0151	345.
O2(aq)	0.00799	0.00799	255.
SO4--	0.00375	0.00375	359.
SiO2(aq)	0.00123	0.00123	73.5

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Bromine	0.0004756	0.0004756	37.91		
Calcium	0.006687	0.006687	267.3		
Carbon	0.01254	0.01254	150.3		
Chlorine	0.005190	0.005190	183.5		
Fluorine	0.0005264	0.0005264	9.976		
Hydrogen	111.0	111.0	1.116e+005		
Magnesium	0.001099	0.001099	26.63		
Nitrogen	0.003871	0.003871	54.08		
Oxygen	55.58	55.58	8.870e+005		
Potassium	0.003223	0.003223	125.7		
Silicon	0.001227	0.001227	34.37		
Sodium	0.01505	0.01505	345.2		
Sulfur	0.003748	0.003748	119.9		

Step # 0–B Xi = 0.0000
Temperature = 25.0 C Pressure = 1.013 bars
pH = 7.023 log fO2 = -0.700
Eh = 0.8032 volts pe = 13.5784
Ionic strength = 0.028471
Activity of water = 0.999818
Solvent mass = 1.000026 kg
Solution mass = 1.001904 kg
Solution density = 1.013 g/cm3
Chlorinity = 0.005190 molal
Dissolved solids = 1875 mg/kg sol'n
Rock mass = 0.000548 kg
Carbonate alkalinity= 384.77 mg/kg as CaCO3

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.003034	-2.518	0.3037	0.1121
Dolomite	0.0009161	-3.038	0.1689	0.05897
Fluorite	0.0001014	-3.994	0.007917	0.002489
Quartz	0.001126	-2.948	0.06767	0.02555
(total)			0.5482	0.1991

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.01478	339.1	0.8522	-1.8999
HCO3-	0.006339	386.0	0.8522	-2.2675
Cl-	0.005179	183.3	0.8456	-2.3586
NO3-	0.003847	238.1	0.8456	-2.4877
SO4--	0.003235	310.2	0.5232	-2.7714
K+	0.003182	124.2	0.8456	-2.5702
Ca++	0.002243	89.73	0.5523	-2.9069
CO2(aq)	0.001133	49.77	1.0000	-2.9458
Br-	0.0004753	37.91	0.8456	-3.3958
F-	0.0003207	6.081	0.8490	-3.5650
CaSO4(aq)	0.0002709	36.81	1.0000	-3.5672
O2(aq)	0.0002522	8.054	1.0000	-3.5983
NaSO4-	0.0001653	19.64	0.8522	-3.8512
Mg++	0.0001403	3.404	0.5782	-4.0908
SiO2(aq)	0.0001002	6.007	1.0000	-3.9993
NaHCO3(aq)	9.701e-005	8.134	1.0000	-4.0132
CaHCO3+	8.745e-005	8.824	0.8522	-4.1277
KSO4-	4.050e-005	5.464	0.8522	-4.4619
MgSO4(aq)	3.544e-005	4.258	1.0000	-4.4505
CaNO3+	2.370e-005	2.415	0.8522	-4.6946
NaCl(aq)	9.216e-006	0.5376	1.0000	-5.0354
CaCO3(aq)	7.031e-006	0.7024	1.0000	-5.1530
MgHCO3+	5.583e-006	0.4755	0.8522	-5.3226
CO3--	5.033e-006	0.3015	0.5308	-5.5732
CaF+	1.902e-006	0.1121	0.8522	-5.7903
CaCl+	1.283e-006	0.09675	0.8522	-5.9611
MgF+	5.834e-007	0.02522	0.8522	-6.3035
KCl(aq)	3.773e-007	0.02807	1.0000	-6.4233
NaF(aq)	3.448e-007	0.01445	1.0000	-6.4625
MgCl+	3.056e-007	0.01823	0.8522	-6.5843

NaBr(aq)	2.226e-007	0.02286	1.0000	-6.6525
MgCO3(aq)	2.065e-007	0.01738	1.0000	-6.6851
HSiO3-	1.382e-007	0.01064	0.8522	-6.9288
NaCO3-	1.291e-007	0.01069	0.8522	-6.9586
OH-	1.256e-007	0.002132	0.8490	-6.9721
H+	1.080e-007	0.0001086	0.8782	-7.0231
NaHSiO3(aq)	6.605e-008	0.006598	1.0000	-7.1802
HF(aq)	3.802e-008	0.0007592	1.0000	-7.4200
KBr(aq)	1.981e-008	0.002353	1.0000	-7.7032
HSO4-	1.795e-008	0.001739	0.8522	-7.8154

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Dolomite-ord	0.0000 sat	Monohydrocalcite	-0.8338
Fluorite	0.0000 sat	Cristobalite(bet	-0.9940
Quartz	0.0000 sat	Gypsum	-1.1962
Dolomite	0.0000 sat	SiO2(am)	-1.2857
Calcite	0.0000 sat	Anhydrite	-1.3719
Ice	-0.1388	Dolomite-dis	-1.5444
Aragonite	-0.1444	Magnesite	-1.6288
Tridymite	-0.1715	Sellaite	-1.8366
Chalcedony	-0.2712	Bassanite	-2.0169
Cristobalite(alp	-0.5505	CaSO4:0.5H2O(bet	-2.1850
Coesite	-0.8100		

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

Gases	fugacity	log fug.
O2(g)	0.1995	-0.700
CO2(g)	0.03335	-1.477
H2O(g)	0.02597	-1.585
HF(g)	1.992e-012	-11.701
N2(g)	2.639e-015	-14.579
HCl(g)	2.055e-016	-15.687
Br2(g)	2.296e-017	-16.639
NO2(g)	1.051e-017	-16.978
HBr(g)	5.007e-020	-19.300
NO(g)	1.577e-023	-22.802
Cl2(g)	2.736e-024	-23.563
SiF4(g)	6.942e-032	-31.159
H2(g)	6.273e-042	-41.203
CO(g)	6.536e-047	-46.185
SO2(g)	1.790e-053	-52.747
NH3(g)	6.153e-067	-66.211
Na(g)	1.441e-075	-74.841
K(g)	5.901e-077	-76.229
F2(g)	2.018e-079	-78.695
Mg(g)	3.199e-131	-130.495
H2S(g)	1.092e-140	-139.962
CH4(g)	4.121e-144	-143.385
Ca(g)	7.253e-153	-152.139
C(g)	3.432e-188	-187.464
Si(g)	4.447e-221	-220.352
S2(g)	6.754e-224	-223.170

C2H4(g)	8.517e-235	-234.070

Original basis	In fluid total moles	In fluid moles	Sorbed mg/kg	Kd moles	Kd mg/kg	Kd L/kg
Br-	0.000476	0.000476	37.9			
Ca++	0.00669	0.00264	105.			
Cl-	0.00519	0.00519	184.			
F-	0.000526	0.000324	6.14			
H+	-0.00762	-0.00275	-2.77			
H2O	55.5	55.5	9.98e+005			
HCO3-	0.0125	0.00767	467.			
K+	0.00322	0.00322	126.			
Mg++	0.00110	0.000182	4.43			
NH3(aq)	0.00387	0.00387	65.8			
Na+	0.0151	0.0151	345.			
O2(aq)	0.00799	0.00799	255.			
SO4--	0.00375	0.00375	359.			
SiO2(aq)	0.00123	0.000100	6.02			

Elemental composition	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg
Bromine	0.0004756	0.0004756	37.93		
Calcium	0.006687	0.002636	105.4		
Carbon	0.01254	0.007674	92.00		
Chlorine	0.005190	0.005190	183.7		
Fluorine	0.0005264	0.0003235	6.135		
Hydrogen	111.0	111.0	1.117e+005		
Magnesium	0.001099	0.0001824	4.425		
Nitrogen	0.003871	0.003871	54.11		
Oxygen	55.58	55.56	8.872e+005		
Potassium	0.003223	0.003223	125.8		
Silicon	0.001227	0.0001004	2.814		
Sodium	0.01505	0.01505	345.3		
Sulfur	0.003748	0.003748	119.9		

The following is the output from StreamAnalyzer after charge balancing:

Reconciliation Summary

	Specification
Charge Balance Method	Make-up Ion
pH Reconciliation Type	Not specified

	Measured	Calculated	Difference %
Temperature, °C	25.0000		
Pressure, atm	1.00000		
pH	0.0	6.72725	100.00
Density, g/ml	0.0	0.998533	
Water, mg H2O/L	1.00000e6	9.96081e5	

Stream Inflows

	Input	Calculated		% Diff
H2O	1.00000e6	9.96081e5	mg/L	-
0.391854				
SiO2	73.7000	73.7000	mg/L	
Ca+2	268.000	268.000	mg/L	
Mg+2	26.7000	26.7000	mg/L	
Na+1	346.000	346.000	mg/L	
K+1	126.000	126.000	mg/L	
Cl-1	184.000	184.000	mg/L	
F-1	10.0000	10.0000	mg/L	
NO3-1	240.000	240.000	mg/L	
SO4-2	360.000	360.000	mg/L	
Br-1	38.0000	38.0000	mg/L	
HCO3-1	0.0	993.733	mg/L	
100.000				

