CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

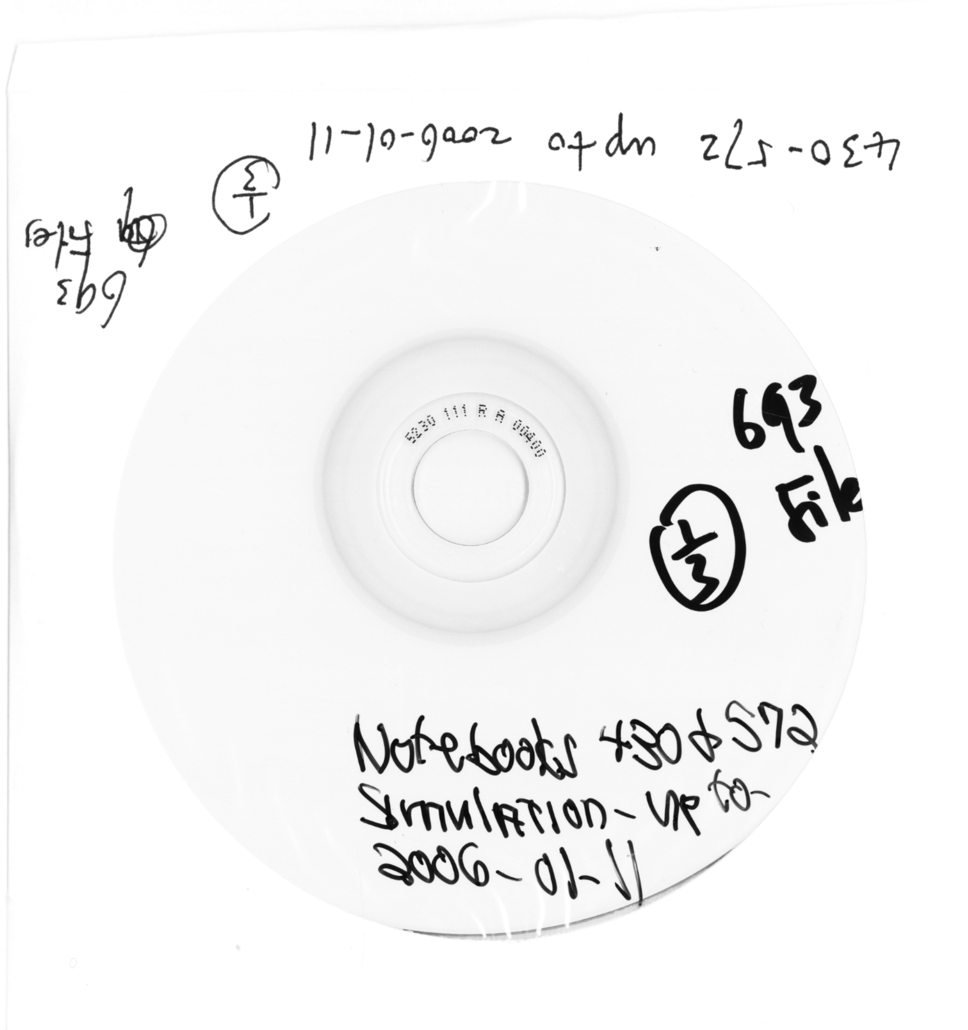
Book #430

J13 Water

Simulation.

Evaporation

CNWRA
CONTROLLED
COPY 430



Lietai Yang

J. Yang J. Y.

Initial Entry. 09/20/00

Project # 20.1402-561

Sub-project Title: Simulation of waters.

* Objective: Simulation of J-13 Water Chemistry During Evaporation.

* Approach: Using OLI Environmental System Program (ESP). V. 6.2d.

4.1.6.2 Groundwater Chemistry

See Table 18, Major Ion Concentrations for J-13 Well Water.

