How water to simulate. (water from Bobby, 10/05/01).

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

SampleID	SD-9/94.2-94.4		SampleID	UZ-14/1277.7-1278	
ater Type	Ca-SO4-Cl		Water Type	Ca-Na-Cl-HCO3	
Ph (Lab)	6.2		Ph (Lab)	not avail.	
Cations	(mg/l)	(meq/l)	Cations	(mg/l)	(meq/l)
Na+	4.30E+01	1.87E+00	Na+	4.50E+01	1.96E+00
K+	0.00E+00	0.00E+00	K+	0.00E+00	0.00E+00
Mg++	2.40E+01	1.97E+00	Mg++	5.10E+00	4.20E-01
Ca++	1.25E+02	6.24E+00	Ca++	7.40E+01	3.69E+00
Anions	(mg/l)	(meq/l)	Anions	(mg/l)	(meq/l)
F-	0.00E+00	0.00E+00	F-	0.00E+00	0.00E+00
Cl-	1.70E+02	4.80E+00	Cl-	1.30E+02	3.67E+00
SO4--	2.60E+02	5.41E+00	SO4--	3.80E+01	7.91E-01
NO3-	1.10E+01	1.77E-01	NO3-	1.50E+01	2.42E-01
HCO3-	3.70E+01	6.07E-01	HCO3-	1.70E+02	2.79E+00
CO3--	0.00E+00	0.00E+00	CO3--	0.00E+00	0.00E+00
Uncharged	(mg/l)		Uncharged	(mg/l)	
SiO2	74		SiO2	38	
Al	0		Al	0	

$T = 110\ ^{\circ}C$

$P_{Total} = 0.85$ ~~bar~~ bar

Juyang 4/12/02.

to use proportionate method to balance the charge — Bobby.

J. Yang 10/15/01

Sample: SD-9/94.2-94.4

Calculate pH Reconcile pH Help

YM_wat2 Study
YMW2 Model
Sample SD-9

Sample SD-9

Measured pH: 0.0

Calculated pH: 7.71422

Template Reconcile Units LastResult Help

YM_wat2 Study
YMW2 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			CL-1	170.	169.997
CA+2	125.	136.2644	CO3-2		
K+1			F-1		
MG+2	24.	26.16287	HCO3-1	37.	36.99935
NA+1	43.	46.87492	NO3-1	11.	10.99978
			SO4-2	260.	259.9959

OLI Stream SD-9

<PgDn>

moles

TEMP	25.0
PRES	1.0
CAOH2	0.340327E-02
H2CO3	0.606962E-03
H2SO4	0.134852E-02
H4SIO4	0.123279E-02
HCL	0.479964E-02
HNO3	0.177573E-03
MGOH2	0.107748E-02
NA3HSO42	0.680300E-03
SCALE CACO3PPT	0.658233D+00

<PgUp>

Converted into OLI Stream.
← after 0.00123279 mol SiO_2
SiO_2 added as neutral species.

Juyang 10/17/01

Sample: UZ-14/1277.7-1278

Calculate pH Reconcile pH Help

YM_wat2 Study
YMW2 Model
Sample UZ-14

Sample UZ-14

Measured pH: 0.0

Calculated pH: 7.949

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			CL-1	130.	129.9964
CA+2	74.	91.26203	CO3-2		
K+1			F-1		
MG+2	5.1	6.2897	HCO3-1	170.	169.9949
NA+1	45.	55.49731	NO3-1	15.	14.99956
			SO4-2	38.	37.99889

YM_wat2 Study
YMW2 Model
OLI Stream UZ-14

OLI Stream UZ-14

TEMP	25.0
PRES	1.0
CAOH2	0.227866E-02
H2CO3	0.259000E-02
H4SIO4	0.632875E-03
HCL	0.366922E-02
HNO3	0.242074E-03
MGOH2	0.258958E-03
NA6SO42CO3	0.197914E-03
NAOH	0.122813E-02
SCALE CACO3PPT	0.429975D+01

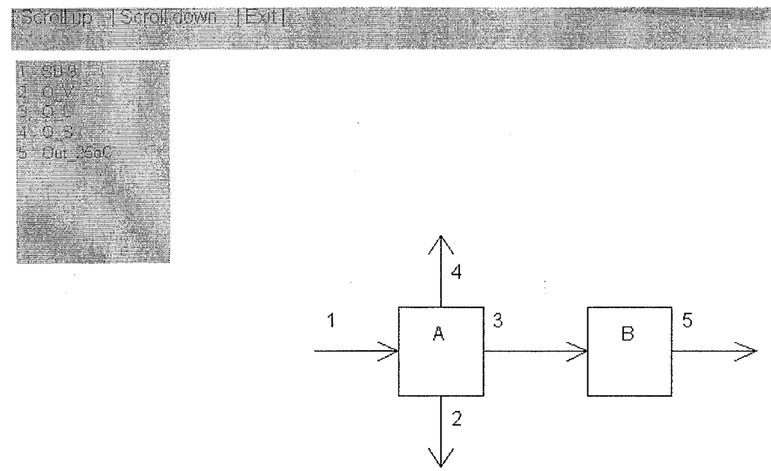
<PgUp>

mols

$0.632875 \times 60 = 38$ mg/L
SiO_2 added as neutral species then ← converted stream for OLI use.

J.Y. 10/15/01

Flow sheet

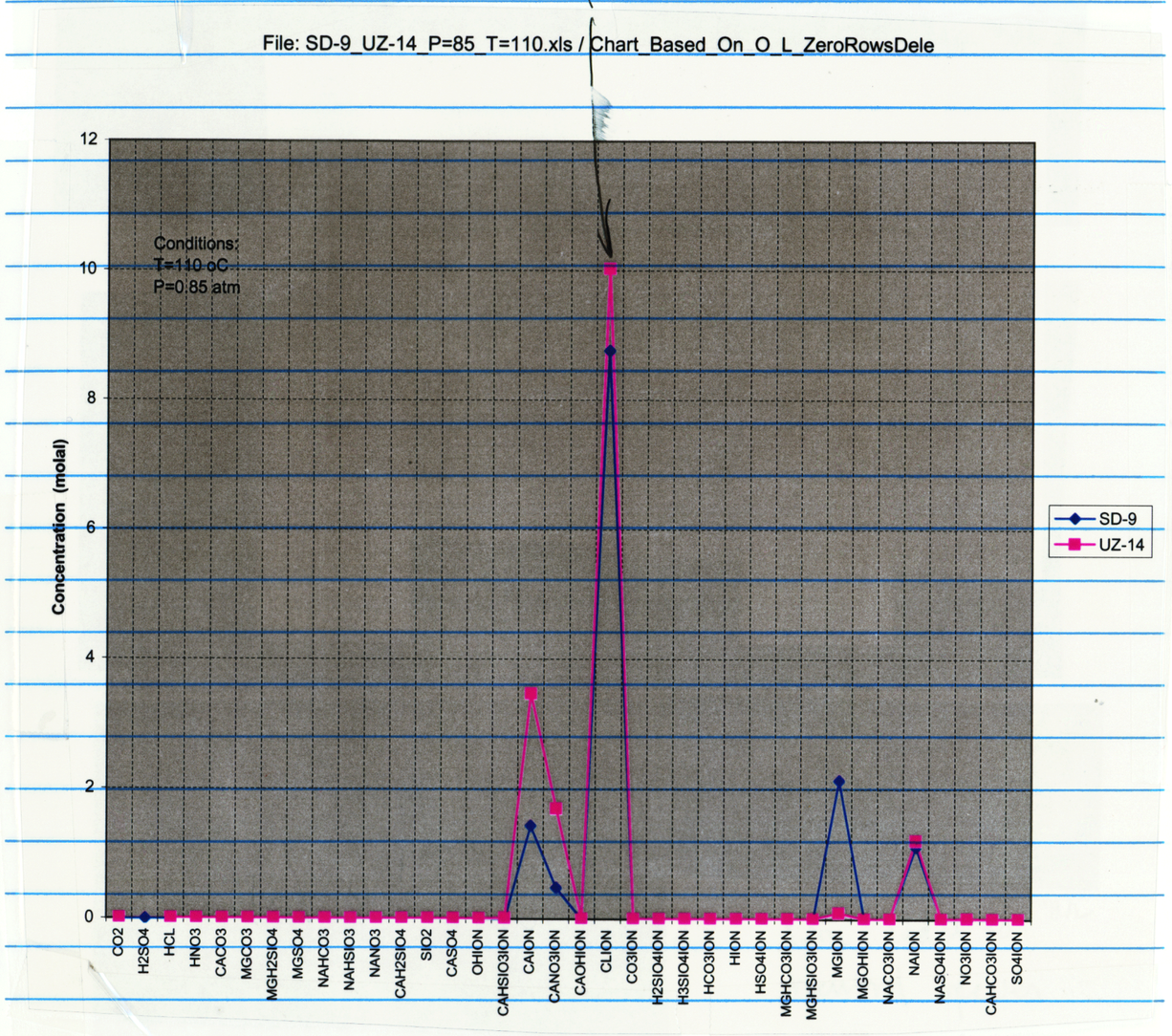


J.Y. 10/15/01

Jy.
2/14/01.

Results:

10.03 molal is 7.85 M
according to the volume in the data file.



Jy. 10/15/01

SD-9 — ~~Cl⁻ – Ca⁺⁺ – Na⁺~~ Cl⁻ – Mg⁺⁺ – Ca⁺⁺ – Na⁺ system

UZ-14 Cl⁻ – Ca⁺⁺ – Na⁺ system,

Jy 10/17/01

More water from Bobby:

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

SampleID	SD-9/94.2changed	
Water Type	Ca-Na-SO4-Cl	
Reference	test chem divide	
Cations	(mg/l)	(meq/l)
Na+	5.536E+01	2.408E+00
K+	0.000E+00	0.000E+00
Mg++	2.399E+01	1.974E+00
Ca++	1.142E+02	5.700E+00
Anions	(mg/l)	(meq/l)
F-	0.000E+00	0.000E+00
Cl-	1.700E+02	4.795E+00
SO4--	2.600E+02	5.414E+00
NO3-	1.100E+01	1.774E-01
HCO3-	3.700E+01	6.065E-01
CO3--	0.000E+00	0.000E+00

ID:
UZ-9B

Na^+ increased from 4.3E+1
Ca^{++} decreased from 1.25E2
others no change.

$(43 - 5.536E1)/23 = -0.537$ mmol

$(1.25E2 - 114.2)/40 = 0.27$ mmol $= 0.54$ eq mmol.

$SiO_2 = 74$ mg/L.

Jy.
10/19/01

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

SampleID	UZ-14/1277.7changed	ID:
Water Type	Ca-Na-Cl-HCO3	
Reference	test of chemical divide	UZ-14B
Cations	(mg/l)	(meq/l)
Na+	5.173E+01	2.250E+00
K+	0.000E+00	0.000E+00
Mg++	5.100E+00	4.196E-01
Ca++	6.814E+01	3.400E+00
Anions	(mg/l)	(meq/l)
F-	0.000E+00	0.000E+00
Cl-	1.300E+02	3.667E+00
SO4--	3.800E+01	7.912E-01
NO3-	1.500E+01	2.419E-01
HCO3-	1.700E+02	2.787E+00
CO3--	0.000E+00	0.000E+00

decreased from 7.40 E+1

increased from 4.50 E+1

~~$\Delta = 22.3/23 = 0.969$ m mol~~

others no change.

J. Yang 10/19/01

$(7.40E1 - 68.14)/40 = 0.1465$ m mol $= 0.293$ eq mol

$(45 - 51.73)/23 = 0.2926$ mmol

$SiO_2 = 38$ mg/L.

J. Yang 10/19/01

Calculate pH Reconcile pH Help

YM_WAT2 Study
YMW2 Model
Sample UZ-14B

Sample UZ-14B

Measured pH: 0.0

Calculated pH: 8.00603

Template Reconcile Units LastResult Help

YM_WAT2 Study
YMW2 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			CL-1	130.	129.9962
CA+2	68.14	84.03099	CO3-2		
K+1			F-1		
MG+2	5.1	6.289374	HCO3-1	170.	169.9951
NA+1	51.73	63.79385	NO3-1	15.	14.99956
			SO4-2	38.	37.99885

<PgDn>

Help

Sample UZ-14B

UZ-14B 10/19/2001

Electroneutrality: reconciled using Proration Method using 23.32% of each cation

pH: not reconciled.

SiO_2: 38 mg/L added as neutral.

J. Yang 10/19/01

Calculate pH Reconcile pH Help

YM_WAT2 Study
YMW2 Model
Sample SD-9B

Sample SD-9B

Measured pH: 0.0

Calculated pH: 7.71315

YM_WAT2 Study
YMW2 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			CL-1	170.	169.9971
CA+2	114.2	124.5074	CO3-2		
K+1			F-1		
MG+2	24.	26.16623	HCO3-1	37.	36.99935
NA+1	55.36	60.35669	NO3-1	11.	10.99983
			SO4-2	260.	259.9955

<PgDn>

Sample SD-9B

SD-9B 10/19/2001

Electroneutrality: reconciled using Proration Method using 9.03% of each cation

pH: not reconciled.

SiO_2: 74 mg/L added as neutral species.

J. Yang 10/19/01

Simulation Flowsheet same as that in Page 149.