Charge Balance

Cation Charge:	0.033844 eq/L
Anion Charge:	-0.017558 eq/L
Imbalance:	0.016286 eq/L
Adjusted Species:	HCO3-1

Charged Species	**Input mg/L**	**Balanced mg/L**	**Difference %**
Ca+2	268.000	268.000	
Mg+2	26.7000	26.7000	
Na+1	346.000	346.000	
K+1	126.000	126.000	
Cl-1	184.000	184.000	
F-1	10.0000	10.0000	
NO3-1	240.000	240.000	
SO4-2	360.000	360.000	
Br-1	38.0000	38.0000	
HCO3-1	0.0	993.733	100.00

Stream Parameters

Row Filter Applied: Only Non Zero Values

Mixture Properties		
Stream Amt - Total Inflow	1.00001	L
Temperature	25.0000	°C
Pressure	1.00000	atm
Aqueous Properties		
pH	6.72725	pH
Ionic Strength	6.00759e-4	mol/mol
Osmotic Pressure	1.31622	atm
Electrical Cond, specific	2.60656e-3	1/(ohm-cm)
Electrical Cond, molar	45.4199	cm2/ohm-mol
Viscosity, absolute	0.898141	cP
Viscosity, relative	1.00833	cP/cP H2O

	Total	**Aqueous**	**Vapor**	**Solid**	**2nd Liquid**
		g/ml	g/ml	g/ml	g/ml
Density		0.998533	0.0	2.72786	0.0
	cal	cal	cal	cal	cal

Enthalpy	-3.78337e6	-3.78238e6	0.0	-983.018	0.0	
	cal/g K	cal/g K	cal/g K	cal/g K	cal/g K	
Heat Capacity	0.989969	0.990236	0.0	0.199608	0.0	
		cal	cal	cal	cal	
Gibbs Free Energy			0.0	0.0	0.0	0.0
		cal	cal	cal	cal	
Gibbs Std State		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy		0.0	0.0	0.0	0.0	
		cal/K	cal/K	cal/K	cal/K	
Entropy Std State		0.0	0.0	0.0	0.0	

Scaling Tendencies

Row Filter Applied: Only Non Zero Values

solids within temperature range		**Temperature Range**		
CaF2	1.00000	data valid through range		inside range
CaCO3	1.00000	data valid through range		inside range
SiO2	0.646726	0.0	300.000 °C	inside range
CaSO4.2H2O	0.0790993	0.0	126.000 °C	inside range
CaSO4	0.0576466	0.0	455.000 °C	inside range
MgF2	0.0170957	data valid through range		inside range
NaHCO3	3.68582e-4	0.0	200.000 °C	inside range
MgCO3.3H2O	1.92471e-4	data valid through range		inside range
MgCO3	1.80596e-4	data valid through range		inside range
MgSO4.7H2O	5.95612e-5	0.0	49.9900 °C	inside range
KHCO3	1.12044e-5	data valid through range		inside range
KNO3	1.11147e-5	0.0	110.000 °C	inside range
NaF	5.86076e-6	0.0	100.000 °C	inside range
Na2SO4.10H2O	5.46489e-6	0.0	32.4000 °C	inside range
NaNO3	3.28823e-6	-30.0000	300.000 °C	inside range
KCl	1.69000e-6	0.0	200.000 °C	inside range
NaCl	1.43000e-6	0.0	350.000 °C	inside range
K2SO4	1.03576e-6	9.70000	292.000 °C	inside range
Na2SO4	5.75238e-7	19.0000	241.000 °C	inside range
Mg(OH)2	2.97997e-7	data valid through range		inside range
NaBr.2H2O	9.39275e-8	0.0	51.0000 °C	inside range
KBr	7.83729e-8	0.0	421.000 °C	inside range

Ca(NO3)2.4H2O	3.60457e-9	0.0	42.5000 °C	inside range
Mg1.25(SO4)(OH)0.5.0.5H2O	1.41312e-9	data valid through range		inside range
Na2CO3.10H2O	1.29313e-9	-2.05000	32.8600 °C	inside range
KF.2H2O	8.35639e-10	17.7000	40.2000 °C	inside range
NaF.Na2SO4	8.91713e-11	20.0000	120.000 °C	inside range
Mg1.5(SO4)(OH)	4.83333e-11	data valid through range		inside range
KHSO4	2.37788e-11	data valid through range		inside range
NaNO3.Na2SO4.2H2O	7.07054e-12	-30.0000	65.0000 °C	inside range
Mg(NO3)2.6H2O	5.91259e-12	1.00000	80.0000 °C	inside range
CaCl2.6H2O	2.53686e-12	-0.0100000	30.1100 °C	inside range
NaHF2	1.93269e-12	data valid through range		inside range
Ca(OH)2	1.14525e-12	data valid through range		inside range
NaHSO4	1.04203e-12	data valid through range		inside range
Na2CO3.NaHCO3.2H2O	7.53290e-13	21.2600	150.000 °C	inside range
MgCl2.6H2O	2.20155e-13	0.0	116.700 °C	inside range
KOH.2H2O	9.16379e-14	0.0	33.0000 °C	inside range
K2CO3.1.5H2O	2.70484e-14	data valid through range		inside range
NaOH.1H2O	1.04073e-14	12.0000	60.0000 °C	inside range
MgClOH	1.30028e-15	data valid through range		inside range
Na2SiO3.9H2O	8.49220e-16	0.600000	46.8000 °C	inside range
CaBr2.6H2O	4.39985e-16	0.0	34.2000 °C	inside range
MgBr2.6H2O	2.65809e-16	-0.830000	100.000 °C	inside range
Na2SO4.NaHSO4	5.87434e-19	0.0	82.5000 °C	inside range
K2CO3	2.23462e-19	data valid through range		inside range
KOH	2.99017e-21	data valid through range		inside range
Mg(NO3)2	8.22683e-24	data valid through range		inside range
K2CO3.2KHCO3.1.5H2O	3.87343e-24	data valid through range		inside range
CaCl2.CaO.2H2O	1.76946e-24	10.0000	50.0000 °C	inside range
K2SiF6	1.55620e-26	0.0	100.000 °C	inside range
CaBr2	5.74403e-27	data valid through range		inside range
Na2SiF6	3.13869e-27	0.0	100.000 °C	inside range

KMgCl3.2H2O	1.09100e-27	data valid through range	inside range
KMgCl3	5.76111e-35	data valid through range	inside range
MgBr2	1.00000e-35	data valid through range	inside range

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

	Total	Aqueous	Vapor	Solid	2nd Liquid
	kgmol	mg/L	mol/mol	g	n/a
H2O	0.055294	9.96E+05	0	0	0
SiO2	1.22E-06	73.5548	0	0	0
Ca+2	3.00E-06	120.444	0	0	0
Mg+2	8.88E-07	21.5891	0	0	0
Na+1	1.47E-05	337.89	0	0	0
K+1	3.18E-06	124.426	0	0	0
Cl-1	5.19E-06	184.019	0	0	0
F-1	1.48E-07	2.80726	0	0	0
NO3-1	3.85E-06	238.762	0	0	0
SO4-2	3.36E-06	322.349	0	0	0
Br-1	4.75E-07	37.9874	0	0	0
HCO3-1	9.37E-06	571.543	0	0	0
(HF)2	2.75E-23	1.10E-15	0	0	0
CaCl2	2.71E-29	3.01E-21	0	0	0
CaCO3	3.23E-06	0.625151	0	0.32223	0
CaF2	1.89E-07	0	0	0.014732	0
CaSiO2(OH)2	3.33E-14	4.46E-06	0	0	0
CaSO4	9.54E-08	12.9842	0	0	0
CO2	3.23E-06	142.303	0	0	0
H2SiF6	1.06E-42	1.53E-34	0	0	0
H2SO4	2.17E-28	2.13E-20	0	0	0
HBr	7.45E-22	6.03E-14	0	0	0
HCl	4.86E-19	1.77E-11	0	0	0
HF	3.74E-11	7.48E-04	0	0	0
HNO3	6.91E-18	4.35E-10	0	0	0
KCl	9.69E-11	7.23E-03	0	0	0
KHSO4	1.53E-15	2.08E-07	0	0	0
MgCO3	8.44E-10	0.071164	0	0	0
MgSiO2(OH)2	9.63E-14	1.14E-05	0	0	0
MgSO4	4.98E-08	5.99094	0	0	0
NaBr	2.16E-10	0.022277	0	0	0
NaF	1.18E-09	0.049659	0	0	0
NaHCO3	1.40E-07	11.7685	0	0	0
NaHSiO3	1.41E-09	0.140842	0	0	0
NaNO3	4.95E-09	0.420907	0	0	0
SiCl4	2.54E-92	4.32E-84	0	0	0
SiF4	1.02E-31	1.06E-23	0	0	0
SO3	2.81E-32	2.25E-24	0	0	0
Ca(NO3)+1	1.55E-08	1.58163	0	0	0