10^{-5} P_{CO_2}

Table 19. Average Composition of Synthetic J-13 Water Used in Reported Tests

Species	Synthetic J-13 Water (mg/L)	Average J-13 Water (mg/L)
Ca	6.4	12
Cl^-	6.9	6.7
F^-	2.2	4.4
HCO_3^-	108	139
K	5.3	4.7
Mg	2.2	1.9
Na	46	46
NO_3^-	8.0	8.8
SO_4^{2-}	18.1	17
Si(aq)	11.3	57.3
pH	7.84	6.8-8.3

DTN: LL991008104241.042 and LL980711104242.054

NOTE: Average J-13 water composition from Table 18.

ANL-EBS-MD-000033, REV 00 55 May 2000

L. Yang 9/16/02

All electronic files are stored in: NoteBooks/NoteBook#430 & 5?? - Simulation

J. Yang 11/17/03

09/20/00

Table 20. Average Composition of SPW Used in Reported Tests

Ions	Synthetic Porewater (mg/L)	Average Porewater (mg/L) [A]
Ca^{2+}	57.3 ± 1.80	101
Cl^{-}	76.6 ± 1.30	117
F^{-}	2.16 ± 0.09	0.86
HCO_3^{-}	20.3 ± 4.30	200 [B]
K^{+}	4.0 ± 0.27	8.0
Mg^{2+}	11.8 ± 0.20	17
Na^{+}	8.56 ± 0.32	61.3
NO_3^{-}	10.7 ± 0.29	Note C
SO_4^{2-}	83.9 ± 1.90	116
SiO_2(aq)	22.2 ± 2.1	70.6
pH	7.55 ± 0.12	8.32 (25°C)

DTN: LL991008004241.041 and LB991200DSTTHC.001 (TBV-4575)

NOTES: A Averages from porewater samples ESF-HD-PERM1(30.1'-30.5').
B Total dissolved inorganic carbon reported as bicarbonate; calculated from charge balance.
C Not analyzed.

Table 16. The Compositions of Evaporatively Concentrated Simulated 100x Well J-13 Water.

Species	Starting Solution (mg/L)	Solution Compositions (mg/L) and the Estimated Boiling Point (°C)						
Sample #	Initial J-13 Batch 3	ECBP 042399-0	ECBP 050699-0	ECBP 051899-0	ECBP 060199-0	ECBP 061099-0	ECBP 061499-0	ECBP 061599-0
DTN: LL990703005924.083								
Boiling Point (°C)		101					108	
Ca	6	735	0	0	48	0	62	587
K	535	3885	7985	15878	21180	24510	21532	8389
Mg	0	0	0	0	0	0	0	0
Na	4360	43317	106465	177301	202726	226721	190711	92279
Si	13	7461	30875	79388	118912	121020	90741	42504
F	210	2230	4392	4393	0	843	0	3020
Cl	729	7446	16130	32814	38125	49021	49831	15715
NO_3	846	9370	14905	34402	40243	51165	50443	15184
SO_4	1790	19326	38594	53455	41150	48408	32913	30480
HCO_3	4773	28712	53990	79599	98307	97053	91637	32372

09/20/00

Table 17. Results of the Evaporative Concentration of a Simulated Well J-13 Water Under Conditions of Constant Temperature and *RH*

Species	Starting Solution (mg/L)	Final Solution 85%*RH*/90°C (mg/L)	
Sample #	Initial J-13 Batch 1	J-13-01	
DTN: LL990703005924.083			
Cl	730	14419	19
NO_3	732	14085	19
SO_4	1632	29783	18
F	208	3630	17
HCO_3 [a]	4142	54614	13
Na	4032	76314	19
K	513	10832	21
Ca	5.0	36	7.2
Mg	2.0	0	0

[a] Total inorganic carbon given as bicarbonate.

09/20/00

Reconciliation of Samples.

J.Y. 09/20/00

Study Name : ~~Jyn_J13~~ Syn_J13

Chemistry Model Syn-J13

Using OLI Sample Manager

(1) Synthetic J-13 Water

Sample Name: Syn_J13

After a few tries, set HCO_3^- to 100 mg/L (original was 108 mg/L, as there must be errors in HCO_3^-)

Reconciled by proration, adding 16.35% of each cations.