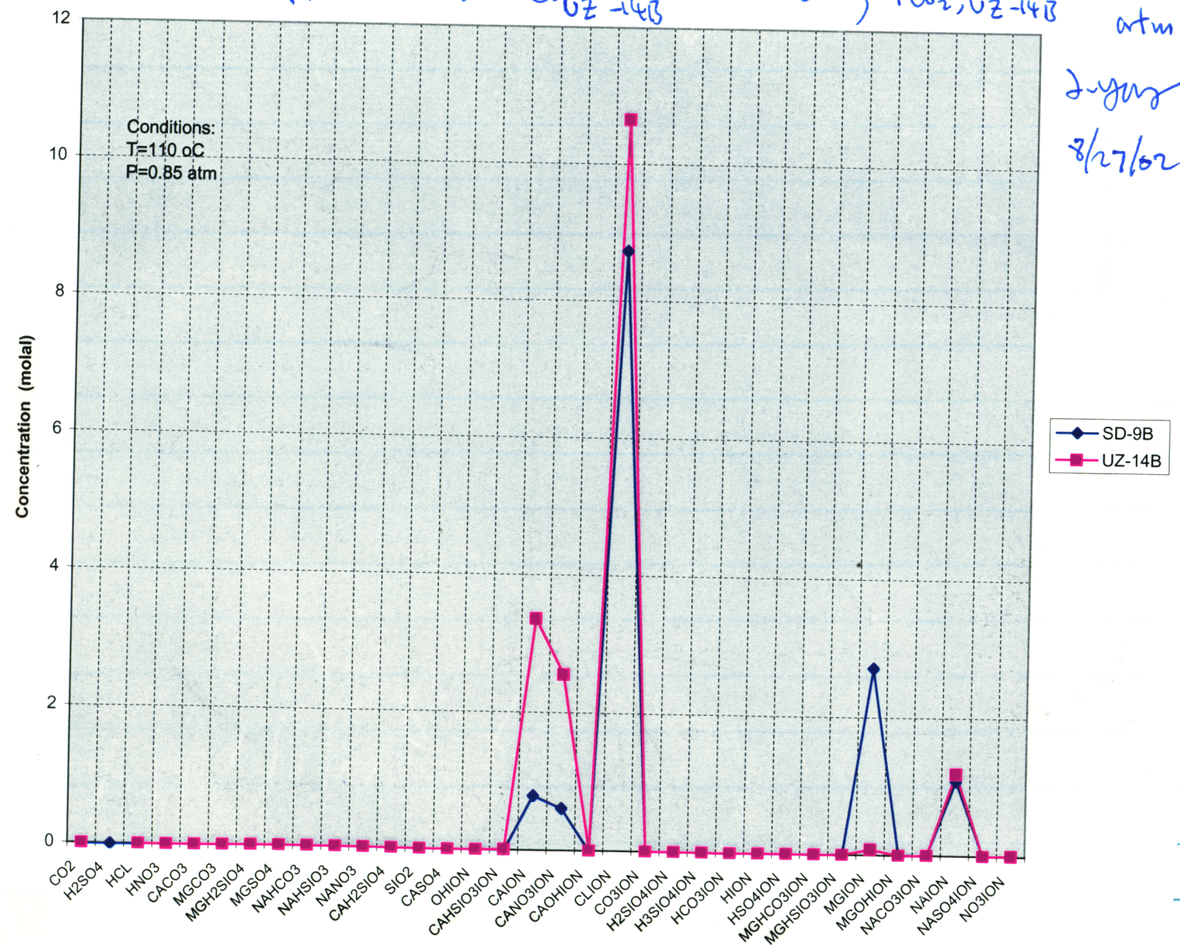
J.Y. 10/19/01.

Results.

File: SD-9B_UZ-14B_P=85_T=110.xls / Chart_Based_On_O_L_ZeroRowsDele

From the file: Cl^-_{UZ-14B} = 10.65 molal; $P_{CO_2,UZ-14B}$ = 2.72E-4 atm.

J.Yang 8/27/02



The free NO_3^- seems too low, most of NO_3^- went to $CaNO_3^+$ - check the data:

SinglePoint1 Results
12/7/01 4:18:49 PM
StreamAnalyzer
Page 3 of 4
OLI Systems, Inc.

User Inflows	Related Inflows	Aqueous Species	Vapor Species	Solid Species	Second Liquid Species
H2O	Ca(NO3)2.4H2O	H2O	H2O - Vap	Ca(NO3)2.4H2O	
Ca(NO3)2	Ca(OH)2	HNO3 - Aq	HNO3 - Vap	Ca(OH)2	
	Ca(NO3)2.3H2O	H+1		Ca(NO3)2.3H2O	
	HNO3	NO3-1		Ca(NO3)2	
		Ca+2			
		CaOH+1			
		OH-1			
		Ca(NO3)+1			

Result obtained using public library.

Species Activity Coefficients

H2O	0.78669	Activity
HNO3 - Aq	1.8332	Act-Coef
H+1	2.0113	Act-Coef
NO3-1	0.63828	Act-Coef
Ca+2	0.047721	Act-Coef
CaOH+1	1.1251	Act-Coef
OH-1	0.49106	Act-Coef
Ca(NO3)+1	1.1251	Act-Coef
H2O - Vap	1.0000	Fug-Coef
HNO3 - Vap	1.0000	Fug-Coef

Species K(eq)-Values 25°C

H2O	1.0144e-14	mol^0
HNO3 - Aq	20.128	mol^0
CaOH+1	0.058762	mol^0
Ca(NO3)+1	0.38045	mol^0
H2O - Vap	31.855	mol^0
HNO3 - Vap	21023	mol^0
Ca(NO3)2.4H2O	4.5041	mol^0
Ca(OH)2	3.8398e-6	mol^0
Ca(NO3)2.3H2O	10.817	mol^0
Ca(NO3)2	1341.5	mol^0

$k = 0.38045$ at 25°C.

Species Mobilities

H+1	9.0010e-4	m2/ohm-mol
NO3-1	1.8383e-4	m2/ohm-mol
Ca+2	1.5397e-4	m2/ohm-mol
CaOH+1	7.6893e-5	m2/ohm-mol
OH-1	5.0721e-4	m2/ohm-mol
Ca(NO3)+1	1.5448e-4	m2/ohm-mol

12/7/01

Species Self Diffusivities

H2O	1.8967e-9	m2/s
HNO3 - Aq	1.4696e-9	m2/s
H+1	6.7865e-9	m2/s
NO3-1	1.3758e-9	m2/s

SinglePoint1 Results
12/7/01 4:20:35 PM
StreamAnalyzer
Page 3 of 4
OLI Systems, Inc.

User Inflows	Related Inflows	Aqueous Species	Vapor Species	Solid Species	Second Liquid Species
H2O	Ca(NO3)2.4H2O	H2O	H2O - Vap	Ca(NO3)2.4H2O	
Ca(NO3)2	Ca(OH)2	HNO3 - Aq	HNO3 - Vap	Ca(OH)2	
	Ca(NO3)2.3H2O	H+1		Ca(NO3)2.3H2O	
	HNO3	NO3-1		Ca(NO3)2	
		Ca+2			
		CaOH+1			
		OH-1			
		Ca(NO3)+1			

1102.

Species Activity Coefficients

H2O	0.71241	Activity
HNO3 - Aq	1.2940	Act-Coef
H+1	1.6110	Act-Coef
NO3-1	0.84575	Act-Coef
Ca+2	0.054095	Act-Coef
CaOH+1	0.97878	Act-Coef
OH-1	0.73409	Act-Coef
Ca(NO3)+1	0.97878	Act-Coef
H2O - Vap	0.99225	Fug-Coef
HNO3 - Vap	0.98619	Fug-Coef

For SD-9
$C_{Ca^{++}} = 1.44$
$C_{NO_3^-} = 0.00547$

Lujun
12/7/01

Species K(eq)-Values (1102)

H2O	7.8230e-13	mol^0
HNO3 - Aq	2.7554	mol^0
CaOH+1	0.010085	mol^0
Ca(NO3)+1	0.14621	mol^0
H2O - Vap	0.71797	mol^0
HNO3 - Vap	215.17	mol^0
Ca(NO3)2.4H2O	30.938	mol^0
Ca(OH)2	2.3230e-7	mol^0
Ca(NO3)2.3H2O	5.5499e7	mol^0
Ca(NO3)2	329.81	mol^0

$CaNO_3 \overset{k}{=} Ca^{++} + NO_3^-$

$k(1102) = 0.14621$

$C_{CaNO_3^+} \doteq \left(\frac{1}{k}\right) C_{Ca^{++}} C_{NO_3^-}$

$= \frac{1}{0.14621 * 1.44 * 0.00547}$

$= 0.0539$ mol/kg.

(print out $C_{CaNO_3^+} = 0.486$ mol/kg)
activity coefficient effect?

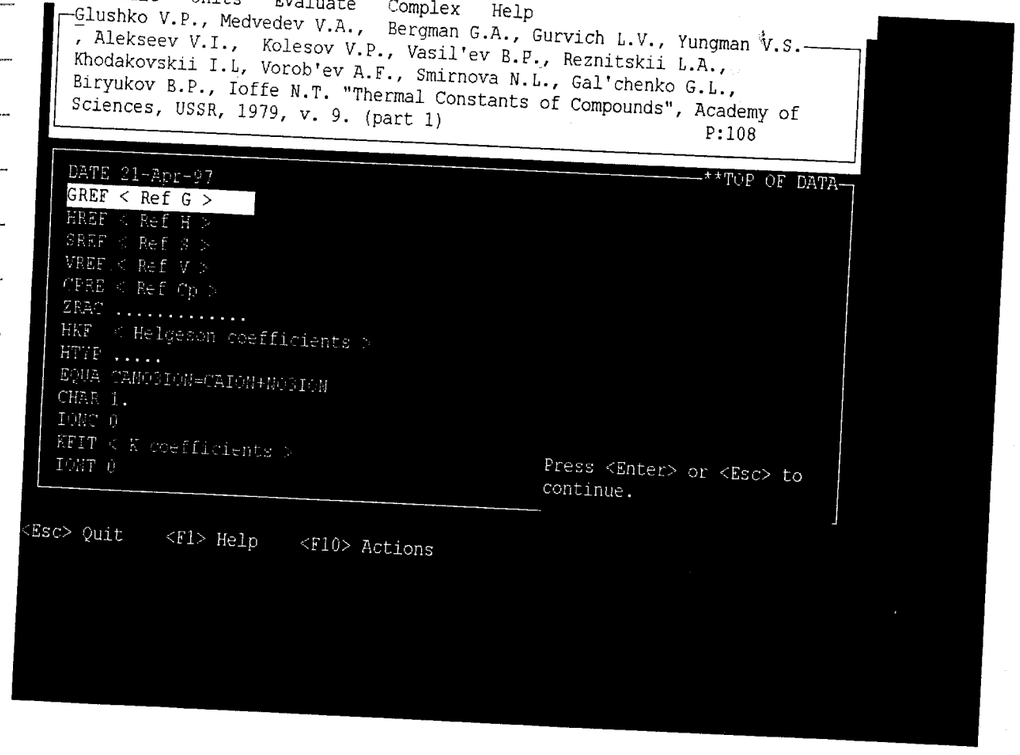
Species Mobilities

H+1	3.1252e-3	m2/ohm-mol
NO3-1	9.6187e-4	m2/ohm-mol
Ca+2	9.6087e-4	m2/ohm-mol
CaOH+1	4.7894e-4	m2/ohm-mol
OH-1	2.2777e-3	m2/ohm-mol
Ca(NO3)+1	9.9105e-4	m2/ohm-mol

Species Self Diffusivities

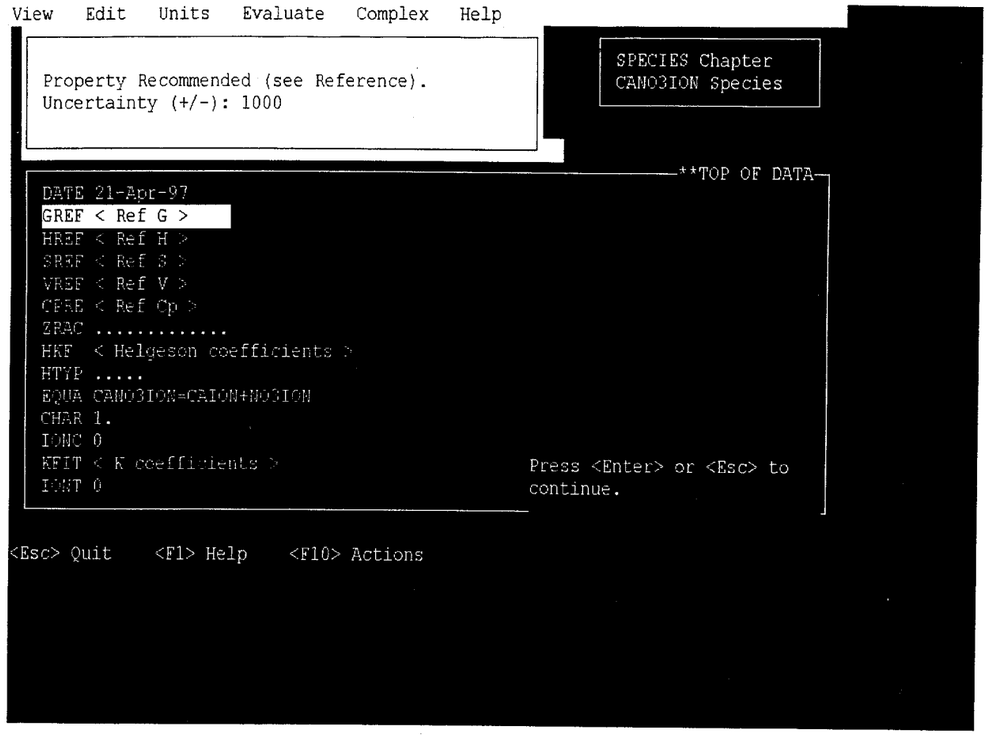
H2O	9.4601e-9	m2/s
HNO3 - Aq	6.5383e-9	m2/s
H+1	2.1178e-8	m2/s
NO3-1	6.1946e-9	m2/s

In the Esp 6.1, go to Databook and check the source for $CaNO_3^+$ species (public library)



Source for $CaNO_3^+$

L. Yang
10/7/01



L. Yang
10/7/01

2/25/02.

Additional Lead Speciation Calculations

Objective: To predict the speciation of the supersaturated $PbCl_2$ solution used for corrosion tests

Solution preparation conditions:

- 25g $PbCl_2$ in 1 liter deaerated deionized water
- 95°C
- pH = 0.5 adjust by HCl (at room temp).

ICP analysis results:

- Total lead – 11,600 ppm
- Total chloride – 10,900 ppm

J. Yang 2/26/02.

Survey1 Results
2/26/02 10:56:40 AM — *StreamAnalyzer* — Page 1 of 7
OLI Systems, Inc.

Calculation Summary

Survey1 Calculation for Survey1 - Workstream

Automatic Chemistry Model
Public Databank

pH survey

Acid - Hydrogen chloride	
Base - Hydrogen chloride	
Range	0.10000 to 1.0000 pH
Step size	0.10000 pH
No. steps	9
No. points	10

cut 2/25. to know how HCl was added.

No secondary survey selected

J. Yang 2/26/02

Stream Inflows

pH	H2O	PbCl2	HCl
pH	mol	g	mol
0.10000	55.508	25.000	0.97792
0.20000	55.508	25.000	0.79789
0.30000	55.508	25.000	0.64558
0.40000	55.508	25.000	0.51855
0.50000	55.508	25.000	0.41401
0.60000	55.508	25.000	0.32897
0.70000	55.508	25.000	0.26046
0.80000	55.508	25.000	0.20572
0.90000	55.508	25.000	0.16228
1.0000	55.508	25.000	0.12798

3.0
3.0
4.5

1.2538E-3
3.0553E-5

therefore 0.41401 mol HCl is needed to get 0.5 pH at room temperature.

Calculation Summary

SinglePoint1 Calculation for Stream2

Automatic Chemistry Model
Public Databank

Isothermal Calculation

Temperatu	95 °C
Pressure	1 atm

Stream Parameters

Stream Am	56.012	mol
Temperatu	95	°C
Pressure	1	atm
pH	0.5345	pH
Osmotic Pı	23.45	atm
Ionic Stren	0.44355	mol/kg H2O
WaterActiv	0.98568	Activity
Electrical C	0.27127	1/ohm
Electrical C	564.32	cm2/ohm-mol
Viscosity, a	0.31583	cP
Viscosity, r	1.063	cP/cP H2O

	Units	Total	Aqueous	Vapor	Solid	2nd Liquid
Density	g/ml	n/a	0.98183	0	5.8499	0
Enthalpy	cal	-3.75E+06	-3.74E+06	0	-3312	0

Stream Inflows

Water	55.508	mol
Lead(II) ch	25	g
Hydrogen (	0.41401	mol

Input based on results on page 161.