CaCl+1	1.81E-13	1.37E-05	0	0	0
CaF+1	1.65E-11	9.77E-04	0	0	0
CaHCO3+1	1.57E-07	15.8525	0	0	0
CaHSiO3+1	3.08E-11	3.61E-03	0	0	0
CaOH+1	1.64E-12	9.38E-05	0	0	0
CO3-2	4.04E-09	0.242431	0	0	0
H+1	2.22E-10	2.23E-04	0	0	0
H2SiO4-2	8.06E-16	7.58E-08	0	0	0
H3SiO4-1	1.11E-09	0.105909	0	0	0
HF2-1	1.34E-15	5.23E-08	0	0	0
HSiF6-1	2.73E-35	3.91E-27	0	0	0
HSO4-1	3.54E-11	3.43E-03	0	0	0
KSO4-1	4.06E-08	5.48203	0	0	0
MgF+1	1.13E-12	4.91E-05	0	0	0
MgHCO3+1	1.60E-07	13.6326	0	0	0
MgHSiO3+1	1.70E-11	1.73E-03	0	0	0
MgOH+1	4.72E-12	1.95E-04	0	0	0
Na2F+1	1.91E-13	1.24E-05	0	0	0
NaCO3-1	1.03E-10	8.56E-03	0	0	0
NaSO4-1	2.07E-07	24.6036	0	0	0
OH-1	6.39E-11	1.09E-03	0	0	0
SiF6-2	1.67E-30	2.37E-22	0	0	0
Total (by phase)	0.055347	9.99E+05	0	0.336962	0

After charge balance reconciliation in StreamAnalyzer, the aqueous stream was exported as input to evaporation simulations. The evaporation 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 25 °C. $pH_2O°$ at 25 °C is 0.0313849 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:

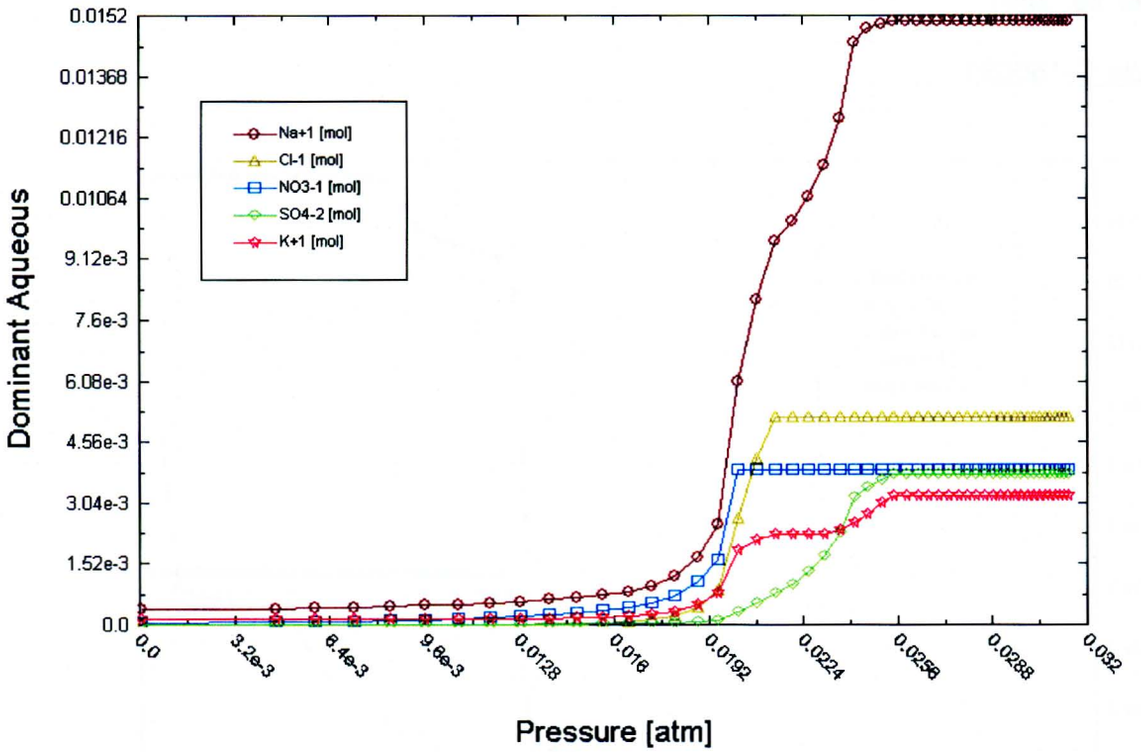
RH	pH2O (25 C)	Ptot
1	0.03138	0.03138
0.95	0.03138	0.02982
0.9	0.03138	0.02825
0.8	0.03138	0.02511
0.7	0.03138	0.02197
0.6	0.03138	0.01883
0.5	0.03138	0.01569
	Did not converge at 0.5	

The runs used the standard H+ ion chemistry model. The output was extracted and copied into an Excel file (Dust leachate composition from ANL-EBS-MD-000001 REV 01 - 2004.xls in the Notes folder). StreamAnalyzer did not converge at a Ptot of 0.01569.

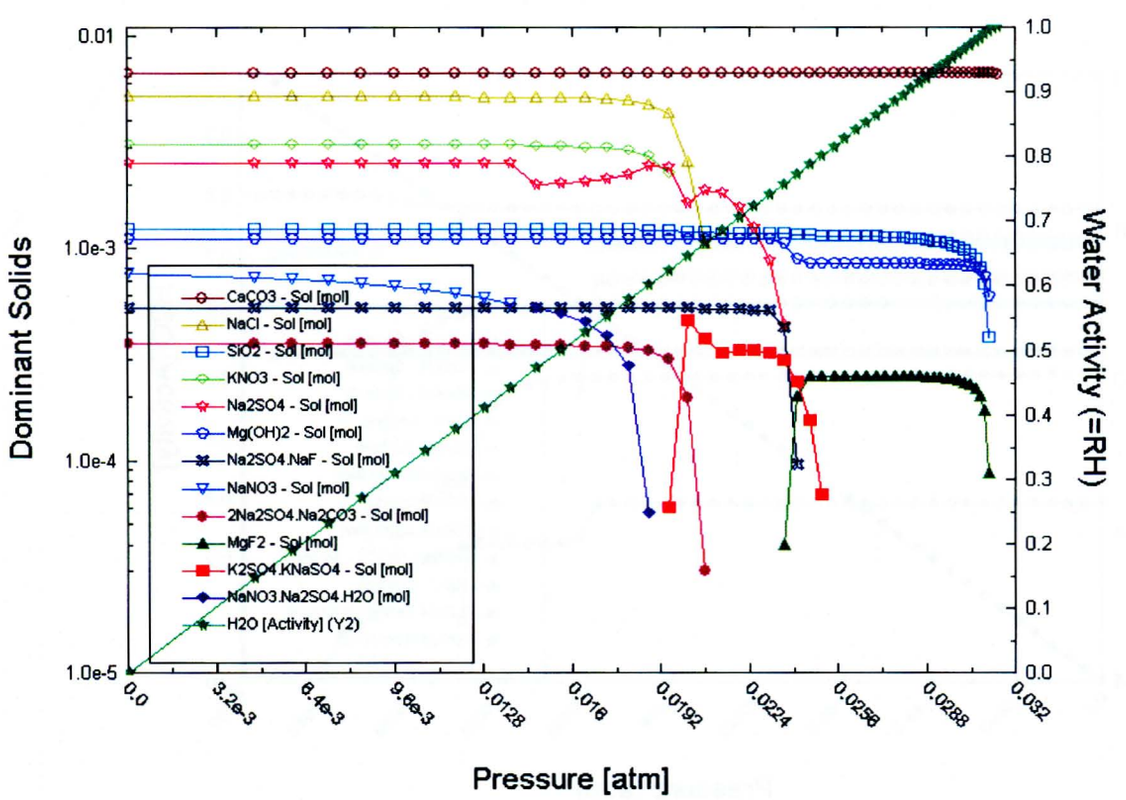
Another series of runs was done using the mixed solvent electrolyte model and the output was copied into the same Excel file. The input Ptot is listed in the following table. Convergence was achieved in all cases.