PH = 8.20529

Sample exported to ESP by using Stream ~~Bank~~ Manager.

J.Y. 09/25/00

Sample Name

Syn_J13

J.Y. 09/25/00

J. Y[illegible] 8/14/02

09/20/00

Sample : Syn-J13.

Sample Name : Syn_J13

Template Reconcile Units LastResult Help — Reconciled by reduce HCO_3^-

Syn_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	6.4	7.44645	CL-1	6.9	6.89992
K+1	5.3	6.16657	F-1	2.2	2.19997
MG+2	2.2	2.55972	HCO3-1	100.*	99.999
NA+1	46.	53.5215	NO3-1	46.	45.9996
			SO4-2	18.1	18.0998

Exported as Jyn_J13 PH=8.205

Changed. from 108 to 100

<PgDn>

Sample Name: Al

Note: HCO_3^{-1} was reduced to 100 mg/L from 108 mg/L.

* Average_J13 water.

Sample Name: Ave-J13

reconciled with 11% Cation proration

Reconciled Sample exported to ESP, Same Name

J. Y[illegible] 8/14/02

~~Sample Name: Ave_J13~~

Template Reconcile ~~AVE~~-J13 Units LastResult Help Reconciled by proration

Syn_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	12.	13.3276	CL-1	6.7	6.69995
K+1	4.7	5.21997	F-1	4.4	4.39997
MG+2	1.9	2.1102	HCO3-1	139.	138.999
NA+1	46.	51.0891	NO3-1	8.8	8.79991
			SO4-2	17.	16.9999

Exported as Ave-J13
pH=8.154

J.Y. 09/20/00
Si: ~~49~~ 57.3 mg/L
= 2.048 mmol/L

<PgDn>

* Synthetic Pore Water.

Sample Name: Syn_Pore

reconciled by proration. 5.51% Cation introduced.

J. Yang 8/14/00

Sample Name: Syn_Pore

reconsiled by proration: 5.51% Cation
very good. basically within error.

pH = 7.997 (measured 7.75).

As HCO_3^- has the biggest error, I
reduce HCO_3^- by 4.30 which is the error
range:
The reconsile by proration: 3.86% of each cation.
J.Y. 09/20/00

Now: pH = 3.413. impossible!!

Try HCO_3^- 20.3 - 1.0 mg/L 5.12% of each cation Required
pH = 7.996

Try HCO_3^- 20.3 - 2 = 18.3 mg/L 4.76% Cation required
pH = 7.9423

Try HCO_3^- 17.3 mg , 4.36% — J. Yang 8/14/00
pH = 7.992

Try HCO_3 16.3 mg/L 3.96% , pH = 7.9897

09/20/00.

J.Y. 09/21/00

Try NO_3^- 15.2 mg/L ~~3.78%~~ 3.6%, P=7.987

Try NO_3^- 16.00 mg/L 3.86% pH=3.4136

Wrong!!

Try HCO_3^- 16.1 mg/L 3.90% pH=7.989

Try HCO_3^- 15.9 mg/L 3.83, pH=3.413

: : 15.8 mg/L 3.79 pH=3.412

15.5 3.67 pH=3.411

: : 15.4 3.63 pH=3.41

Try NO_3^- again 15.3 mg/L 3.60 pH=7.987

15.2 3.56 pH=7.987

14.3 mg/L 3.21% pH=3.405

Try NO_3^- again,

(OLI Jim said may form complex.)

: 15.1 3.52% pH=7.9864

: 15.0 3.48% pH=3.4086

use original HCO_3^- (20.3).

* Reconsile by 5.51% each cation. (proration)

Export as Syn-Pore (original, HCO_3^{-1} = 20.3) pH=7.997.

Jim at OLI said I should not use proration then I can find out which one causes the problem.