Scaling Tendencies

solids withi Temperature Range

Lead(II) ch	1	0	287.00 °C	inside range
Lead(II) ox	2.81E-13	data valid thr		inside range

Total and Phase Flows

	Units	Total	Aqueous	Vapor	Solid	2nd Liquid
Mole	mol	56.012	56.4	0	0.039155	0
Mass	g	1040.1	1029.2	0	10.889	0
Volume	L	1.0501	1.0482	0	1.86E-03	0

total aqueous mass

Species Output (True Species)

	Total mol	Aqueous mol	Vapor mol	Solid mol	2nd Liquid n/a
H2O	55.508	55.508	0	0	0
PbCl2	0.060699	0.021544	0	0.039155	0

HCl	2.60E-06	2.60E-06	0	0	0
PbO	9.03E-17	9.03E-17	0	0	0
PbCl4-2	2.78E-03	2.78E-03	0	0	0
H+1	0.41401	0.41401	0	0	0
PbOH+1	8.66E-09	8.66E-09	0	0	0
Pb+2	2.89E-03	2.89E-03	0	0	0
PbCl3-1	5.44E-03	5.44E-03	0	0	0
HPbO2-1	8.14E-26	8.14E-26	0	0	0
PbCl+1	0.018083	0.018083	0	0	0
OH-1	2.66E-12	2.66E-12	0	0	0
Cl-1	0.42688	0.42688	0	0	0

Molecular Output (Apparent Species)

	Total mol	Aqueous mol	Vapor mol	Solid mol	2nd Liquid n/a
H2O	55.457	55.457	0	0	0
PbCl2	0.039155	0	0	0.039155	0
HCl	0.51549	0.51549	0	0	0
PbO	0.050739	0.050739	0	0	0

Results.

Element Balance

	Total mol	Aqueous mol	Vapor mol	Solid mol	2nd Liquid n/a		Concentration of Dissolved Species FW	gram	ppm
CL(-1)	0.5938	0.51549	0	0.07831	0	Cl	35.5	18.3	17780.7
H(+1)	111.43	111.43	0	0	0				
O(-2)	55.508	55.508	0	0	0				
PB(+2)	0.089894	0.050739	0	0.039155	0	Pb	207.2	10.513	10214.85

Speciation Summary

User Inflows	Related Inflows	Aqueous Species	Vapor Species	Solid Species	Second Liquid Species
H2O	Pb(OH)2	H2O	H2O - Vap	PbCl2	
PbCl2	PbO	PbCl2 - Aq	HCl - Vap	PbO	
HCl		PbO - Aq			
		HCl - Aq			
		PbCl4-2			
		H+1			
		PbOH+1			
		Pb+2			
		PbCl3-1			
		HPbO2-1			
		PbCl+1			
		OH-1			
		Cl-1			

Note.

① $= \frac{18.3}{1029.2} * 10^6$

$= 17780.7$

Species Activity Coefficients

H2O	0.98568	Activity
PbCl2 - Aq	1.0105	Act-Coef
PbO - Aq	1.0105	Act-Coef
HCl - Aq	1.0105	Act-Coef
PbCl4-2	0.11853	Act-Coef

Similarly, For pH = 3.0, 4.5 and at T = 25°C, 95°C

the values were calculated and the main results are as follows:

pH = 0.5, T = 25°C

uid	Concen. of Dissolved Species	FW	gram	ppm
0	Cl- total	35.5	15.13862	14888.49
0				
0				
0	Pb++ total	207.2	1.287686	1266.41

pH = 0.5, T = 95°C (25°C)

Concen. of Dissolved Species	FW	gram	ppm
Cl- total	35.5	18.3	17780.7
Pb++ total	207.2	10.513	10214.85

pH(95°C) = 0.534

pH = 3.0, T = 25°C

Concen. of Dissolved Species	FW	gram	ppm
Cl-	35.5	2.823777	2793.329
Pb++ total	207.2	8.110637	8023.184

pH(25°C) = 3, T = 95°C

Concen. of Dissolved Species	FW	gram	ppm
Cl- total	35.5	6.42692	6270.166
Pb++ total	207.2	18.62604	18171.74

pH(95°C) = 3.021

pH(25°C) = 4.5, 25°C

Concen. of Dissolved Species	FW	gram	ppm
Cl- total	35.5	2.811955	2781.36
Pb++ total	207.2	8.203048	8113.796

pH(25°C) = 4.5, T = 95°C

Concen. of Dissolved Species	FW	gram	ppm
Cl- total	35.5	6.38361	6227.912
Pb++ total	207.2	18.62604	18171.74

pH(95°C) = 3.812

L. Yang 2/26/02

Evaporation Analysis.

Lietai Yang

From: Roberto Pabalan [rpabalan@cnwra.swri.edu]
Sent: Monday, January 28, 2002 2:28 PM
To: Lietai Yang
Subject: input file for ESP

2/27/02 L.Yang

For LYang analyses 012802.xls

Lietai:

Attached is an Excel file with the YM pore water compositions. Units are in millimoles/liter.

Thanks.

bobby

These are modified waters for testing purpose, 2/6/03 L.Y.

For LYang analyses 012802.xls

mMol/L ≒ m molal

SampleID	pHLab	Na	K	Mg	Ca	F	Cl	SO4	NO3	HCO3	CO3	SiO2	Al
UE-25 NRG-6	7.4	4.31927	0	0.172768	0.606287	n.a.	2.17189	0.801616	0.7579423	1.507999	0	1.021801	3.71E-02
UE-25 NRG-7a	8.3	3.566768	0	0.152201	1.072854	n.a.	1.511861	0.681894	0.7047251	2.098085	0	1.146613	3.71E-02
UE-25 UZ-N2	0	1.091779	0	0.160428	0.359281	n.a.	0.282064	0.218623	0.4402516	0.953973	0	9.65E-02	0
USW SD-9	7.5	4.132232	0	0.390786	1.072854	n.a.	1.805207	1.290914	3.06E-02	1.999738	0	0.97354	0
USW UZ-14-a	0	2.131361	0	0.185109	1.546906	n.a.	2.453953	0.468477	0.2741493	2.78652	0	0.732235	0
USW UZ-14-b	6.9	1.892127	0	0.542987	1.24501	n.a.	1.692382	0.687099	0.3547815	2.147259	0	1.494425	1.11E-02
USW UZ-14-c	0	1.739887	0.161125	0.12752	0.923154	n.a.	0.203086	0.596527	0.2048057	2.360346	0	0.356133	0
USW UZ-14-d	7	1.796433	0	0.567668	1.27495	n.a.	1.24108	0.864079	0.3709079	2.098085	0	1.527709	0
USW UZ-14-e	8.3	3.827751	0.148338	0.168655	1.122754	n.a.	0.437199	2.321563	0	1.739116	0	0.128141	0

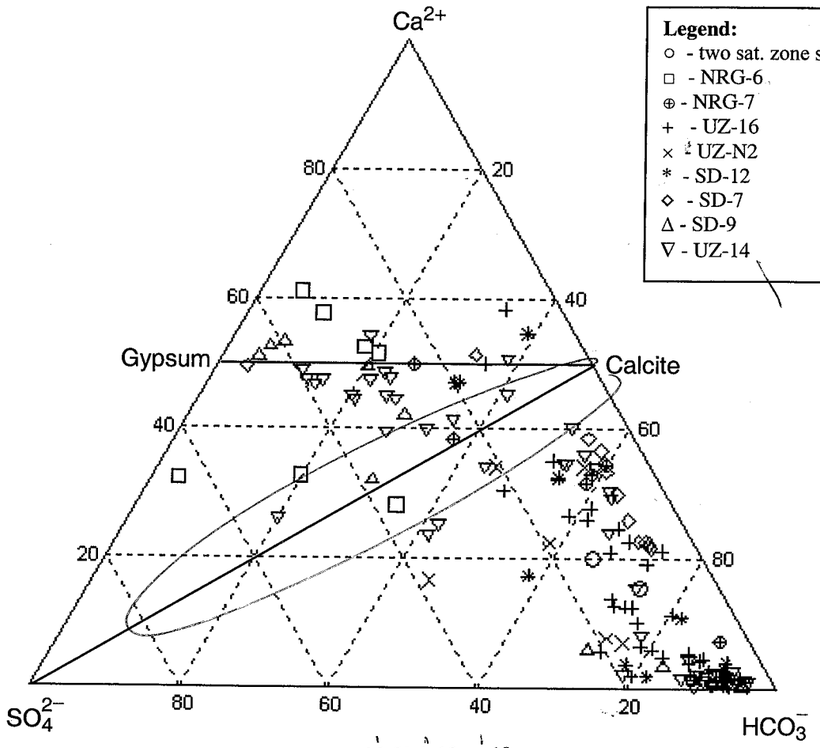
2/27/02

Bobby wants to do just UZ-2r NRG-6 and ① USW SD-9 two kinds. These two are on the border line of divide diagram. (See next page)

① — Na-Ca-Cl-SO4-HCO3 type

② — ~~Na-Ca-HCO3-NO3-SO4~~ L.Yang 2/27/02.
Na-Ca-SO4-HCO3-Cl type

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



Notebook#185, Vol. 10; p. 18
RTP; January 21, 2002

Analyses to be conducted at 110°C, using Eqp 6.5
see pages 121 – 133 for details.

J. Yang
2/27/02

Sample reconciliation using Water Analyzer; Sample manager.

NRG-6

Template Reconcile Units LastResult Help

YMW2 Study
YM2 Model
Concentrations

Values in molality

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3	3.71000E-05	3.71000E-05	OH-1		
CA+2	6.06287E-04	6.06287E-04	CL-1	0.00217189	0.00217189
H+1			CO3-2		
K+1			F-1		
MG+2	1.72768E-04	1.72768E-04	H3SIO4-1		
NA+1	0.00431927	0.00437162	HCO3-1	0.001508	0.001508
			HSO4-1		
			NO3-1	7.57900E-04	7.57900E-04
			SO4-2	8.01620E-04	8.01620E-04

<PgDn>

Unit: molal

5.23E-5 molality Na^+ added to reconcile the sample.

YMW2 Study
YM2 Model
Sample NRG-6

Sample NRG-6

Measured pH: 0.0

Calculated pH: 7.36044

Neutrals/Organics	Input	Values in molality Reconciled
NAHSIO3	0.0	
NANO3	0.0	
ALF3	0.0	
CACO3	0.0	
SIO2	0.001021801	
CAH2SIO4	0.0	

J. Yang
2/27/02

SD-9

YMW2 Study
YM2 Model
Concentrations

Values in molality

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			OH-1		
CA+2	0.001072854	0.00107285	CL-1	0.00180521	0.00180521
H+1			CO3-2		
K+1			F-1		
MG+2	3.90786E-04	3.90786E-04	H3SIO4-1		
NA+1	0.004132232	0.00413223	HCO3-1	0.00199974	0.00264189
			HSO4-1		
			NO3-1	3.06000E-05	3.06000E-05
			SO4-2	0.0012909	0.0012909

6.421E-4 molality of HCO_3^- added during reconciliation

YMW2 Study
YM2 Model
Sample SD-9

Sample SD-9

Measured pH: 0.0

Calculated pH: 7.71497

Neutrals/Organics	Input	Values in molality Reconciled
NAHSIO3		
NANO3		
ALF3		
CACO3		
SIO2	9.73540E-04	

Lyons
2/7/02

Samples were converted into OLI Stream File using StreamAnalyzer of OLI Tool kit.

Utility Send Help

YMW2 Study
YM2 Model
OLI Stream NRG-6

OLI Stream NRG-6

UNITS	USER	CALORI	GMOLE	HOUR	CENTIG	ATMOSP	METER	LITER	MOLALI
TEMP	25.0								
PRES	1.0								
ALOH3	0.371038E-04								
CAOH2	0.606349E-03								
H2CO3	0.110730E-02								
H4SIO4	0.102191E-02								
HCL	0.217211E-02								
HNO3	0.757978E-03								
MGOH2	0.172786E-03								
NA6SO42CO3	0.400851E-03								
NAOH	0.196696E-02								
SCALE ALOH3PPT	0.100000D+01	273.150	373.150						
SCALE ALOOHPPT	0.738497D+00	373.250	523.150	EXCL TR					
SCALE SIO2PPT	0.533725D+00	273.150	573.150						
SCALE CACO3PPT	0.162726D+00								
SCALE NAALCO3OH2PPT	0.104325D-01								
END									

<PgUp>

Lyons
2/7/02

```
Utility   Send   Help
```

```
YMW2 Study
YM2 Model
OLI Stream SD-9
```

OLI Stream SD-9

UNITS	USER	CALORI GMOLE	HOUR	CENTIG ATMOSP METER	LITER	MOLALI
TEMP	25.0					
PRES	1.0					
CAOH2	0.107295E-02					
H2CO3	0.199662E-02					
H4SIO4	0.973630E-03					
HCL	0.180538E-02					
HNO3	0.306028E-04					
MGOH2	0.390822E-03					
NA6SO42CO3	0.645510E-03					
NAOH	0.259554E-03					
SCALE CACO3PPT	0.100000D+01					
SCALE SIO2PPT	0.505309D+00	273.150	573.150			
SCALE CASO4.2H2O	0.183923D-01	273.150	373.150			
SCALE CASO4PPT	0.131595D-01	373.150	523.150	EXCL TR		
END						