RH	pH2O	Ptot
1	0.03138	0.03138
0.95	0.03138	0.02982
0.9	0.03138	0.02825
0.8	0.03138	0.02511
0.7	0.03138	0.02197
0.6	0.03138	0.01883
0.5	0.03138	0.01569
0.4	0.03138	0.01255
0.3	0.03138	0.00942
0.2	0.03138	0.00628
0.1	0.03138	0.00314
0.05	0.03138	0.00157
0.01	0.03138	0.00031
0.001	0.03138	3.1E-05

A survey calculation was done in StreamAnalyzer. The total pressure was varied from 0.031385 atm to 0.0000313849 atm (logarithmic spacing was used). The resulting dominant aqueous concentrations are plotted in the following figure:



All the solid precipitates (14 maximum specified in options) are shown in the following figure:



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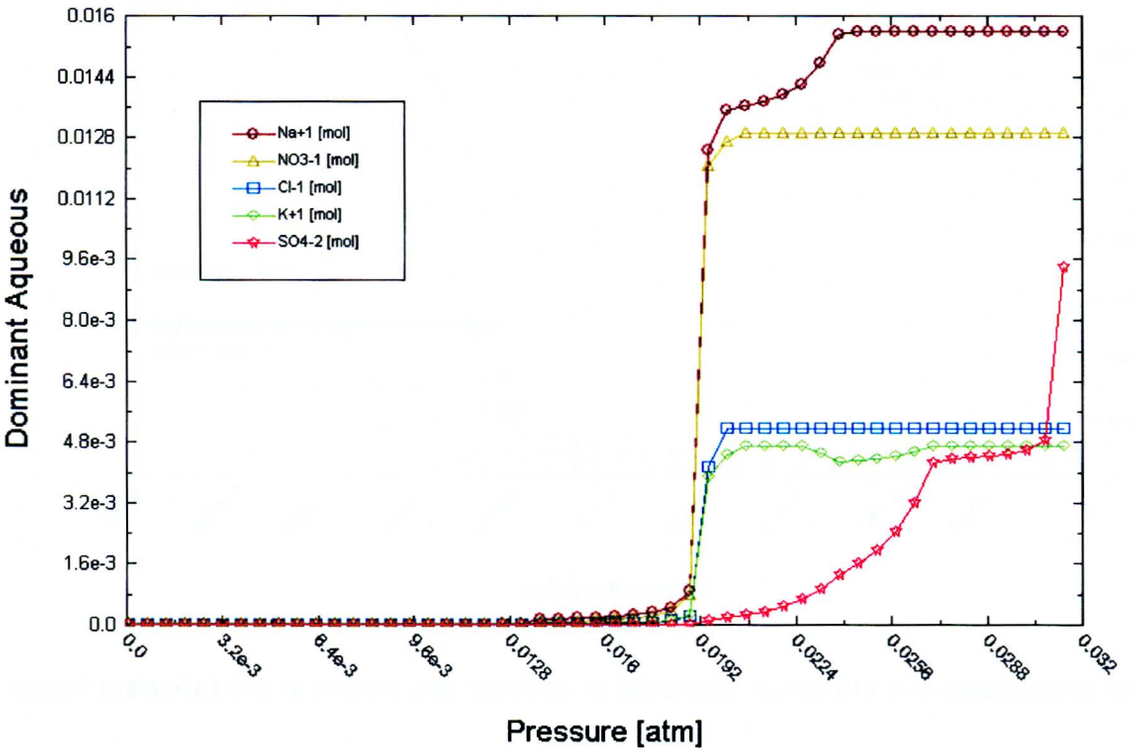
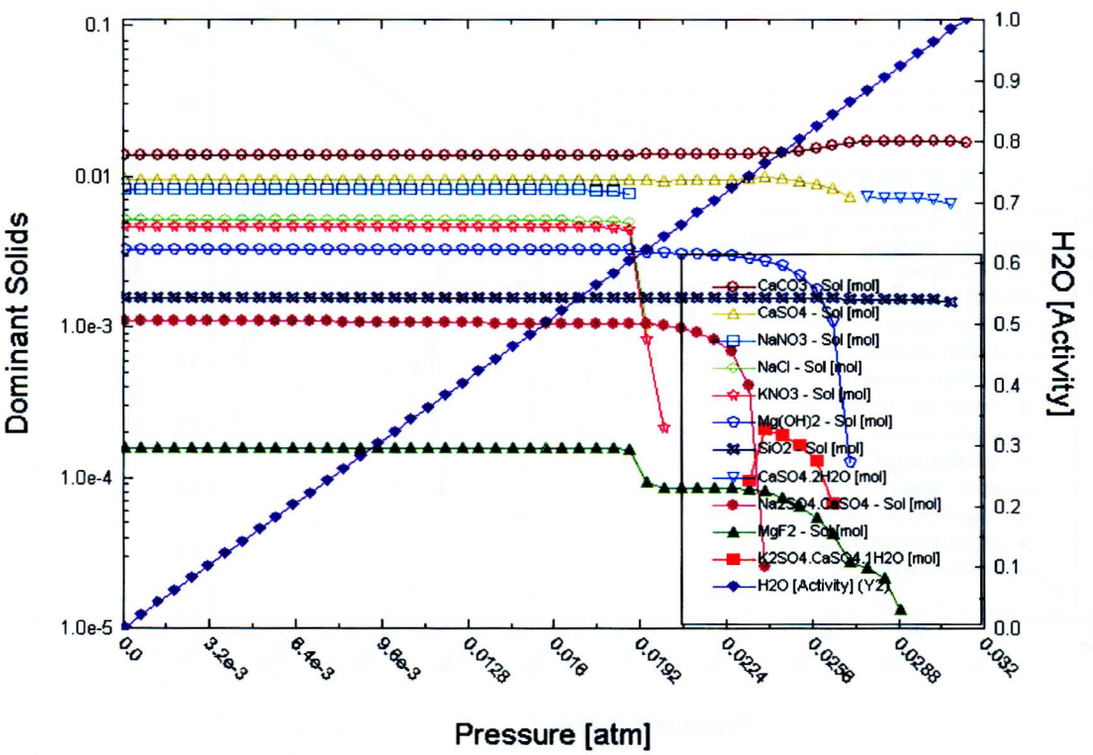
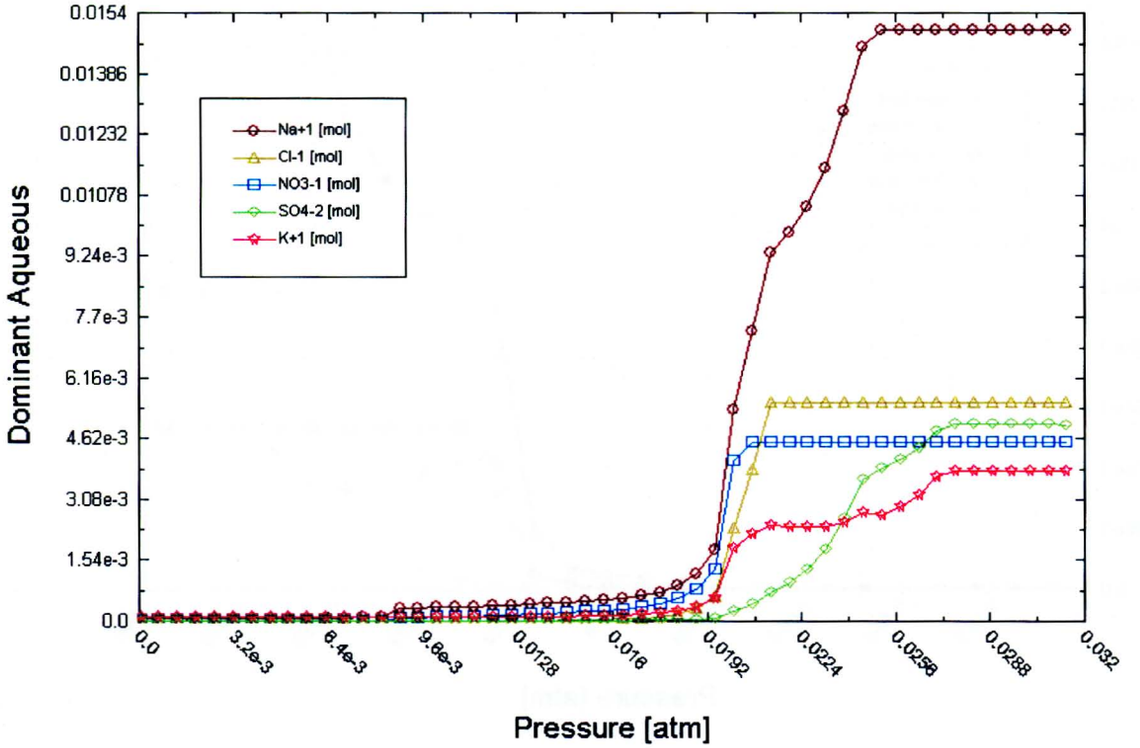
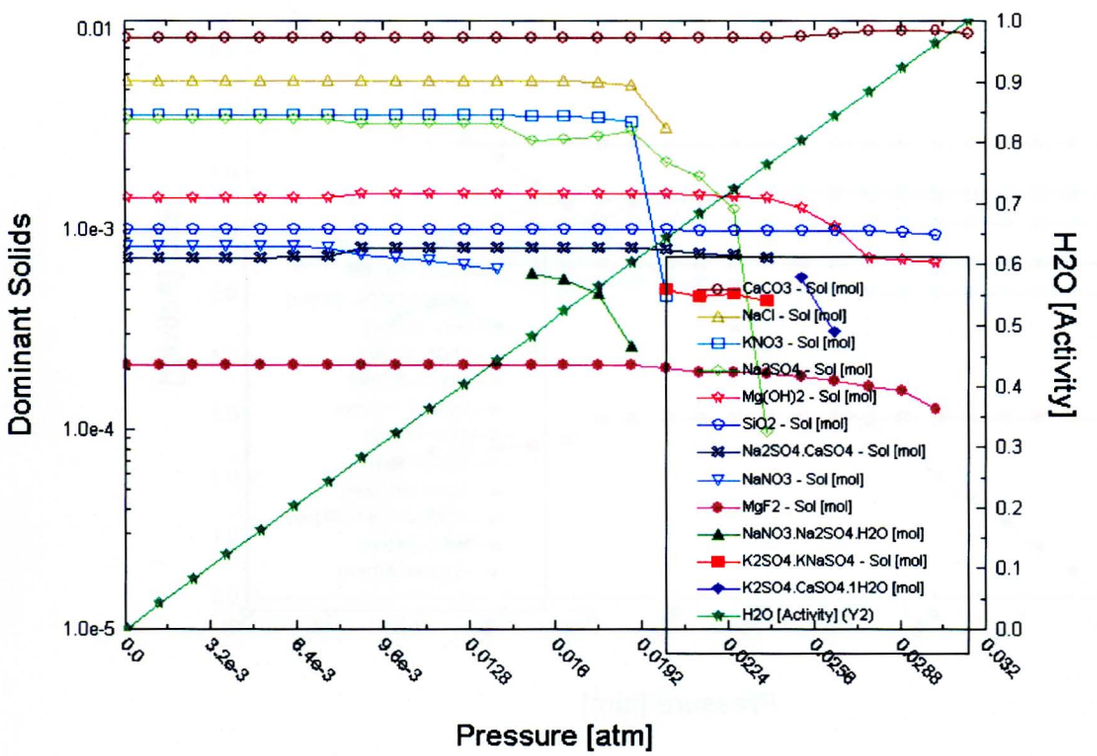
Lab sample C-186091