J. Yang 8/14/02

Sample Name: Syn_Pore.

Template Reconcile Units LastResult Help

SYN_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	57.	60.1383	CL-1	76.6	76.5996
K+1	4.	4.22022	F-1	2.16	2.15999
MG+2	11.8	12.4497	HCO3-1	20.3	20.2999
NA+1	8.56	9.0313	NO3-1	10.7	10.6999
			SO4-2	83.9	83.8996

Sample Name J.Y. ~~Ave-pore.~~ 09/21/00 Syn-pore

pH=7.997

<PgDn>

Reconciled by adding 5.51% each cation.

Exported to ESP: Syn-pore.

* Average Pore water:

Sample Name: Ave-Pore

NO_3^- Not analyzed, I assign the same value as in Syn-Pore. (10.7 mg/L)

AS HCO_3^- in the Assay was calculated, I shall use HCO_3^- to balance the charge.

J. Yang 8/14/02

Sample: Ave-Pore

Template Reconcile Units LastResult Help

SYN_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	101.	100.999	CL-1	117.	116.999
K+1	8.	7.99996	F-1	0.86	0.859995
MG+2	17.	16.9999	HCO3-1	200.	206.743
NA+1	61.3	61.2996	NO3-1	10.	9.9999
			SO4-2	116.	116.

Sample Name Ave-Pore

pH=8.205

<PgDn>

Reconciled by adding 6.744 mg/L HCO_3^-.

~~pH= 8.205~~.

* Reconcile water from Table 16 of (ANL-EBS-MD-000001 Rev 00C, 1999) and from Table 17

Sample Name: Table16, added 2609.17 HCO_3^- mg/L, pH=7.989

Sample Name: Table17 added 2660.04 mg/L HCO_3^-, pH= 7.9977

Table16 + Table17 Exported to Esp Files. [signature]

Sample: Table16

Template Reconcile Units LastResult Help

SYN_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	6.	5.98434	CL-1	729.	727.097
K+1	535.	533.604	F-1	210.	209.452
MG+2			HCO3-1	4773.	7370.09
NA+1	4360.	4348.62	NO3-1	846.	843.794
			SO4-2	1790.	1785.33

Sample Name Table 16

Si = 13 mg/L (= 0.4629 mM)

pH=7.989

added 2609.17 mg to balance

<PgDn>

Template Reconcile Units LastResult Help

SYN_J13 Study
SYN_J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	5.	4.98668	CL-1	730.	728.057
K+1	513.	511.636	F-1	208.	207.446
MG+2	2.	1.99468	HCO3-1	4142.	6791.06
NA+1	4032.	4021.27	NO3-1	732.	730.055
			SO4-2	1632.	1627.66

Sample Name Table 17

Si = 0.

pH=7.998

<PgDn>

Sample Table 17. [initials] 09/25/02

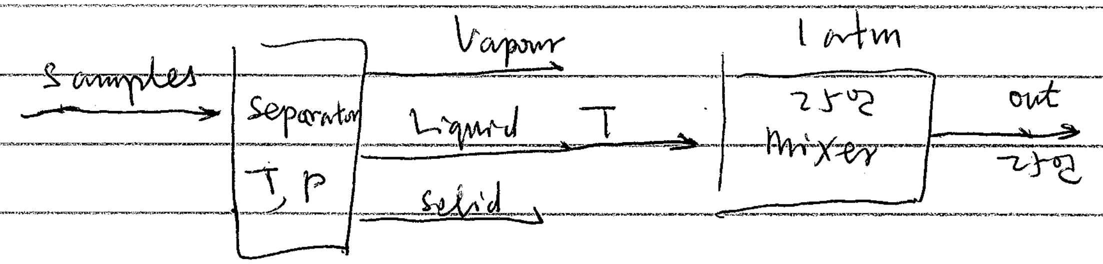
09/25/00

Simulation

* Evaporation at Constant T & T

In Esp:

Process Build:



Isothermal: T = 90C ; P = 0.588021 atm*

*: P_{H_2O} (T = 90C) = 525.76 mmHg, Page 3-45

Perry's Chem. Eng. Hand Book.