<PgUp>

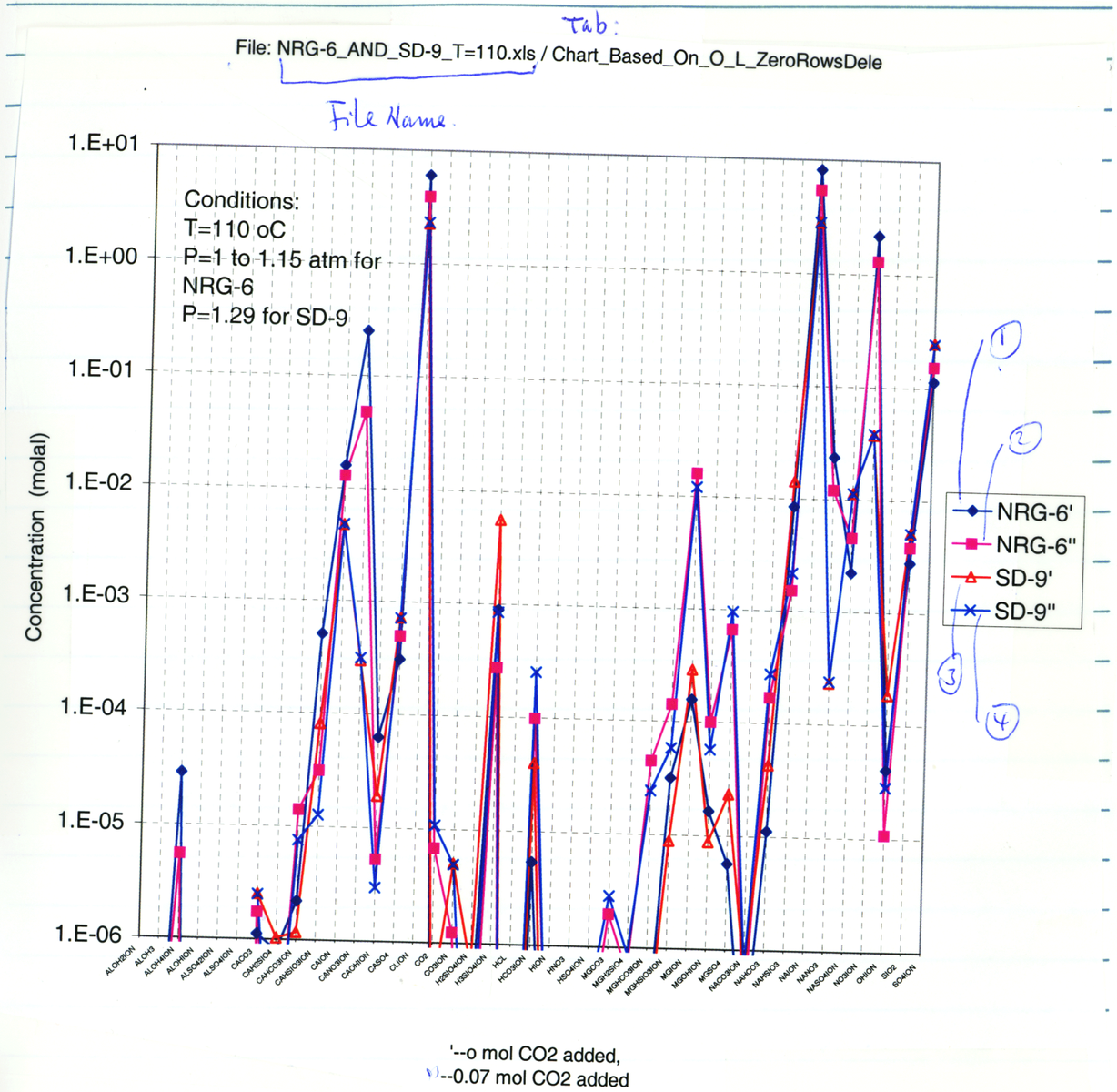
From Right page:

② Calculated by ~~setting~~ f = 0.999, got C. factor = 1200
P = 1.2902 atm, a_{water} = 0.916, P_{CO_2} = 4E-4 atm.

① Calculated by ~~setting~~ P = 1.29, got C. factor = 1300
f = 0.99903 ~~atm~~ by 2/27/02 a_{water} = 0.9147, P_{CO_2} = 1.67 E-3 atm

Note ⓐ f => the vapour faction
ⓑ all calculations are at the highest concentration factors that converges.

by. 2/27/02



'--o mol CO2 added,
--0.07 mol CO2 added

① Calculated by setting f = 0.9995, got C. factor = 3200,
P = 0.9918 atm a_{water} = 0.7042, P_{CO_2} = 1.76 E-3

② Calculated by setting f = 0.99925, got C.factor = 1800
P = 1.148 atm, a_{water} = 0.814, P_{CO_2} = 1.47 E-3

by. 02/27/02.

Lietai Yang

Subject: FW: F-added NRG-6 results

-----Original Message-----
From: Lietai Yang [mailto:LTyang@swri.org]
Sent: Tuesday, April 02, 2002 11:02 AM
To: Roberto Pabalan
Subject: F-added NRG-6 results

Enclosed is the simulation results for NRG-6: water with added F

Conditions the same as the previous plot for NRG-6", i.e.
T=110 oC,
Vapor fraction: 0.99925 (molar basis)
added H6F6: 0.191296E-4 molal (2.18 mg/L for F, same as J13 water)
added CO2: 0.07 molal and 0.0 molal.

↑ See page 132

Thanks

L. Yang

Lietai

NRG-6_T=110_added_H6F6_Zero_Ro...

All simulation conditions and parameters are the same as in Page 167.

L. Yang
4/02/02

NRG-6_T=110_added_H6F6_Zero_Rows_Deleted.xls

CO2=0.07 mola added

Stream	NRG-6	NRG-6	O_V	O_L	O_S	O_L25oC	O_L25oC
Phase	Aqueous	Vapor	Vapor	Aqueous	Solid	Aqueous	Solid
Temperature, C	25	25	110	110	110	25	25
Pressure, atm	1	1	1.14713	1.14713	1.14713	1	1
pH	4.93585			7.0522		7.67993	
Total mol/hr	55.48702	0.0388647	55.485	0.03700234	0.00246332	0.037	1.54E-06
Flow Units	molal	mol/hr	mol/hr	molal	mol/hr	molal	mol/hr
H2O	55.5555556	0.0012349	55.41412	55.55555556		55.55556	
H2F2	6.6489E-18	1.373E-23	1.24E-19	2.76845E-19		1.64E-23	
CO2	0.03244826	0.0376298	0.070884	6.80045E-06		1.6E-06	
H2SO4	2.6296E-22	2.85E-29	1.75E-25	7.69148E-26		#VALUE!	
HCL	1.3601E-14	5.728E-16	9.1E-09	6.26395E-12		1.85E-14	
HF	5.8434E-07	1.214E-12	1.15E-08	7.29998E-09		3.8E-10	
HNO3	3.9736E-10	7.513E-16	4.12E-09	1.1756E-08		1.11E-10	
CASO4	2.7013E-05			0.000495105	3.7564E-05	0.001255	
ALOH3	1.0033E-09			2.20835E-08		9.76E-10	3.06E-09
MGCO3	5.5941E-10			1.94532E-06		1.92E-06	
MGH2SIO4	5.3015E-15			6.11403E-07		2.02E-07	
MGSO4	3.9727E-06			0.00066298		0.001421	
NAF	9.6182E-08			5.80566E-05		5.2E-05	
NAHCO3	2.124E-06			0.000167917		5.14E-05	
NAHSIO3	6.1336E-09			0.001520646		0.002036	
NANO3	5.0803E-08			0.012054542		0.016468	
ALF3	8.3681E-06			3.55875E-14		2.28E-13	
CACO3	4.3348E-09			1.72872E-06	0.00053369	1.93E-06	
SIO2	0.00102267			0.003795398	0.00101741	0.000954	1.52E-06
CAH2SIO4	1.9183E-15			1.71496E-08		9.49E-09	
OHION	9.5788E-10			1.07444E-05		2.39E-07	
ALF4ION	7.0424E-08			1.39985E-15		1.35E-14	
ALF5ION	6.34E-11			1.20119E-17		1.51E-16	
ALF6ION	9.9116E-15			4.36003E-20		1.28E-18	
ALFION	2.6623E-06			7.75028E-14		1.82E-12	
ALION	1.4091E-08			7.65724E-19		1.48E-16	
ALOH2ION	2.3337E-09			2.85464E-11		1.27E-11	
ALOH4ION	2.3761E-11			5.5091E-06		3.8E-08	
ALOHION	7.736E-09			1.16635E-14		5.33E-14	
ALSO42ION	1.5435E-10			3.65254E-19		1.07E-16	
ALSO4ION	3.7112E-09			5.2357E-18		7.25E-16	
CAFION	1.0055E-09			7.02364E-06		9.27E-08	
CAHCO3ION	6.1956E-06			1.40455E-05		1.5E-05	
CAHSIO3ION	1.0038E-10			3.13258E-05		5.68E-06	
CAION	0.0005728			0.012900787		0.023698	
CANO3ION	7.9187E-07			0.048144811		0.036594	
CAOHION	6.4808E-12			5.2951E-06		9.61E-08	
CLION	0.00217376			3.892727138		3.892702	
CO3ION	7.4591E-09			1.23123E-06		5.09E-06	
FION	3.4131E-05			8.13583E-05		6.95E-05	
H2SIO4ION	1.2459E-16			3.69864E-09		9.36E-10	
H3SIO4ION	1.3871E-08			0.000270913		9.13E-06	
HCO3ION	0.00139399			9.80876E-05		0.000146	
HF2ION	4.829E-12			1.42727E-12		1.59E-14	
HION	1.2703E-05			6.53999E-08		1.04E-08	
HSO4ION	6.3915E-07			8.55126E-08		3.93E-09	
MGFION	6.5786E-11			4.37257E-06		4.67E-08	
MGHCO3ION	5.9956E-06			4.4498E-05		0.000111	
MGHSIO3ION	5.3033E-11			0.000142066		2.31E-05	
MGION	0.00016295			0.015984718		0.015382	
MGOHION	1.777E-11			0.000100602		2.03E-06	
NA2FION	4.5617E-12			4.5031E-05		1.24E-05	
NACO3ION	7.9561E-11			2.32084E-07		2.61E-06	
NAION	0.00437069			5.396409093		5.384495	
NASO4ION	2.4254E-06			0.004534176		0.011684	
NO3ION	0.00075771			1.298203757		1.305333	
ALF2ION	2.6002E-05			2.15353E-13		2.67E-12	
SO4ION	0.00076826			0.153388013		0.144741	
ALOOH				#VALUE!	3.7054E-05	#VALUE!	
CAF2				#VALUE!		#VALUE!	1.72E-08
MGF2				#VALUE!	5.7256E-05	#VALUE!	
MGOH2				#VALUE!	0.00010587	#VALUE!	
NA2SO4				#VALUE!	0.00067447	#VALUE!	
Total g/hr	1000.73	1.67833	1001.42	0.761336	0.227429	0.761243	9.31E-05
Volume, L/hr	1.00316	0.945866	1507.15	0.000669894	8.9607E-05	0.000632	4.21E-08
Enthalpy, cal/hr	-3791810	-3610.9	-3172340	-2390.18	-652.901	-2436.33	-0.334138
Density, g/L	997.587	1.77439	0.66445	1136.5	2538.07	1204.55	2213.7
Vapor fraction		1	1				
Solid fraction					1		1
Organic fraction							
Osmotic Pres, atm	1.03427			354.808		301.87	
Redox Pot, volts							
E-Con, 1/ohm-cm	0.00065374			0.664426		0.225769	
E-Con, cm2/ohm-n	8.39014			5.46383		23.4673	
Abs Visc, cP	0.892481			0.50402		1.66683	
Rel Visc	1.00198			1.9798		1.87133	
Ionic Strength	0.00739976			5.68019		5.67846	

CO2=0.0

Stream	NRG-6	NRG-6	O_V	O_L	O_S	O_L25oC	O_L25oC
Phase	Aqueous	Solid	Vapor	Aqueous	Solid	Aqueous	Solid
Temperatu	25	25	110	110	110	25	25
Pressure, a	1	1	1.14517	1.14517	1.14517	1	1
pH	7.04274			7.96534		8.54771	
Total mol/h	55.52588	3.71E-05	55.485	0.037051	0.00245511	0.037049	1.58E-06
Flow Units	molal	mol/hr	mol/hr	molal	mol/hr	molal	mol/hr
H2O	55.55556		55.48396	55.55556		55.55556	
H2F2	4.58E-21		7.29E-21	1.62E-20		2.97E-25	
CO2	0.00023		0.001044	9.99E-08		2.82E-08	
H2SO4	1.61E-26		2.58E-27	#VALUE!		#VALUE!	
HCL	1.07E-16		1.11E-09	7.61E-13		2.49E-15	
HF	1.53E-08		2.79E-09	1.77E-09		5.13E-11	
HNO3	3.11E-12		5E-10	1.43E-09		1.49E-11	
CASO4	2.71E-05			0.000497	5.02048E-05	0.001278	
ALOH3	2.4E-09	3.71E-05		2.21E-08		9.78E-10	2.5E-08
MGCO3	6.52E-08			2.87E-08		3.01E-08	
	0	0	0	0	0	0	0
MGSO4	3.99E-06			9.77E-06		2.33E-05	
NAF	3.22E-07			0.000116		5.21E-05	
NAHCO3	1.92E-06			2.04E-05		6.75E-06	
NAHSIO3	7.81E-07			0.012557		0.015132	
NANO3	5.07E-08			0.012057		0.016467	
ALF3	3.62E-10			5.06E-16		5.58E-16	
CACO3	5.04E-07			1.73E-06	0.000464138	1.88E-06	
SIO2	0.00102			0.003803	0.001011389	0.000956	1.49E-06
CAH2SIO4	3.14E-11			1.17E-06		5.24E-07	
OHION	1.23E-07			8.76E-05		1.75E-06	
ALF4ION	1.02E-11			3.94E-17		3.27E-17	
ALF5ION	3.08E-14			6.69E-19		3.63E-19	
ALF6ION	1.62E-17			4.81E-21		3.05E-21	
ALFION	1.02E-11			2.8E-16		4.51E-15	
ALION	1.61E-14			1.38E-21		3.65E-19	
ALOH2ION	4.37E-11			3.48E-12		1.72E-12	
ALOH4ION	7.29E-09			4.51E-05		2.8E-07	
ALOHION	1.13E-12			1.73E-16		9.76E-16	
ALSO42IO	1.77E-16			6.46E-22		2.67E-19	
ALSO4ION	4.25E-15			9.4E-21		1.81E-18	
CAFION	3.38E-09			1.41E-05		9.34E-08	
CAHCO3IO	5.63E-06			1.71E-06		1.98E-06	
CAHSIO3IO	1.28E-08			0.00026		4.25E-05	
CAION	0.000573			0.013023		0.023984	
CANO3IOI	7.93E-07			0.048421		0.036828	
CAOHION	8.3E-10			4.39E-05		7.19E-07	
CLION	0.002174			3.894806		3.894655	
CO3ION	8.65E-07			1.22E-06		4.89E-06	
FION	0.000115			0.00016		6.85E-05	
H2SIO4IOI	2.03E-12			2.49E-07		5.11E-08	
H3SIO4IOI	1.77E-06			0.002229		6.76E-05	
HCO3ION	0.001265			1.19E-05		1.9E-05	
HF2ION	4.25E-13			6.81E-13		2.11E-15	
HION	9.93E-08			7.97E-09		1.41E-09	
HSO4ION	5E-09			1.03E-08		5.37E-10	
MGFION	2.22E-10			1.29E-07		7.57E-10	
MGHCO3I	5.46E-06			7.99E-08		2.37E-07	
MGHSIO3I	6.79E-09			1.74E-05		2.78E-06	
MGION	0.000163			0.000237		0.000251	
MGOHION	2.28E-09			1.23E-05		2.44E-07	
NA2FION	1.52E-11			9.06E-05		1.25E-05	
NACO3IOI	9.21E-09			2.29E-07		2.51E-06	
NAION	0.00437			5.434665		5.420451	
NASO4IOI	2.42E-06			0.004483		0.011729	
NO3ION	0.000758			1.298649		1.305778	
ALF2ION	3.35E-10			1.54E-15		6.57E-15	
SO4ION	0.000769			0.154788		0.146741	
ALOOH	#VALUE!			#VALUE!	3.70786E-05	#VALUE!	
CAF2	#VALUE!			#VALUE!	5.72809E-05	#VALUE!	6.92E-08
	0	0	0	0	0	0	0
MGOH2	#VALUE!			#VALUE!	0.000172631	#VALUE!	
NA2SO4	#VALUE!			#VALUE!	0.000662388	#VALUE!	
Total g/hr	1000.59	0.002893	999.608	0.762994	0.22491	0.762897	9.67E-05
Volume, L/	1.00338	1.19E-06	1509.74	0.000671	8.87279E-05	0.000633	4.3E-08
Enthalpy, c	-3793470	-11.4675	-3169820	-2394.7	-648.222	-2440.92	-0.348518
Density, g/	997.22	2440.66	0.662108	1137.16	2534.83	1205.55	2246.31
Vapor fract			1				
Solid fracti		1			1		1
Organic fra							
Osmotic Pi	0.247779			355.467		302.462	
Redox Pot,							
E-Con, 1/o	0.000648			0.666084		0.226357	
E-Con, cm	78.7175			38.6442		23.4359	
Abs Visc, c	0.892409			0.503624		1.66358	
Rel Visc	1.0019			1.97825		1.86768	
Ionic Stren	0.007354			5.67331		5.672	