Lab sample C-186099





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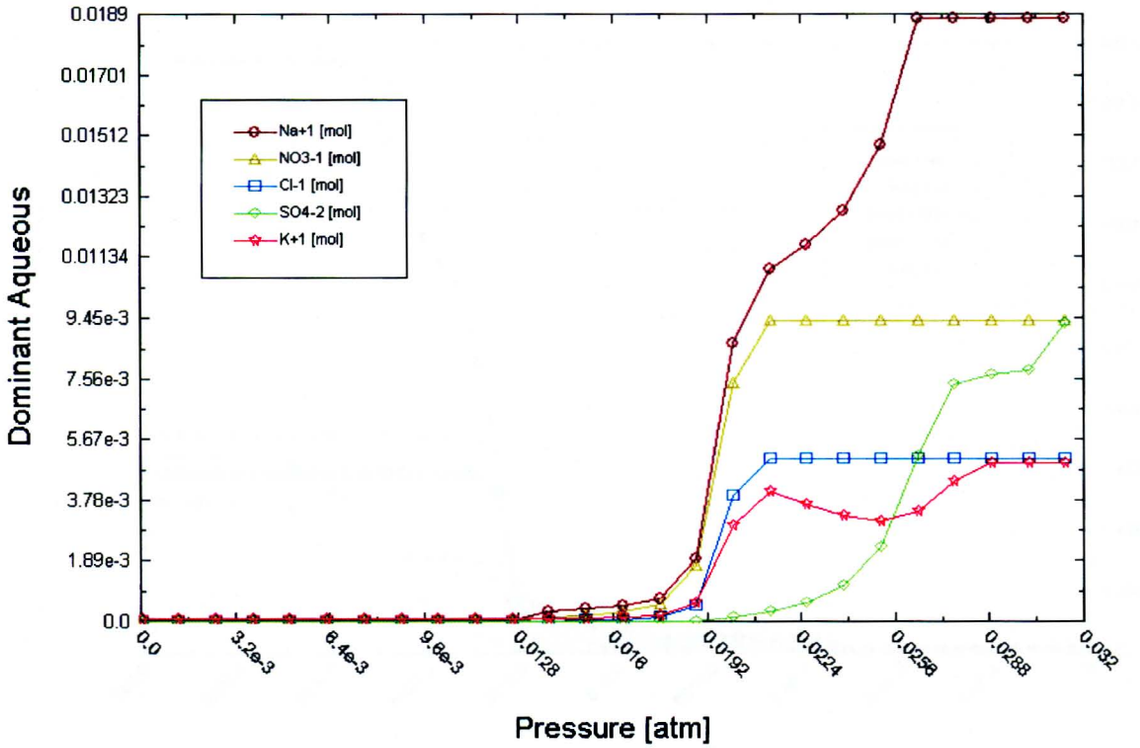