~~at 85% RH at 90C~~ : 525.76 * 0.85 = 446.896 mmHg

= 0.588021 atm

use Syn_J13 as input Sample.

Chemistry Model: Syn_J13 (same)

~~Also. This model does not allow Regenerate the~~

chemistry. I use a new one: "J13Z"

Regenerate the model, turn on all solid

and add 11.3 mg/L Si → $\frac{11.3}{28.08}$ = 0.4023 * 10^{-3} m/L

J. Yang 3/19/02

09/25/00

Save Results to spreadsheet Files

turn on all zero print (to have same format of print out).

After trying many times, I found it is better to export the Total species (Molecules) data.

In Spreadsheet: Two sheets, Summary sheet and Data sheet.

Syn_J13_Evap_90.xls Summary_sheet Page 1 9/25/00

(after reconciled → input; from data sheet → Amount lost)

	input 25oC	Amount lost during evapor.	Amout left after evap	C of liquid after evap at 90oC	C of liquid if analyzed at 25oC
	mg/L	mg	mg	mg/L	mg/L
Ca	7.446	7.4342	0.0118	2.79E+01	2.95E+01
Cl	6.9	3.017E-09	6.9	1.63E+04	1.73E+04
F	2.2	1.3161431	0.883857	2.09E+03	2.21E+03
HCO3	100	78.08732	21.91268	5.18E+04	5.49E+04
K	6.16657	0	6.16657	1.46E+04	1.54E+04
Mg	2.5597	2.560005	-0.000305	-7.21E-01	-7.64E-01
Na	53.5215	0	53.5215	1.27E+05	1.34E+05
NO3	46	2.055E-08	46	1.09E+05	1.15E+05
SO4	18.1	0	18.1	4.28E+04	4.53E+04
Si	11.3	0	11.3	2.67E+04	2.83E+04
pH	8.08679			10.9112	11.9083
Sum (mg/L)				3.90E+05	4.13E+05
Density (kg/m^3)	0.99706			1.268084	1.343401943
Volume of liquid (m^3/hr or m^3)				4.23E-07	3.99E-07

Note: pH= 8.205 (before SiO2 introduced for input)

Moles (mM): 0.40242

J. Yang 3/19/02

09/25/00

Syn_J13_Evap_90.xls Data_sheet Page 1/ 2 9/25/00

Exported by Esp

Calculated to see contributions to elements or compou.

Stream	Syn_J13	V_Syn_J13	L_Syn_J13	S_Syn_J 13	Out
Phase	Aqueous	Vapor	Aqueous	Solid	Mixed
Temperature, C	25	90	90	90	25
Pressure, atm	1	0.588021	0.588021	0.588021	1
pH	8.08679		10.9112		11.9083
Total mol/hr	55.5142	55.4931	0.0212966	2.91E-04	0.0213019
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.5115	55.492	0.0195573		0.0195519
H2F2	3.72E-05	3.44E-22	5.54E-06		
CO2	6.11E-04	0.0011289	1.42E-11		2.56E-13
H2SO4					
HCL		8.50E-14	3.69E-05		7.37E-06
HF	1.44E-09	6.91E-10	2.00E-13		7.76E-15
HNO3	3.02E-04	3.31E-13	3.38E-16		
SICL4					
SIF4	1.03E-05				
SO3					
H2SIO3	1.96E-04		6.14E-08		1.26E-08
KCL	2.24E-10		1.58E-04		1.58E-04
KHSO4			3.23E-17		
MGCO3	6.28E-07		3.83E-11		2.70E-11
MGH2SIO4	1.38E-09		2.74E-10		2.88E-10
MGSO4	7.21E-07		1.35E-13		4.16E-13
NAF	1.83E-07		3.55E-05		4.05E-05
NAHCO3	1.36E-06		2.43E-06		1.04E-07
NAHSIO3	9.10E-07		3.46E-04		3.95E-04
NANO3	2.79E-08		7.42E-04		7.42E-04
CASO4	2.50E-06		1.74E-12		1.20E-12
CAH2SIO4	2.54E-10		2.00E-10		4.40E-11
SIO2	1.95E-04		2.20E-07		1.46E-08
CACO3	2.48E-06		7.81E-10	1.51E-04	8.84E-11
H2CO3					
H6F6					
KMGCL3	6.49E-05		2.02E-11		1.71E-11
KOH					
NA3HSO42					
NA6SO42CO3	9.26E-05		9.42E-05		9.12E-05
MGOH2				1.05E-04	
NAOH					5.21E-06
CAOH2					
CA2CL2O.2H2C					
CACL2.1H2O					
CACL2.2H2O					
CACL2.4H2O					
CACL2.6H2O					
CACL2			1.10E-10		5.80E-11
CAF2				3.46E-05	9.01E-10
CANO32.3H2O					
CANO32.4H2O					
CANO32	1.81E-04				
CASO4.2H2O					
K2CO3.1.5H2O					
K2CO3	4.64E-05				
K2SO4.1H2O					
K2SO4					