L. Yang
4/02/02

Pages 141 – 173 copied

for QA records

J. Yang 4/2/02

Continued from page 114; OLI set up see page 61

Input to Yiming's IM

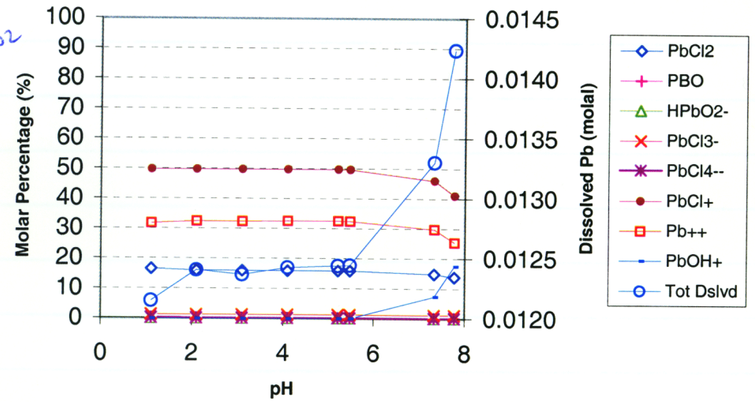
File: Lead_Speciation_Yiming_IM_PbCl2.xls | Tab: %PLot_pH

pH	1.10927	2.10938	3.10945	4.10681	5.21947	5.48284	7.33254	7.77858
PbCl2	16.66708	16.07168	16.0919	16.01434	15.99777	15.99049	14.95699	13.95163
PBO	1.78E-14	1.79E-12	1.78E-10	1.76E-08	2.96E-06	9.96E-06	0.045732	0.300283
HPbO2-	3.45E-24	3.52E-21	3.52E-18	3.47E-15	7.55E-12	4.65E-11	1.51E-05	0.000279
PbCl3-	1.422213	1.329284	1.334328	1.320775	1.318726	1.318222	1.246929	1.232518
PbCl4--	0.305905	0.277541	0.279679	0.275057	0.274462	0.27438	0.263072	0.279003
PbCl+	49.77055	49.78583	49.81056	49.78634	49.75551	49.72997	46.11127	41.11131
Pb++	31.83425	32.53561	32.48305	32.59868	32.59117	32.57264	29.95216	25.5668
PbOH+	4.73E-06	4.83E-05	0.000482	0.004812	0.06236	0.114294	7.423836	17.55817
Tot Dslvd	0.012151	0.012405	0.012368	0.012428	0.012441	0.012446	0.013303	0.014238

(molal)

%

J.Y. 8/14/02



Molar percent of dissolved lead species and total dissolved lead in chloride solutions
(Total added lead: 0.025 molal)

By OLI ESP 6.1

Inputs see file in attached CD (to be done at end of interval)

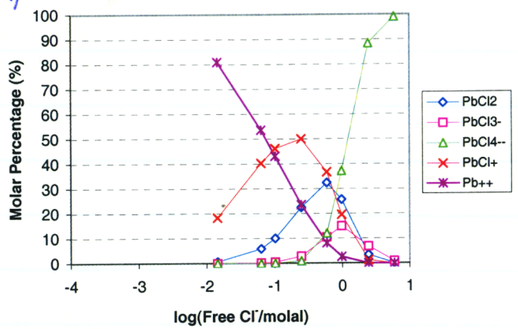
J. Yang 7/19/02

Input to Yiming's IM.

File: Lead_Speciation_Yiming_IM_PbCl2.xls Tab: %Plot_Cl

pH	5.01192	5.16124	5.23213	5.40088	5.7186	5.91782	6.58849	6.94064
log(free Cl-	-1.841179	-1.195266	-0.98909	-0.603128	-0.226916	-0.005353	0.394	0.776417
PbCl2	0.724926	5.928996	10.12876	22.50168	32.43912	25.67919	3.490358	0.095971
PbCl3-	0.0051	0.186368	0.515713	2.867368	10.51334	14.9735	6.824549	0.89334
PbCl4--	6.23E-05	0.012224	0.059871	1.019571	12.12633	37.15759	88.39772	98.99618
PbCl+	18.37179	40.24995	46.21777	50.05989	36.7325	19.56661	1.239669	0.014454
Pb++	80.89812	53.62247	43.07789	23.55149	8.188708	2.623116	0.047701	5.86E-05
Cl- molal	0.014415	0.063787	0.102544	0.249386	0.59304	0.98775	2.47742	5.97609
Sum of Pb (molal)	0.007989	0.007992	0.007993	0.007995	0.005641	0.006596	0.008	0.008

(%)



J.Y. 8/14/02

Molar percent of dissolved lead species in chloride solutions
(Total disolved lead: ~ 1600 ppm)

By OLI ESP6.5

Input see File.

J yang 7/19/02

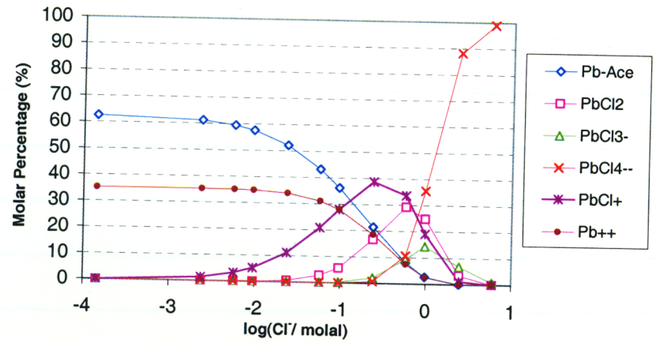
Input to Yiming's IM.

File: Lead_Speciation_Yiming_IM.xls Tab: %Plot_25C

log(molal)

log(Free Cl-)	-3.844664	-2.622413	-2.241678	-2.019311	-1.619901	-1.237584	-1.014253	-0.613512	-0.231853	-0.00859	0.392671	0.775903
Pb-Ace	62.61055	61.30561	59.54144	57.72801	52.18715	43.25832	36.29913	21.61884	8.262122	2.77122	0.068031	0.000326
PbCl2	3.59E-05	0.009503	0.051312	0.133366	0.678854	2.767815	5.741341	16.88696	29.38757	24.95229	3.504452	0.096266
PbCl3-	2.5E-09	1.11E-05	0.000143	0.000623	0.007974	0.07893	0.275894	2.101294	9.416146	14.43859	6.828058	0.894447
PbCl4--	2.85E-13	2.14E-08	6.86E-07	5.1E-06	0.000176	0.004751	0.03058	0.735522	10.78414	35.66142	88.26183	98.99411
PbCl+	0.087716	1.416521	3.255727	5.187034	11.2427	21.01132	28.11692	38.78839	33.78705	19.19574	1.249305	0.014519
Pb++	35.2209	35.21044	35.12498	34.95758	33.99494	31.17397	27.98819	18.70893	7.598153	2.584242	0.048087	5.89E-05
Cl-	1.787216	29.81444	71.64112	119.5441	299.8745	723.1988	1209.45	3043.196	9416.58	14439.11	30868.3	74601.06

(%)



J.Y. 8/14/02

Molar percent of dissolved lead species in chloride-acetate solutions
(Pb-Ace is for the total lead acetates; total dissolved lead is about 1600 ppm)

By OLI ESP V.6.2.

Input data see File.

J yang 7/19/02

-----Original Message-----
From: R Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Tuesday, June 18, 2002 10:27 AM
To: Lietai Yang
Subject: seawater evaporation

Lietai:

Here is the seawater composition:

Ca++ = 411 mg/kg
Mg++ = 1290 mg/kg
Na+ = 10760 mg/kg
K+ = 399 mg/kg
Cl - = 19350 mg/kg
SO4-- = 2710 mg/kg
HCO3- = 142 mg/kg

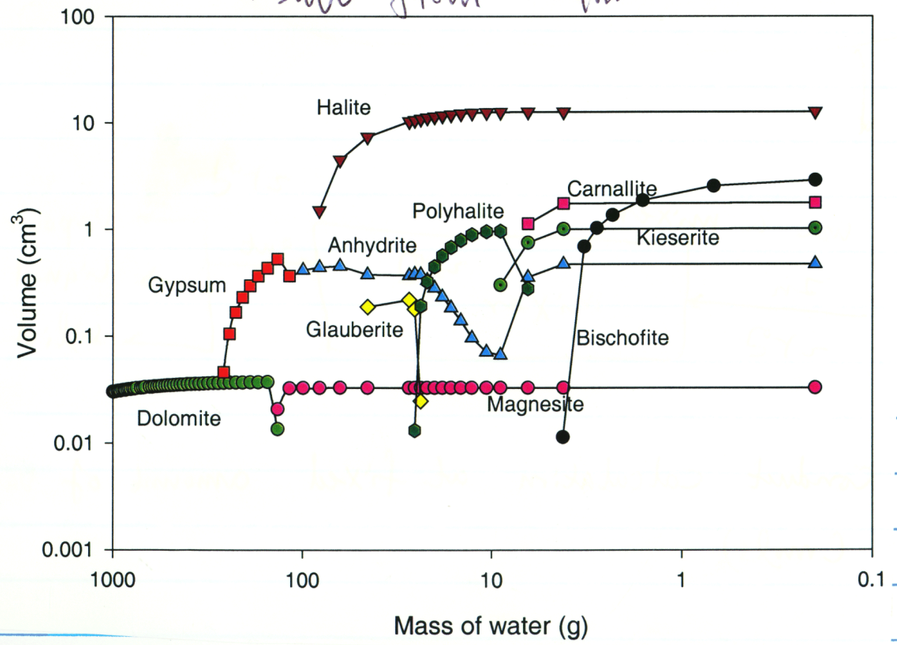
fix log (pCO2) = -3.5 atm

Evaporate until 4 gms H2O are left. Determine amount of precipitates and solution composition as a function of mass of water left in solution.
Attached is a plot of the mineral precipitates calculated using TEQUIL.

Thanks.

bobby

Results from Tequil.



L. Yang 7/24/2002

File: SeaWater_Evaporation_Using_ESP_V65.xls / Tab:Input_data

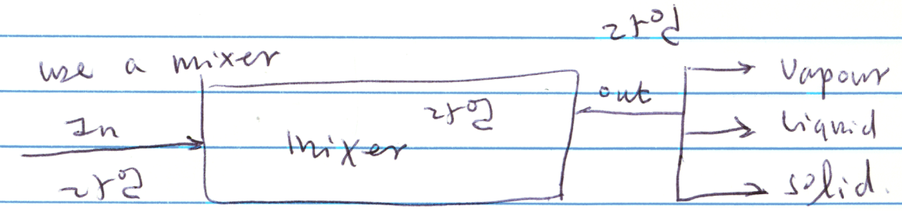
Conversion to molecular basis.

	Input			Balanced Results		
	mg/kg	MW	mol/kg	mol/kg	Val	Eq Charge
Water	1.00E+06	18	55.55555556	55.556		
Calcium ion(+2)	411	40	0.010275	0.010255	2	0.02051
Magnesium ion(+2)	1290	24.3	0.05308642	0.053075	2	0.10615
Sodium ion(+1)	10760	23	0.467826087	0.46803	1	0.46803
Potassium ion(+1)	399	39.1	0.010204604	0.010205	1	0.010205
Sum Cation						0.604895
Chloride ion(-1)	19350	35.5	0.545070423	0.546145	1	0.546145
Sulfate ion(-2)	2710	96	0.028229167	0.02821	2	0.05642
Bicarbonate ion(-1)	142	61	0.002327869	2.33E-03	1	0.002327
Sum Anio						0.604892
Anio-Cation						-2.8E-06
Carbon dioxide				2.27E-03		

Molecular Distribution for Input to OLI

	based on	mol/kg
Na2SO4	Sulfate ion(-2)	0.02821
NaHCO3	Bicarbonate ion(-1)	2.33E-03
CaCL2	Calcium ion(+2)	0.010255
MgCl2	Magnesium ion(+2)	0.053075
KCl	Potassium ion(+1)	0.010205
NaCL	Balance on Na	4.09E-01

Note: CO2 varies to get log(PCO2) =-3.5



Conduct calculation at fixed amount of vapour (mols).