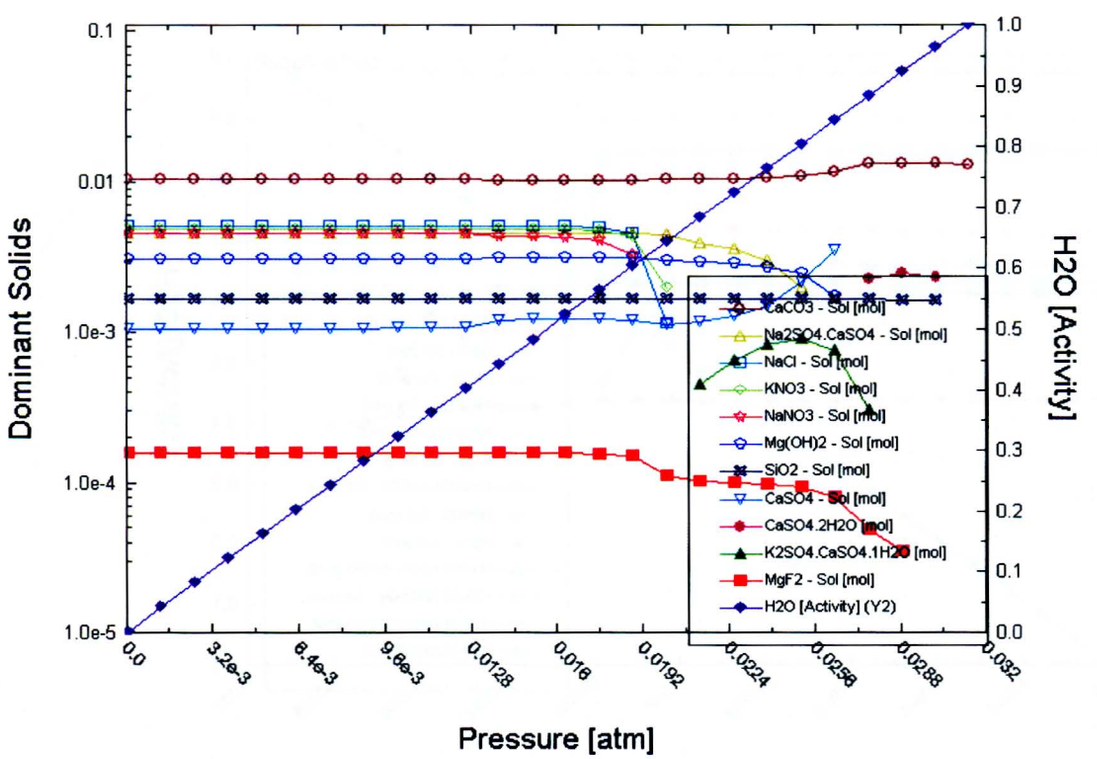

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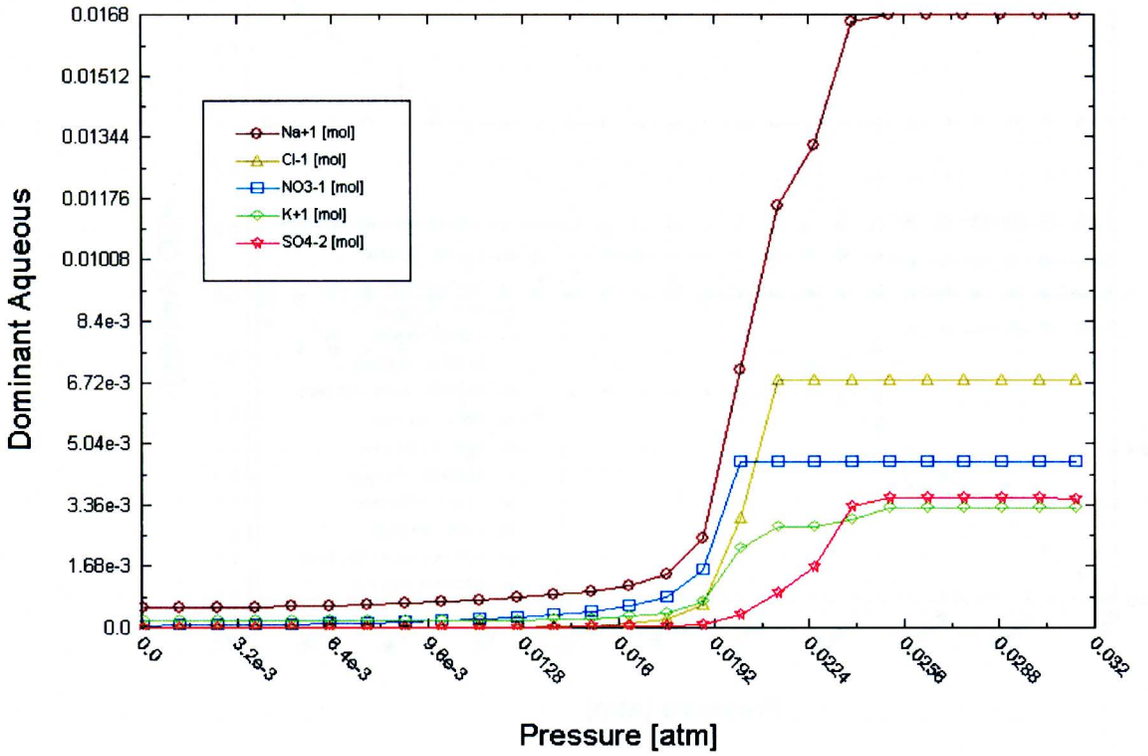
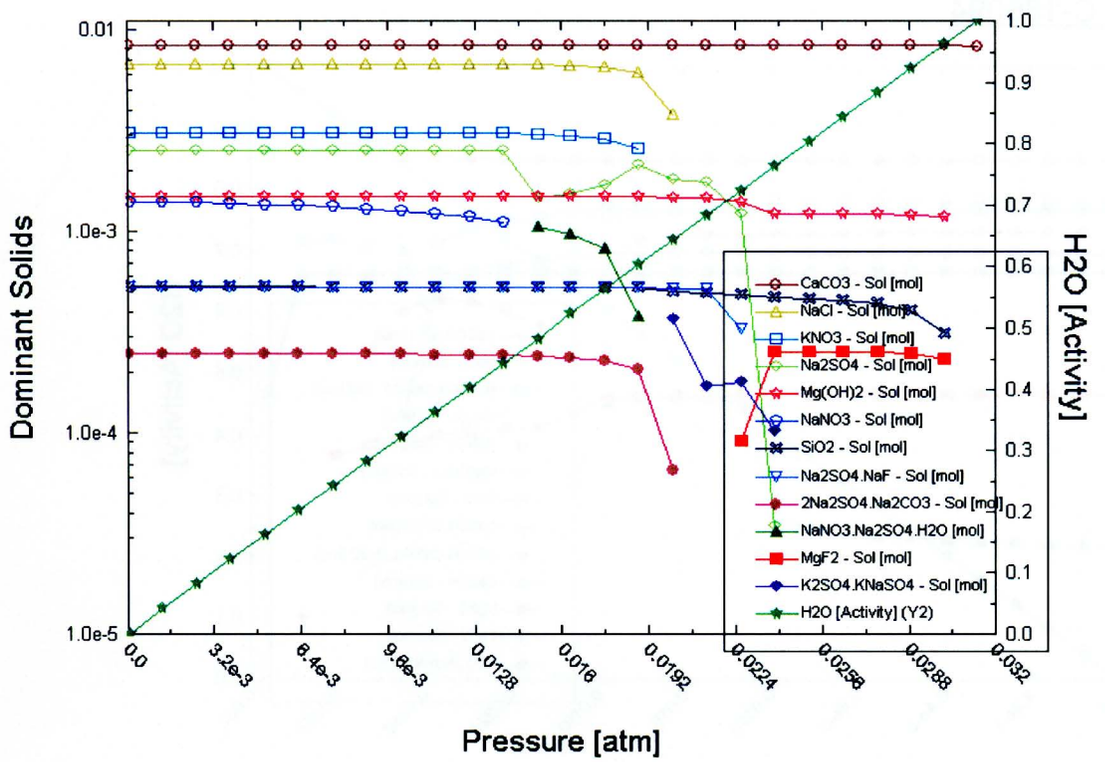
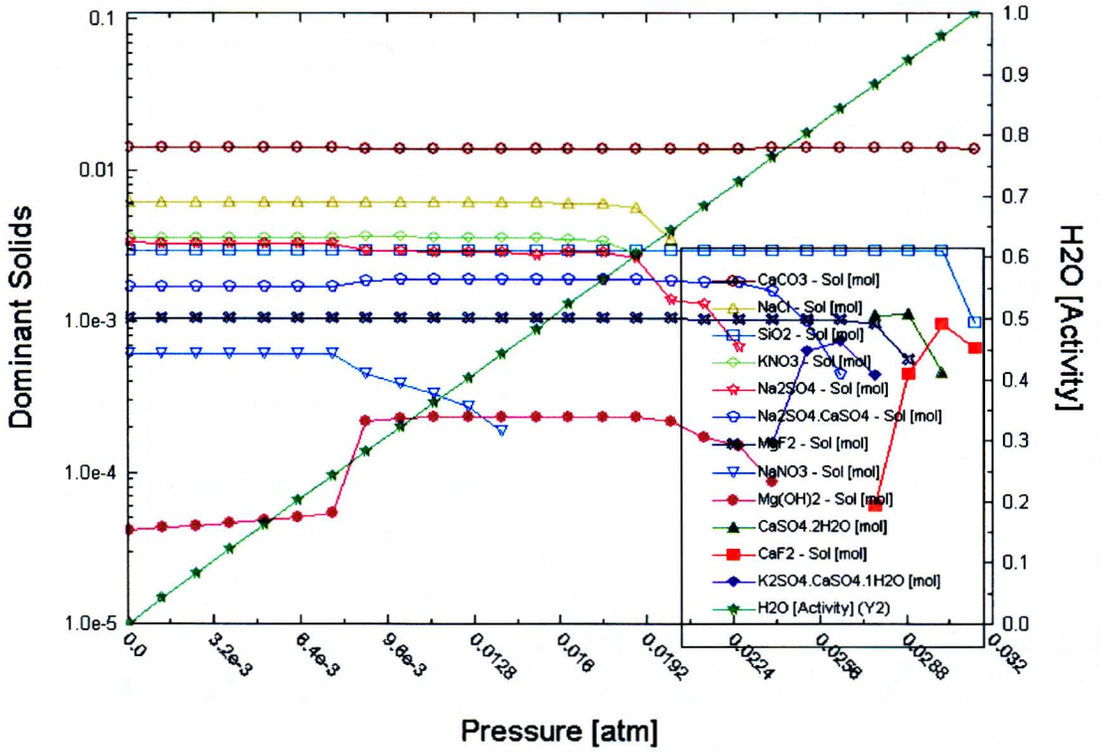