Species	FW	amount to vapour mole	amount to Solid mole	Total lost in Evapora mg
Ca	40		1.86E-04	7.4342
CL	35.5	8.50E-14		3.0173E-09
F	19	6.91E-10	6.93E-05	1.31614313
HCO3	61	0.0011289	1.51E-04	78.08732
K				0
Mg	24.3		1.05E-04	2.560005
Na				0
NO3	62	3.31E-13		2.0549E-08
SO4				0
Si				0

Contributed from different rows.

J. Yang 8/19/02

09/25/00

Syn_J13_Evap_90.xls Data_sheet Page 2/ 2 9/25/00

	Syn_J13	V_Syn_J13	L_Syn_J13	S_Syn_J13	Out
K3NASO42					
KF.2H2O					
KF.4H2O					
KF					
KHCO3					
KMGCL3.2H2O					
KNO3					
KOH.1H2O					
KOH.2H2O					
MGCL2.2H2O					
MGCL2.4H2O					
MGCL2.6H2O					
MGCL2					
MGCLOH					
MGCO3.3H2O					
MGF2					
MGNO32.2H2O					
MGNO32.6H2O					
MGNO32	3.91E-05				
MGSO4.1H2O					
MGSO4.6H2O					
MGSO4.7H2O					
MGSO4OH.0.5I					
MGSO4OH					
NA2CO3.10H2C					
NA2CO3.1H2O					
NA2CO3.7H2O					
NA2CO3	8.85E-04		2.63E-04		2.68E-04
NA2SIO3.5H2O					
NA2SIO3.6H2O					
NA2SIO3.9H2O					
NA2SIO3			5.62E-05		7.76E-06
NA2SO4.10H2C					
NA2SO4					
NA3FSO4					6.07E-06
NACL					2.95E-05
NAHF2					
NAHSO4					
NAOH.1H2O					
Total g/hr	1000.32	999.755	0.536501	0.023983	0.536501
Volume, m3/hr	0.0010033	2.79744	4.23E-07	3.03E-09	3.99E-07
Enthalpy, cal/hr	-3.79E+06	-3.18E+06	-1713.45	-76.6669	-1737.3
Vapor fraction		1			
Solid fraction				1	2.85E-04
Organic fraction					
Osmotic Pres, a	0.135279		265.473		222.626
Redox Pot, volts					
E-Con, 1/ohm-c	3.18E-04		0.4274		0.178569
E-Con, cm2/ohr	64.4057		67.7448		41.0006
Abs Visc, cP	0.891946		1.02723		2.83186
Rel Visc	1.00138		3.26916		3.1793
Ionic Strength	0.0035189		7.29586		6.81646

$$\text{density} = \frac{0.536501 \times 10^{-6}\ t}{0.423 \times 10^{-6}\ m^3} = 1.268\ t/m^3$$

J.Y. 12/04/00.