L. Yang 4/24/02

Lietai Yang

To: rpabalan@cnwra.swri.edu
Subject: RE: seawater evaporation

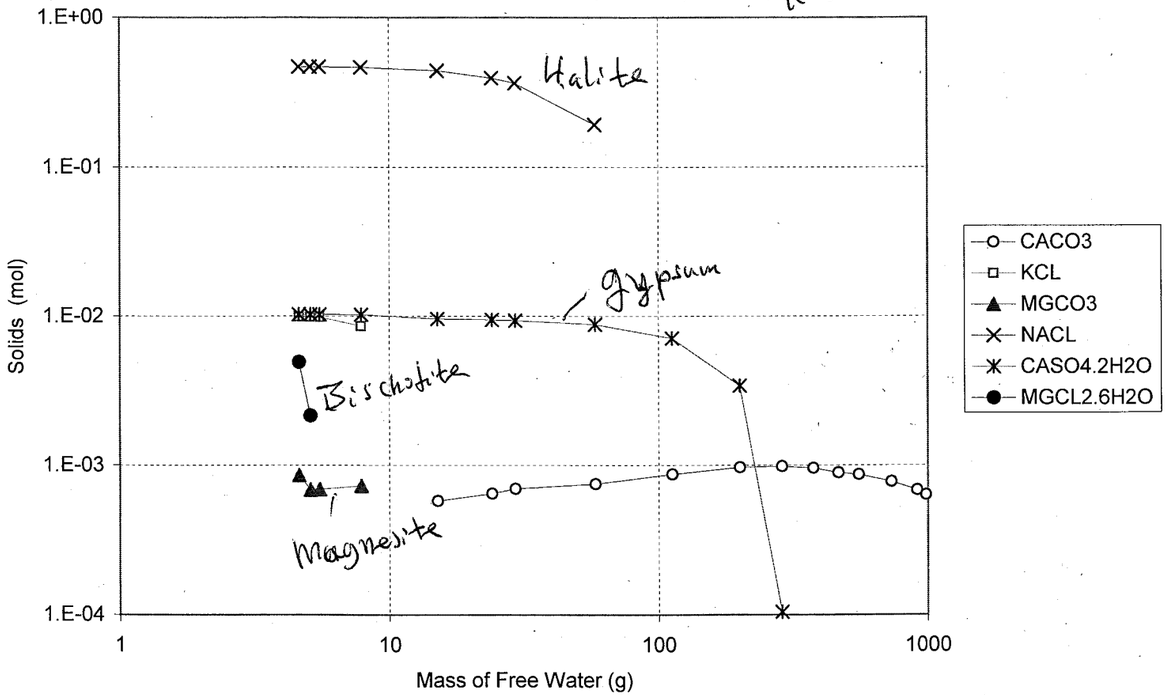
SeaWater_Evaporation_Using_ESP...

Enclosed are the results of simulation with sea water. I cann't go beyond 5 g.

-Lietai

File: SeaWater_Evaporation_Using_ESP_V65.xls / Tab: Chart

Detailed data see the file in folder of "Notebook#430"



L. Yang 7/24/02

Lietai Yang

To: rpabalan@cnwra.swri.edu
Subject: RE: ESP simulations

ym_water_F_addod.xls

Bobby,

Enclosed are the results of simulation conducted with and without 0.07 mol CO2 added at 110 oC and 0.85 atm (except NRG_B at 1.3 atm). It seems most of them end up with lot of Flourides.

Water	ID used	Composition in NoteBook Page#
UZ-14/85.2	--UZ_B	127
UZ-14/1277.7	--UZ_14	148
UZ-14/1542.3	--UZ_A	127
NRG-6/158.2	--NRG_A	128
NRG-6/244.6	--NRG_B	128
SD-9/94.2	--SD_9	147

F- was added as H6F6 (1.91308E-5 molal H6F6) (page 129 of notebook)
ESP version 6.5.
All conditions and procedures are the same as previous calculations (described on page 133 of notebook).

-Lietai

-----Original Message-----
From: R Pabalan [mailto:rpabalan@cnwra.swri.edu]
Sent: Friday, June 21, 2002 8:55 AM
To: Lietai Yang
Subject: ESP simulations

Lietai:

When you get a chance, please rerun the calculations you did for UZ-14/85.2, UZ-14/1277.7, UZ-14/1542.3, NRG-6/158.2, NRG-6/244.6, and SD-9/94.2, but add 1.15E-4 molal F- (same as J-13) to each. I want to find out what happens to the fluoride ion concentration during evaporation.

thanks.

bobby

Results see page 182

Input Compositions see pages 183-184.

L. Yang 7/24/02

Results

File: ym_water_F_added.xls / Tab:F_Only_Molal

Molal Concentration for liquid streams ONLY (Ignored those whose C<1e-7 molal)

Water	UZ_A		UZ_A		UZ_B		UZ_B		UZ_14		UZ_14	
Variable T, oC	110		110		110		110		110		110	
Variable Con of added CO2 to Feec	0.07		0		0.07		0		0.07		0	
Variable, Pressure,atm	0.85		0.85		0.85		0.85		0.85		0.85	
Conc. Factor (Derived)	126826.5		73229.3		28991.52		28862.71		6857.106		7035.711	
P of Pure H2O at T	1.40844		1.40844		1.40844		1.40844		1.40844		1.40844	
R Humidity at T	0.603505		0.603505		0.603505		0.603505		0.603505		0.603505	
P(CO2, atm)	0.00114		7.09E-05		0.001095		2.59E-05		0.001093		2.6E-05	
Ionic Strg.* (Maximum, 30)	14.7036		12.4042		13.0306		12.9949		13.1871		13.5885	
X(H2O) (Minimum, 0.65)	0.665297		0.67576		0.683765		0.684067		0.776382		0.770789	
Stream	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	
Temperature, C	110	25	110	25	110	25	110	25	110	25	110	25
Pressure, atm	0.85	1	0.85	1	0.85	1	0.85	1	0.85	1	0.85	1
pH	10.006	10.4948	10.6252	11.752	6.65205	7.50806	7.46319	8.09032	5.63055	7.07749	6.30726	7.94292
Total mol/hr	0.000658	0.000629	0.001122	0.001107	0.002797	0.002639	0.002812	0.002656	0.010428	0.010338	0.010237	0.010146
H2O	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556
NAF	0.0816	0.044467	0.087665	0.046924	2.21E-05	1.43E-05	4.43E-05	1.43E-05	2.29E-07	1.51E-07	2.87E-07	1.3E-07
CAFION					2.64E-05	4.04E-07	5.3E-05	4.06E-07	0.000377	3.08E-06	0.000762	4.23E-06
FION	0.094759	0.049025	0.102908	0.053004	2.31E-05	1.73E-05	4.59E-05	1.71E-05	7.03E-06	6.62E-06	7.15E-06	4.49E-06
MGFION					1.65E-05		7.84E-07		0.000128	1.58E-06	1.13E-05	
NA2FION	0.350704	0.038348	0.330921	0.036884	5.76E-05	7.31E-06	0.000115	7.38E-06	2.15E-07		2.71E-07	
Total	0.527063	0.13184	0.521495	0.136812	0.000146	3.93E-05	0.000259	3.92E-05	0.000513	1.14E-05	0.000781	8.85E-06

NRG_A	NRG_A	NRG_B	NRG_B	SD_9	SD_9		
110	110	110	110	110	110		
0.07	0	0.07	0	0.07	0		
0.85	0.85	1.3	0.85	0.85	0.85		
2212.874	2228.161	1089.347	15360.55	2778.243	2770.905		
1.40844	1.40844	1.40844	1.40844	1.40844	1.40844		
0.603505	0.603505	0.923007	0.603505	0.603505	0.603505		
0.001076	8.54E-06	0.001656	1.21E-05	0.00108	9.3E-06		
12.7435	12.8507	3.19751	13.8434	12.3582	12.336		
0.787171	0.78558	0.91145	0.6743	0.798931	0.799133		
O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC	O_L	O_L25oC
Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
25	110	25	110	25	110	25	110	25	110	25	110	25
1	0.85	1	0.85	1	1.3	1	0.85	1	0.85	1	0.85	1
7.94292	5.7434	7.38463	5.78872	7.56373	7.40233	8.05772	7.8491	8.38795	5.78071	7.43598	5.78195	7.60634
0.010146	0.031871	0.031603	0.031717	0.031446	0.055908	0.055894	0.005359	0.004997	0.025012	0.024806	0.025072	0.024865
55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556	55.55556
1.3E-07	2.03E-07	1.81E-07	2.39E-07	1.67E-07	9.07E-05	9.99E-05	6.75E-05	2.65E-05	2.12E-07	2.03E-07	2.15E-07	2.06E-07
4.23E-06	0.000217	2.37E-06	0.000323	2.74E-06	2.54E-06		3.21E-05	2.23E-07	0.000176	2.03E-06	0.000175	2.02E-06
4.49E-06	6.93E-06	8.97E-06	7.53E-06	7.55E-06	0.000224	0.00023	6.9E-05	2.72E-05	7.65E-06	1.08E-05	7.67E-06	1.08E-05
	0.000134	2.18E-06	0.00012	1.53E-06	1.58E-06		2.23E-07		0.000122	2.1E-06	0.000122	2.09E-06
	1.83E-07		2.16E-07		1.63E-05	5.61E-06	0.000206	1.56E-05	1.81E-07		1.84E-07	
8.85E-06	0.000358	1.37E-05	0.000451	1.2E-05	0.000335	0.000335	0.000374	6.95E-05	0.000306	1.51E-05	0.000305	1.51E-05

Total F Tank

J. Yans

7/27/02

Input Compositions

Process Build
Y2A Model
UZ_A Stream

**TOP OF DATA

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.52858	mol/hr
H2O	55.508	moles
HCL	5.64627E-04	moles
HNO3	6.45682E-05	moles
CAOH2	8.99044E-05	moles
MGOH2	2.05902E-05	moles
NA6SO42CO3	1.45866E-04	moles
NAOH	0.00813669	moles
CO2		moles
NACL		moles
H6F6	1.91308E-05	moles
ALOH3	5.11910E-04	moles
H2CO3	0.00864287	moles
SIO2	0.00238	moles
H2SO4		moles
NA3HSO42	[redacted]	moles

Process Build
Y2A Model
UZ_B Stream

18 LINES

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.5156	mol/hr
H2O	55.508	moles
HCL	0.00169314	moles
HNO3	3.54971E-04	moles
CAOH2	0.00127884	moles
MGOH2	5.43344E-04	moles
NA6SO42CO3	2.87317E-04	moles
NAOH		moles
CO2		moles
NACL		moles
H6F6	1.91308E-05	moles
ALOH3	1.11237E-05	moles
H2CO3	0.00186058	moles
SIO2	0.001495	moles
H2SO4		moles
NA3HSO42	5.63604E-05	moles

<PgUp>

Process Build
Y2A Model
UZ_14 Stream

18 LINES

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.51912	mol/hr
H2O	55.508	moles
HCL	0.00366922	moles
HNO3	2.42074E-04	moles
CAOH2	0.00227866	moles
MGOH2	2.58958E-04	moles
NA6SO42CO3	1.97914E-04	moles
NAOH	0.00122813	moles
CO2	0.00	moles
NACL		moles
H6F6	1.91308E-05	moles
ALOH3		moles
H2CO3	0.00259	moles
SIO2	6.32875E-04	moles
H2SO4		moles
NA3HSO42	[redacted]	moles

J. Yans

7/27/02

Input Compositions

NRG_A Stream

Process Build
Y2A Model
NRG_B Stream

18 LINES

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.5218	mol/hr
H2O	55.50868	molality
HCL	0.005222078	molality
HNO3	5.16474E-04	molality
CAOH2	0.003070299	molality
MGOH2	9.59368E-04	molality
NA6SO42CO3		molality
NAOH		molality
CO2		molality
NACL		molality
H6F6	1.91310E-05	molality
ALOH3		molality
H2CO3	5.57637E-04	molality
SIO2	0.001621019	molality
H2SO4	6.23288E-04	molality
NA3HSO42	5.16551E-04	molality

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.51304	mol/hr
H2O	55.508	moles
HCL	0.00138268	moles
HNO3	6.45378E-04	moles
CAOH2	8.23735E-04	moles
MGOH2	2.01688E-04	moles
NA6SO42CO3	5.03138E-04	moles
NAOH		moles
CO2		moles
NACL		moles
H6F6	1.91308E-05	moles
ALOH3	2.22466E-05	moles
H2CO3	4.96991E-04	moles
SIO2	8.49000E-04	moles
H2SO4		moles
NA3HSO42	9.56701E-05	moles

Process Build
Y2A Model
SD_9 Stream

**TOP OF DATA

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.59135	mol/hr
H2O	55.508	moles
HCL	0.00479964	moles
HNO3	1.77573E-04	moles
CAOH2	0.00340327	moles
MGOH2	0.00107748	moles
NA6SO42CO3		moles
NAOH		moles
CO2	0.07	moles
NACL		moles
H6F6	1.91308E-05	moles
ALOH3		moles
H2CO3	6.06962E-04	moles
SIO2	0.00123279	moles
H2SO4	0.00134852	moles
NA3HSO42	6.80300E-04	moles

L. Yang

7/24/02

Letai Yang

From: Letai Yang [ltyang@cnwra.swri.edu]
Sent: Tuesday, August 27, 2002 11:14 AM
To: 'lbrowning@cnwra.swri.edu'
Subject: RE: data

Lauren:

For free F-, the maximum Concentration is 0.135 molal (see Report Table 4.2, page 17) at CO2 Vapour Pressure of 2.36E-5 atm (page 137 of BK#430).

For free Cl-, the maximum Concentration is 10.65 molal at CO2 vapour pressure of 2.52E-5 atm (see page 152 and 155, BK #430).

The value we came up with (0.527 molal) the other day is the total F which includes the complexed ones.

These pages has been photocopied and put in the mail for you.

Thanks

-Lietai

-----Original Message-----
From: Lauren Browning [mailto:lbrowning@cnwra.swri.edu]
Sent: Friday, August 23, 2002 7:20 PM
To: Lietai Yang
Subject: data

Hi Lietai,

Please send me the TPA5.0 information that we discussed asap (e.g. [max. [F-] = 0.52 (what is the exact number, and what is the associated fCO2(g)? What is the sci. notebook number this data?)

Thank You,
Lauren

Pages 175 – 184
Copied for QA Records.
L. Yang 10/3/02.

L. Yang

8/27/02

Simulation of waters at 110°C, 0.87 Bar. No CO_2 added.

For each water b) add F^- 1.1 E-4 molal (2.18 mg/L)

a) add no F^-

SampleID	USW UZ-14-1068	
Water Type	Na-Ca-HCO3-Cl	
Reference	Yang et al. 1996	
Date	1/14/94	
Ph (Lab)	0	
Cond 20°C (µS)	0	
Sampling depth (m)	383.65	
UTM(east)	548033	
UTM(west)	4080262	
Elev(masl)	1068.5	
Cations	(mg/l)	(meq/l)
Na+	6.700E+01	2.914E+00
K+	0.000E+00	0.000E+00
Mg++	3.700E+00	3.044E-01
Ca++	4.300E+01	2.146E+00
Anions	(mg/l)	(meq/l)
Cl-	8.800E+01	2.482E+00
SO4--	1.900E+01	3.956E-01
NO3-	1.600E+01	2.580E-01
HCO3-	1.700E+02	2.787E+00
CO3--	0.000E+00	0.000E+00
Uncharged	(mg/l)	
SiO2	35 = $\frac{35}{60.1}$ = 0.5824 mmol/L	
Al	0	

(3) Water from Bobby 9/16/02

SampleID	USW SD-9orig	
Water Type	Na-Ca-SO4-HCO3-Cl	
Date	3/7/97	
Ph (Lab)	7.5	
Cond 20°C (µS)	720	
Sampling depth (m)	53.74	
Cations	(mg/l)	(meq/l)
Na+	9.500E+01	4.132E+00
K+	0.000E+00	0.000E+00
Mg++	9.500E+00	7.816E-01
Ca++	4.300E+01	2.146E+00
Anions	(mg/l)	(meq/l)
Cl-	6.400E+01	1.805E+00
SO4--	1.240E+02	2.582E+00
NO3-	1.900E+00	3.064E-02
HCO3-	1.220E+02	2.000E+00
CO3--	0.000E+00	0.000E+00
Uncharged	(mg/l)	
SiO2	58.5	
Al	0	

(9) Water from Bobby, 9/16/02.