Lab sample C-186100



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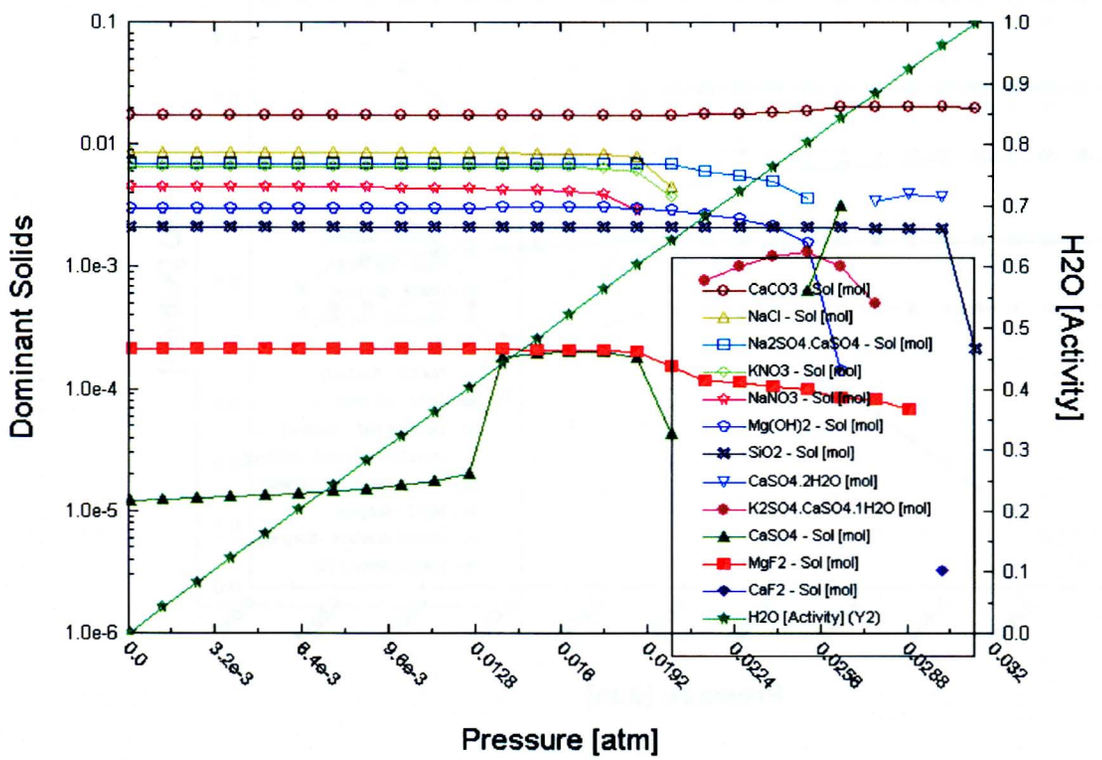
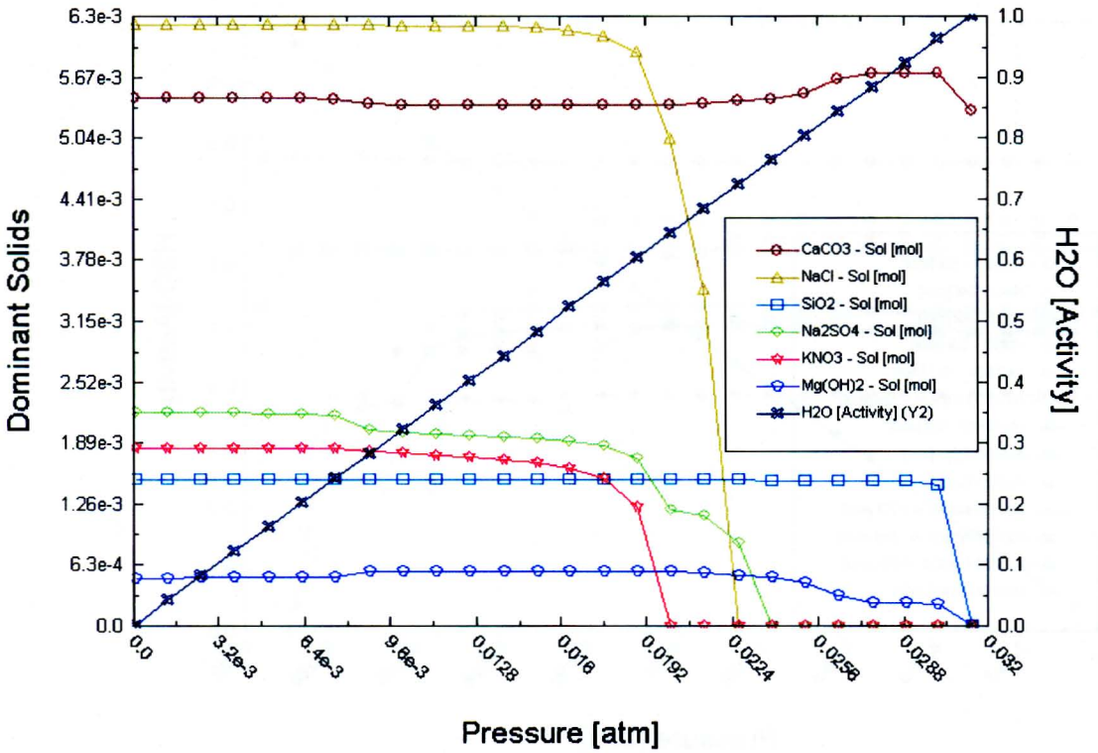
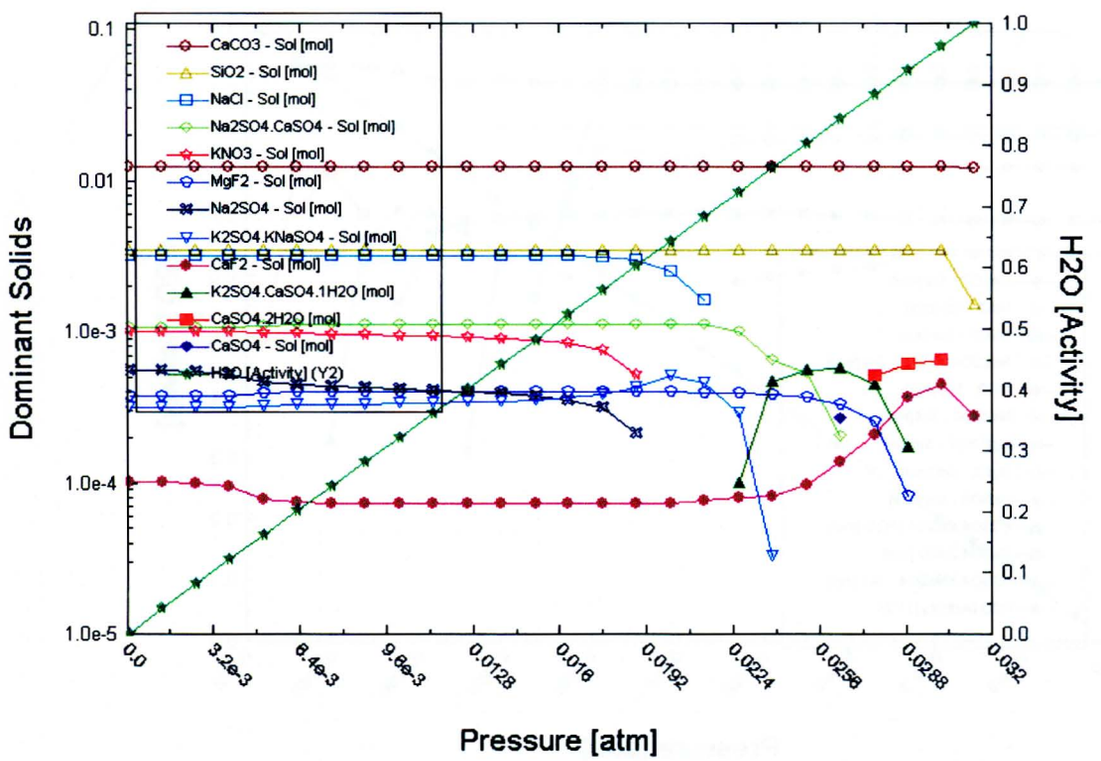