J. Yang 10/14/02

UZ-14-1068

Cations	Input	Reconciled	Anions	Input	Reconciled
	Values in mg/l				
AL+3			CL-1	88.	87.99868
CA+2	43.	48.38604	CO3-2		
K+1			F-1	2.18	2.17996
MG+2	3.7	4.163458	HCO3-1	170.	169.9974
NA+1	67.	75.39196	NO3-1	16.	15.99979
			SO4-2	19.	18.99968

<PgDn>

added SiO_2 = 35 mg/L = 0.5824 mmol/L

Reconciled on prorated basis

SD-9 orig

Cations	Input	Reconciled	Anions	Input	Reconciled
	Values in mg/l				
AL+3			CL-1	64.	69.17304
CA+2	43.	42.99878	CO3-2		
K+1			F-1	2.18	2.356193
MG+2	9.5	9.499769	HCO3-1	122.	131.8612
NA+1	95.	94.9976	NO3-1	1.9	2.053569
			SO4-2	124.	134.0232

<PgDn>

Reconciled on prorated basis, added SiO_2 58.5 mg/L = 0.9734 mol/L

J. Yang 10/14/02

Mix: Mix

Process Build
OCT14 Model
UZ-14_1068 Stream

UZ-14_1068

(optional)

14 LINES

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.5189	mol/hr
H2O	55.50868	molality
CAOH2	0.00120799	molality
H2CO3	0.002688709	molality
H4SIO4	5.82851E-04	molality
H6F6	1.91351E-05	molality
HCL	0.002483559	molality
HNO3	2.58190E-04	molality
MGOH2	1.71399E-04	molality
NA6SO42CO3	9.89483E-05	molality
NA6SO42CO3	9.89483E-05	molality
NAOH	0.002687539	molality
SIO2	5.82400E-04	molality

Mix:

Process Build
OCT14 Model
SD-9orig Stream

SD-9orig

(optional)

**TOP OF DATA

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.5163	mol/hr
H2O	55.50868	molality
CAOH2	0.00107349	molality
H2CO3	0.001482099	molality
H4SIO4	9.74192E-04	molality
H6F6	2.06820E-05	molality
HCL	0.001952239	molality
HNO3	3.31385E-05	molality
MGOH2	3.91081E-04	molality
NA6SO42CO3	6.80191E-04	molality
NAOH	[redacted]	molality
SIO2	9.73400E-04	molality
NA3HSO42	1.77853E-05	molality

10/14/02

UZ-14-1608

SD-9orig

File: UZ-14_1608_&_SD-9orig/Tab: UZ-14_1608

Summary for Liquid Streams at 110 oC in Molal

Stream	Added F- Liq	No F- Liq
Phase	Aqueous	Aqueous
Temperature, C	110	110
Pressure, atm	0.85	0.85
pH	10.4133	10.4261
Total mol/hr	0.003123122	0.0031659
	moal	moal
H2O	5.56E+01	55.555556
H2F2	8.13E-21	#VALUE!
CO2	4.42E-08	4.31E-08
H2SO4	#VALUE!	#VALUE!
HCL	2.72E-15	2.667E-15
HF	3.88E-11	#VALUE!
HNO3	2.50E-11	2.409E-11
SICL4	#VALUE!	#VALUE!
SIF4	#VALUE!	#VALUE!
SO3	#VALUE!	#VALUE!
MGCO3	2.60E-08	2.526E-08
MGH2SIO4	3.56E-07	3.583E-07
MGSO4	3.17E-11	3.025E-11
NAF	3.56E-02	#VALUE!
NAHCO3	5.81E-03	0.0058125
NAHSIO3	3.09E+00	3.1969933
NANO3	6.91E-02	0.0684879
CAH2SIO4	4.36E-07	4.543E-07
CACO3	1.01E-06	1.014E-06
SIO2	2.31E-03	0.002325
CASO4	1.04E-09	1.022E-09
OHION	1.14E-02	0.0117254
CAHCO3ION	7.11E-09	6.888E-09
CAHSIO3ION	8.64E-07	8.663E-07
CAION	1.73E-07	1.667E-07
CANO3ION	2.14E-06	2.074E-06
CAOHION	8.50E-08	8.629E-08
CLION	4.13E+00	4.1259452
CO3ION	1.05E-01	0.1062757
FION	3.58E-02	#VALUE!
H2SIO4ION	1.39E-02	0.0145385
H3SIO4ION	2.13E-01	0.2182931
HCO3ION	2.64E-03	0.0026246
HF2ION	1.01E-10	#VALUE!
HION	1.41E-11	1.388E-11
HSO4ION	5.55E-12	5.395E-12
MGFION	8.57E-10	#VALUE!
MGHCO3ION	4.82E-10	4.511E-10
MGHSIO3ION	8.97E-08	8.691E-08
MGION	6.54E-10	6.312E-10
MGOHION	3.74E-08	3.654E-08
NA2FION	1.07E-01	#VALUE!
NACO3ION	1.91E-02	0.019541
NAION	1.17E+01	11.703868
NASO4ION	1.79E-03	0.0017871
NO3ION	6.72E+00	6.6090384
CAFION	5.98E-08	#VALUE!
SIF6ION	#VALUE!	#VALUE!
SO4ION	2.36E-01	0.2366388
Total g/hr	0.0841232	0.0852888
Volume, L/hr	5.69557E-05	5.772E-05
Enthalpy, cal/hr	-231.718	-235.585
Density, g/L	1476.99	1477.6
Vapor fraction		
Solid fraction		
Organic fraction		
Osmotic Pres, atm	862.605	862.816
Redox Pot, volts		
E-Con, 1/ohm-cm	0.680822	0.668802
E-Con, cm2/ohm-mol	3.35202	3.39913
Abs Visc, cP	1.39018	1.36422
Rel Visc	5.46068	5.35869
Ionic Strength	12.1823	12.0512

File: UZ-14_1608_&_SD-9orig /Tab:SD-9orig

Summary for Liquid Streams at 110 oC in Molal

Stream	Added F- L	No F- L
Phase	Aqueous	Aqueous
Temperature, C	110	110
Pressure, atm	1	0.85
pH	7.69359	7.72409
Total mol/hr	0.00117868	0.0002751
	moal	moal
H2O	5.56E+01	55.555556
H2F2	1.12E-20	#VALUE!
CO2	8.93E-08	3.433E-08
H2SO4	#VALUE!	#VALUE!
HCL	1.78E-12	1.336E-12
HF	8.88E-10	#VALUE!
HNO3	2.92E-09	1.928E-08
SICL4	#VALUE!	#VALUE!
SIF4	#VALUE!	#VALUE!
SO3	#VALUE!	#VALUE!
MGCO3	2.60E-08	2.245E-08
MGH2SIO4	3.94E-07	3.555E-07
MGSO4	8.85E-06	7.649E-06
NAF	7.47E-05	#VALUE!
NAHCO3	1.36E-05	1.023E-05
NAHSIO3	6.81E-03	0.0062831
NANO3	1.91E-02	0.0993374
CAH2SIO4	5.33E-07	5.033E-07
CACO3	1.11E-06	1.006E-06
SIO2	2.80E-03	0.0022887
CASO4	3.20E-04	0.0002885
OHION	3.34E-05	2.025E-05
CAHCO3ION	2.66E-06	3.741E-06
CAHSIO3ION	4.17E-04	0.0005088
CAION	1.51E-02	0.0601348
CANO3ION	2.17E-01	0.6862979
CAOHION	5.28E-05	4.208E-05
CLION	6.15E+00	3.8503841
CO3ION	4.22E-07	4.068E-07
FION	8.31E-05	#VALUE!
H2SIO4ION	6.15E-08	6.144E-08
H3SIO4ION	7.41E-04	0.0004035
HCO3ION	6.61E-06	4.62E-06
HF2ION	3.19E-13	#VALUE!
HION	9.76E-09	5.573E-09
HSO4ION	4.75E-09	2.358E-09
MGFION	3.46E-07	#VALUE!
MGHCO3ION	1.75E-07	2.348E-07
MGHSIO3ION	3.91E-05	4.572E-05
MGION	2.58E-04	8.659E-05
MGOHION	2.08E-05	1.584E-05
NA2FION	1.72E-04	#VALUE!
NACO3ION	1.03E-07	6.634E-08
NAION	7.90E+00	12.720433
NASO4ION	2.27E-03	0.0018036
NO3ION	1.78E+00	9.1379192
CAFION	2.68E-05	#VALUE!
SIF6ION	#VALUE!	#VALUE!
SO4ION	1.08E-01	0.268625
Total g/hr	0.0254116	0.0070251
Volume, L/hr	2.1115E-05	5.173E-06
Enthalpy, cal/hr	-75.011	-17.5066
Density, g/L	1203.47	1358.13
Vapor fraction		
Solid fraction		
Organic fraction		
Osmotic Pres, atm	595.105	836.528
Redox Pot, volts		
E-Con, 1/ohm-cm	0.789521	0.738973
E-Con, cm2/ohm-m	1.26386	0.294957
Abs Visc, cP	0.689495	1.15856
Rel Visc	2.70836	4.55088
Ionic Strength	8.26894	13.8449

1

Five given to Bobby 10/15/02

10/15/02

TABLE 1
RECIPES FOR VARIOUS GROUDWATERS

Solute	Introduced Concentration, mg/L					
	1xUZ	62xUZ	UZx1243	J13x1	J13x157	250xJ13 rewetted
$CaCl_2 \cdot 2H_2O$	159	6512	57767	15	0.2	11
$CaSO_4 \cdot 2H_2O$	73					
$MgSO_4 \cdot 7H_2O$	111	3961	5382	21	12	0.8
$Mg(NO_3)_2 \cdot 6H_2O$	16					
KNO_3	5.2	719	4205	4.1	1533	3456
KF	3.3					
NaF	2.4	84	1198	5.1	707	1748
$NaHCO_3$	28	14	61	145	8197	18210
$SiO_2 \cdot xH_2O$, 84% SiO_2	12	599	644	12	1671	3950
$MgCl_2 \cdot 6H_2O$		1499	42264			
NaCl		982	14211		1810	4342
KCl			1975			
$Ca(NO_3)_2 \cdot 4H_2O$				10		
K_2SO_4				8.0		
$NaNO_3$		207			626	988
			Introduced NaOH (g/L)*			
0.001 M NaOH	.007	.32	.12	.24	.724	1.992

*added to achieve mass balance for Na

from the Draft paper by Catholic University of America ; submitted to Corrosion / 2003, paper 03693

This paper reported very low pH values in the condensate. The purpose of the following simulation is to verify their results. using OLI Esp 6.1.

12/23/02

conversion of mg/L to mol/L or M unit.

File: Simulated_Water_CUA_Test / Tab: Sheet1

	MW	cheched	UZx1243 mg/L	mol/L	assuming mol/kg H2O
CaCl2.2H2O	147.02	y	57767	0.392919	0.392919
CaSO4.2H2O	172.17	y			
MgSO4.7H2O	246.48	y	5382	0.021835	0.021835
Mg(NO3)2.6H2O	256.41	y			
KNO3	101.11	y	4205	0.041588	0.041588
KF	58.1	y			
NaF	41.99	y	1198	0.028531	0.028531
NaHCO3	84.01	y	61	0.000726	0.000726
SiO2.xH2O, 84%SiO2 *	60.09	y	540.96	0.009002	0.009002
MgCl2.6H2O	203.31	y	42264	0.20788	0.20788
NaCl	58.44	y	14211	0.243172	0.243172
KCl	74.55	y	1975	0.026492	0.026492
Ca(NO3)2.4H2O	236.15	y			
K2SO4	174.27	y			
NaNO3	84.99	y			
0.001 M NaOH	40	y	0.12	0.003	

*How come contain water?, MW is for SiO2
Weight of mixture (mg/L): 644

Input Stream Data

Process Build
COND Model
In Stream

Vapor →

22 LINES

Temperature	25.	C
Pressure	1.	atm
Total Flow	55.56	mol/hr
H2O	55.56	moles
CACL2.2H2O	0.392919	moles
CASO4.2H2O		moles
MGSO4.7H2O	0.021835	moles
MGNO32.6H2O		moles
KNO3	0.041588	moles
KF		moles
\F	0.028531	moles
NAHCO3	7.26000E-04	moles
SIO2	0.009002	moles
MGCL2.6H2O	0.20788	moles
NACL	0.243172	moles
KCL	0.026492	moles
CANO32.4H2O		moles
K2SO4		moles
NANO3		moles
NAOH		moles
O2		moles
CO2		moles

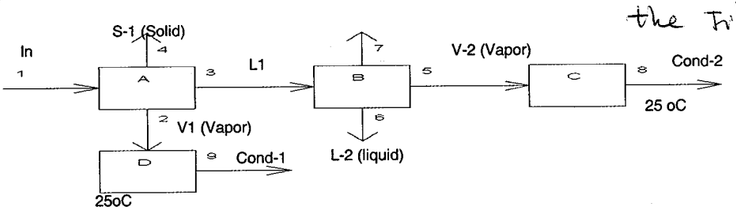
12/23/02

PH-Simulated_1243xUZ_2 J.Y. 2/6/03

File: ~~Simulation_1243xUZ_V65 / Tab:Summary~~

Detailed data are given in the file

Simulation Results.



these are identifiers for the worksheets.

values are from the corresponding worksheets.

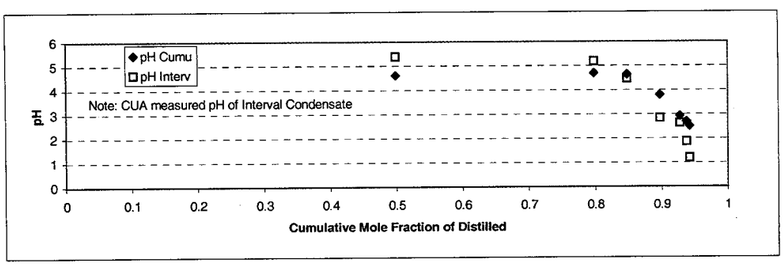
Simulation using ESP 6.5,
Two stage Evaporators.
The Cumullative Fraction is set in the first stage of the evaporators
The Cond-1 and cumulative pH are from the first stage evaporator
The Cond-2 and interval pH are from the second stage evaporator (by evaporate 20% of what left from the first stage in Method 1)
The data files are in the different TABs of this spreadsheet file.