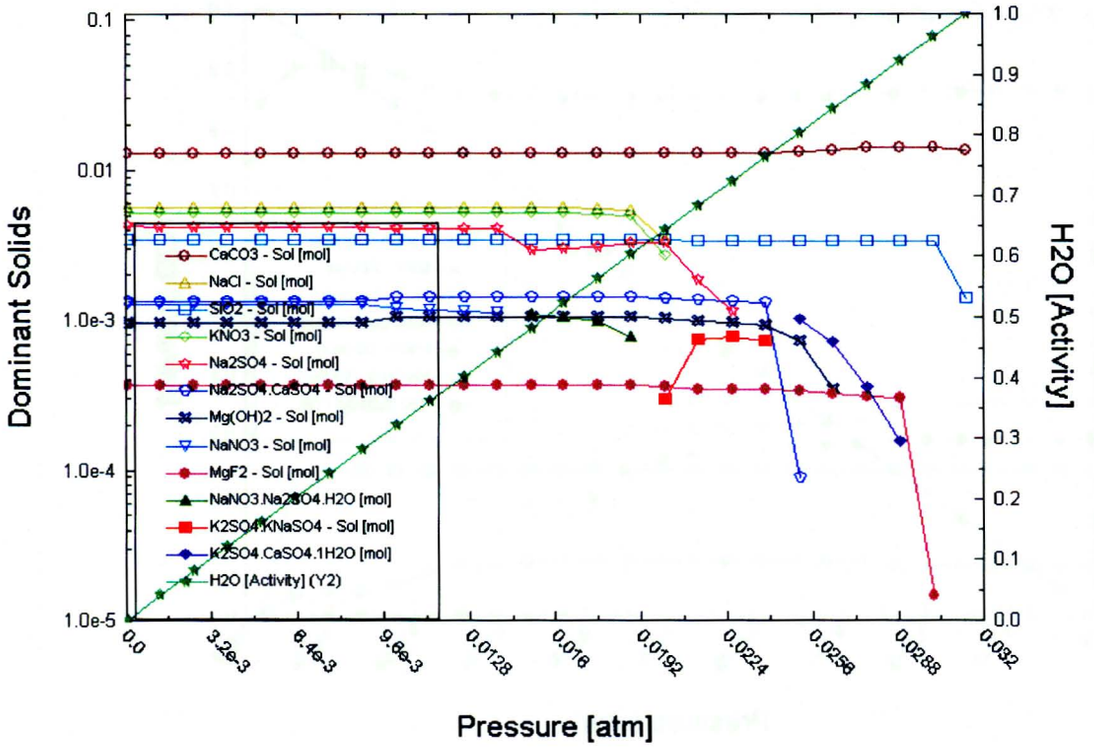
Lab sample C-186101



Lab sample C-186102



Lab sample C-186095



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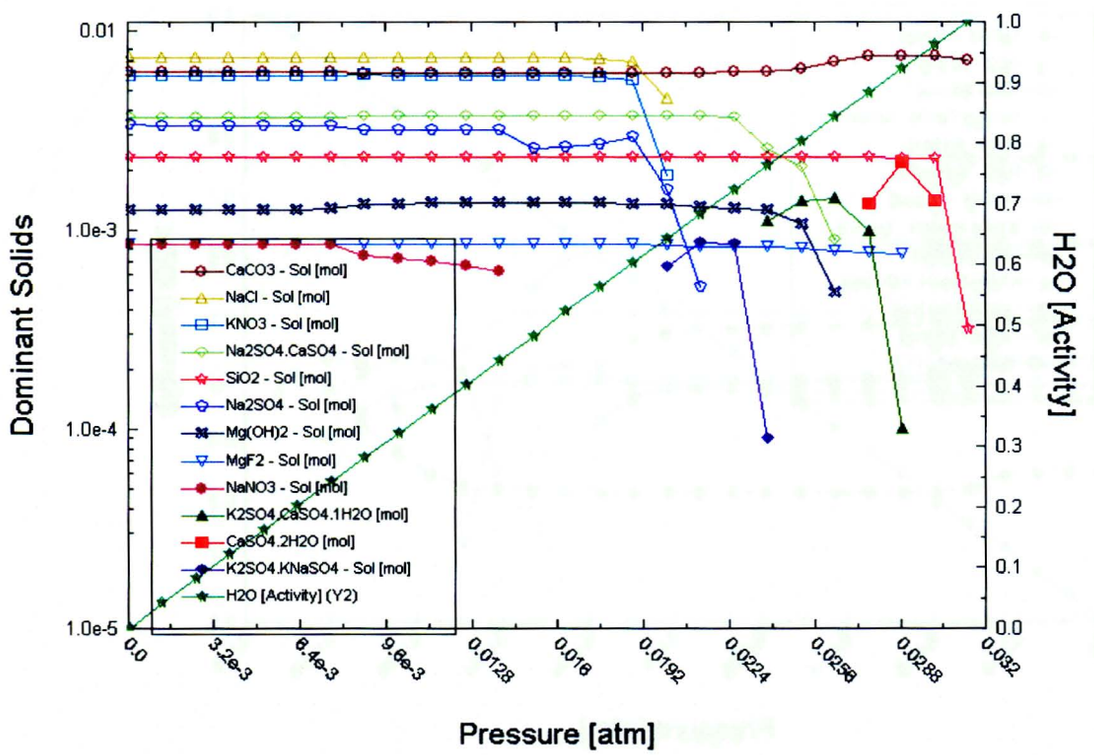

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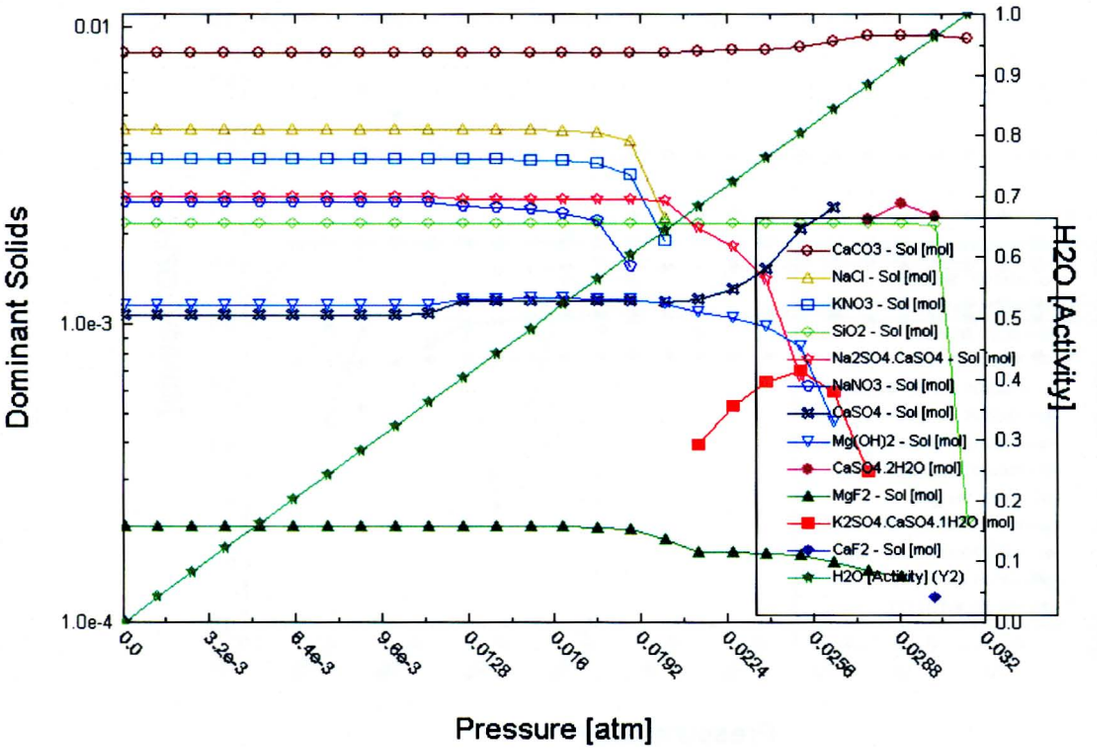
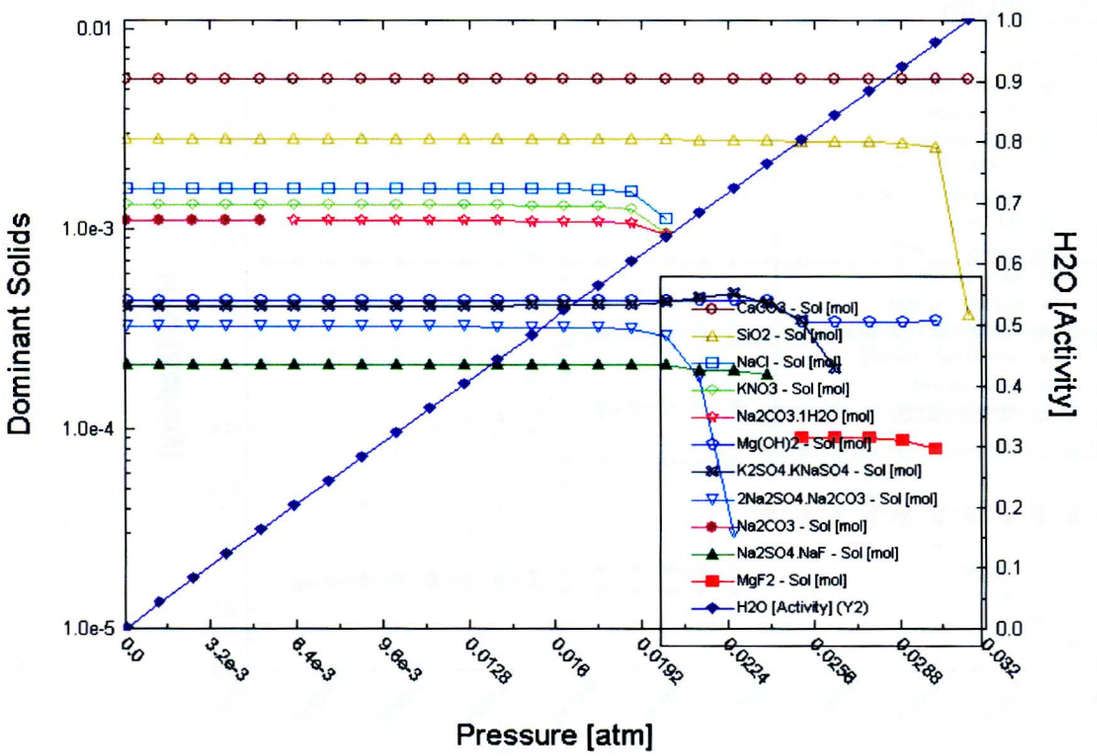
Lab sample C-186090