1 atm		Cumulative Solution			Interval Solution			Residual Liquid				
		Cond-1			Cond-2			L1		L2		
Specified Condition for A	Specified Condition for B	Cumul. Evap. Fraction	pH Cumu	I strength (molal)	pH Interv	I strength (molal)	Cation* (molal)	I strength (molal)	Temp (oC)	I strength (molal)	Temp (oC)	Method
f=50%	f=20%	0.499	4.608	2.48E-05	5.4	3.99E-06		4.01	102.9	5.01	104	1
80%	f=20%	0.798171	4.698	2.26E-05	5.194	3.41E-05		10.3491	111.43	12.6009	115.195	1
85%	f=20%	0.848057	4.648	2.26E-05	4.47	3.41E-05		13.2751	116.36	16.2506	121.943	1
90%	f=20%	0.897941	3.795	1.63E-04	2.836	0.00152		19.6632	129.06	24.8213	140.786	1
93%	f=20%	0.927872	2.922	0.001244	2.625	0.00251		25.534	142.99	26.3818	146.266	1
93.80%	f=20%	0.937849	2.69	0.002141	1.87	0.01526		26.141	145.43	28.6491	153.202	1
T=148	f=20%	0.942235	2.497	0.003391	1.19	0.07815		26.9205	148	30.8814	159.655	2
T=148	f=20%	0.942489	2.49	0.003413	1.18	0.08002	None	26.936	148	30.9159	159.752	2

Notes
Method 1 not converging
CO_2 added to input (0.007 molal)

* Total of None H+ Cations

Method 1: using vapor target method for 1st and 2nd evaporators (20% evaporated in the second evaporator) at 1 atm
Method 2: using isotherm method for 1st evaporator and vapor target method for 2nd (20%) at 1 atm



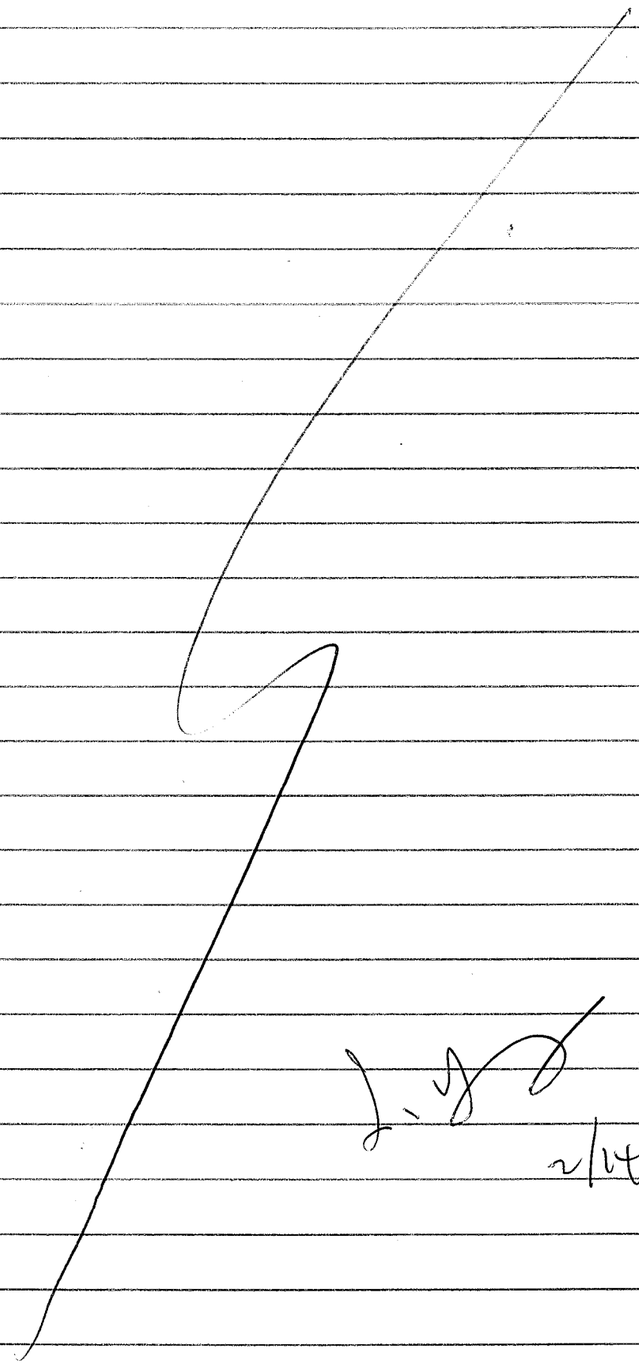
2/6/03

Pages 186 - 192 copied for QA records.

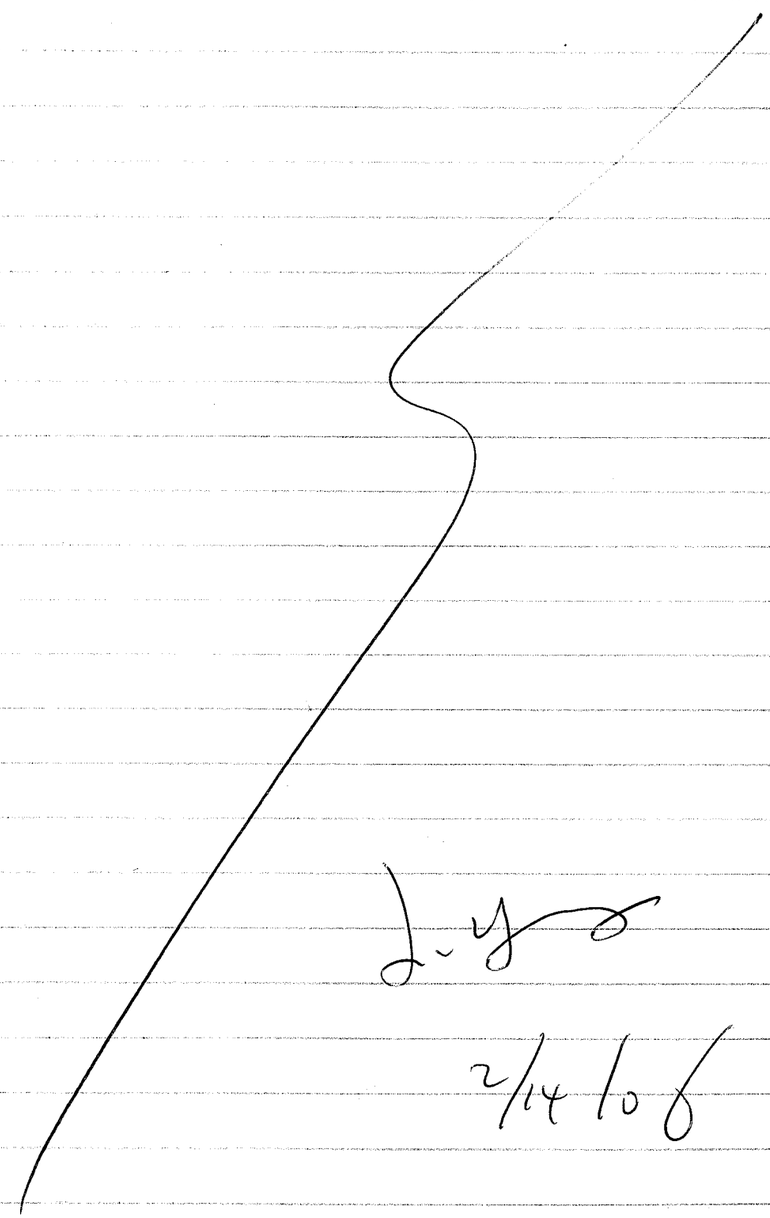
4/3/03 J.Y.

Work continued in Work #572.

2/4/03



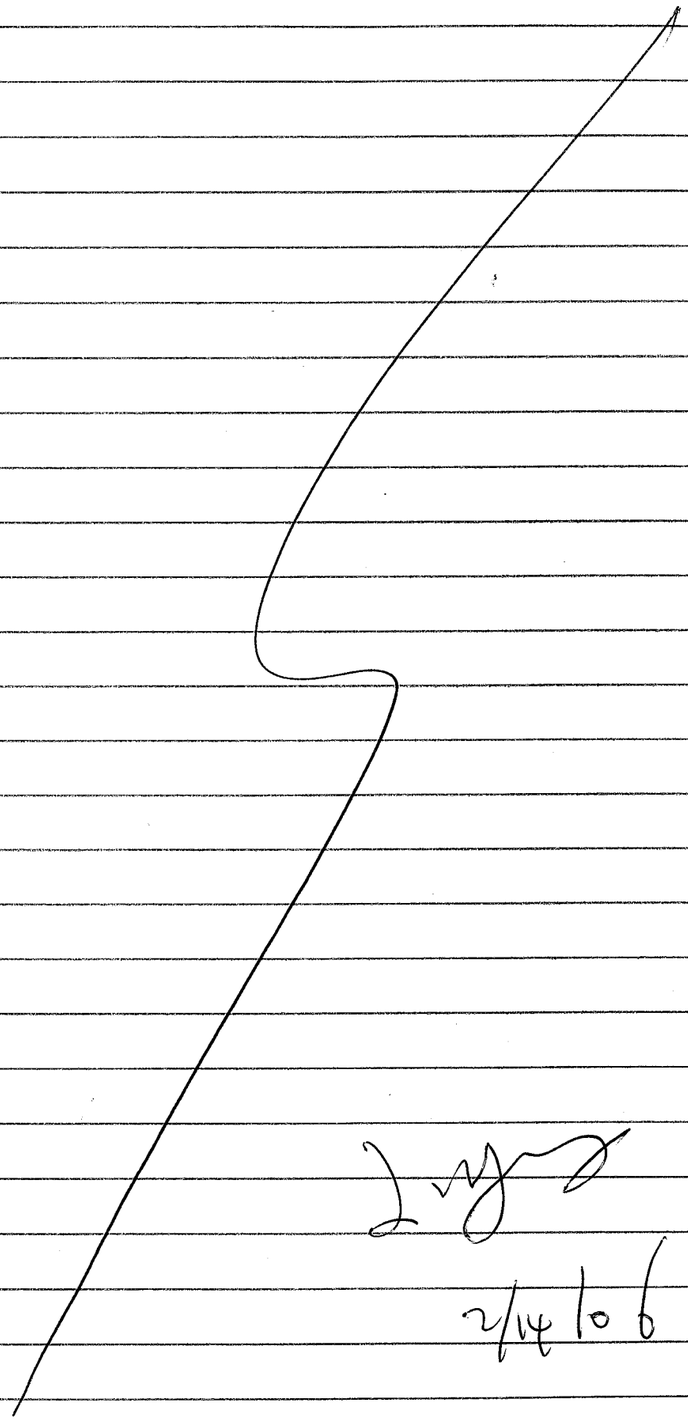
2/14/06



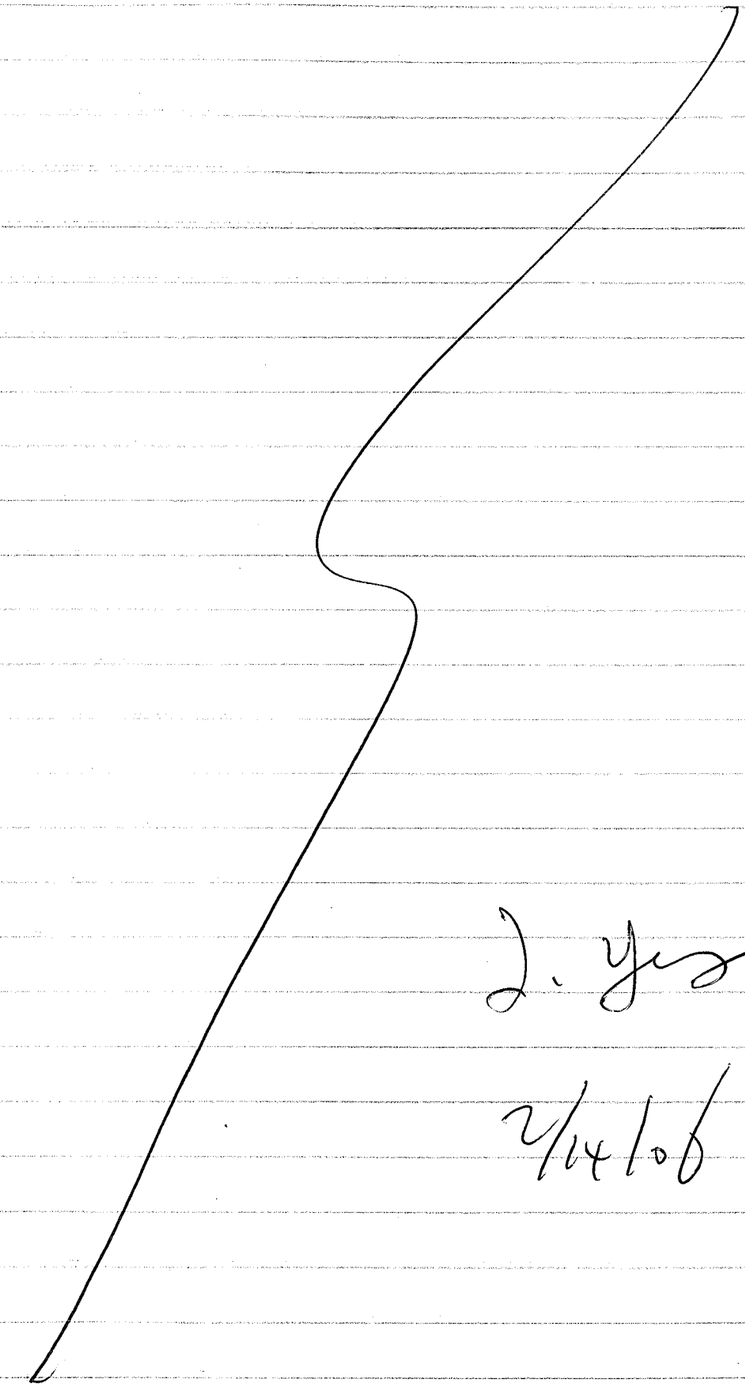
2/14/06

2/14/06

2/14/06



L. Yang
2/14/06



L. Yang
2/14/06

Work continued in
Book #572

J. Yang
2/14/06

The following paper/rport were published based on the work in this scientific notebook (#430):

R. T. Pabalan, L. Yang and L. Browning, "Deliquescence Behavior of Multicomponent Salts: Effects on the Drip Shield and Waste Package Chemical Environment at the Proposed Nuclear Waste Repository at Yucca Mountain, Nevada" in Scientific Basis for Nuclear Waste Management XXV, B. P. McGrail and G.A. Cragnolino eds, Warrendale, PA: Materials Research Society, Symposium Proceedings Vol. 713, pp. 37-44, 2002.

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R. Pabalan, Lietai Yang and L. Browning, "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 Report, CNWRA 2002-03, (San Antonio, TX: Center for Nuclear Waste Regulatory Analyses, May 2002).

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

4/11/06

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 430

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