J. Yang 8/19/02

Note. OLI does not print out concentration of element or basic compound. I did it the following way:

~~Weight (i) =~~ J.Y. 09/25/00

Weight (i, in liquid) = Weight (i, input) - Weight (i, vapor) - Weight (i, solid)

As there are only a few vapor and solid species.

J.Y. 09/25/00

C_i (90°C) = Weight (i, in liquid) ~~at 90°C~~ [90°C] / ~~volum at 90°C~~

C_i (25°C) = Weight (i, in liquid [90°C]) / Volume cooled to 25°C.

J.Y. 09/25/00

Working with different Samples. (Evap. at 90°C, 85%RH)

1. Syn_J13 : adding SiO_2: 11.3mg/L of Si → 0.40242 × 10^{-3} mol/L

Saved spreadsheet file as Syn-J13-Evap-90.XLS

J.Y. 09/26/00

2. Ave_J13 : Adding SiO_2: 57.3/28.08 (of Si) ⇒ ~~4.025E-4~~ 2.04 E-3 mol/L

Spreadsheet file saved as Ave-J13-Evap_90. XLS

3. Syn_pore : Specify : SiO_2 = 22.2 mg/L → 0.3645 E-3 mol/L

Spreadsheet file saved as : Syn-pore-Evap-90 .XLS

4. Ave_pore : Specify : SiO_2 = 70.6 mg/L → 1.175E-3 mol/L

Spreadsheet file saved as : Ave-Pore-Evap_90. XLS

5. Table17 : Specify : SiO_2 = 0

Spreadsheet file saved as : Table17_Evap_90.XLS

~~6. Table 16 : Specify~~ J.Y. 09/25/00

* Note : File Directory C:\work\J13_Water

[signature]

3/19/02

Working with Different samples
Boiling at 1 atm

1. Table16 Sample
~~adding: Si: 13 mg/L~~

① 101℃: Spread sheet file saved as Table16_Evap_101.XLS
~~② 104℃ Table16_Evap_104.XLS~~
③ 108℃ —108.XLS
④ 112℃ —112.XLS
⑤ 120℃ spreadsheet file saved as Table16_Evap_120.XLS
⑥ 110℃ spreadsheet file saved as Table16_Evap_120.XLS
⑦ 111℃ spread sheet file saved as Table16_Evap_111.XLS
J.Y. 09/27/00

2. Syn_J13 sample
~~adding Si: 11.3 mg/L~~

① 101℃: Spread sheet file saved as Syn_J13_Evap_101.XLS
② 104℃ —104.XLS
③ 108℃ —108.XLS
④ 112℃ —112.XLS
⑤ 120℃ spreadsheet file saved as Syn_J13_Evap_120.XLS

J.Y. 09/25/00

Note: All Files in Directory C:\work\J13_Water

3. Ave_J13 sample. adding SiO_2: 57.3 mg/L of Si ⇒ ~~4.023E-4 mol~~ ~~4.023E-4 mol~~ ~~2.04~~ 2.04E-3 mol/L
~~ado~~ J.Y. 09/26/00 J.Y. 09/26

① 101℃ Spread sheet file saved as: Ave_J13_Evap_101.XLS
② 104℃ —104.XLS
③ 108℃ —108.XLS
④ 112℃ —112.XLS
⑤ 120℃ Spread sheet file saved as Ave_J13_Evap_120.XLS

Note: at 108℃ Na_2SO_4 were found to be solid.
only at this temperature.

4. Syn_Pore sample: adding SiO_2: 22.2 mg/L of SiO_2 ⇒ 0.3695E-3 mol/L

① 101℃ Spreadsheet file saved as: Syn_Pore_Evap_101.XLS
② 104℃ —104.XLS
③ 108℃ —108.XLS
④ 112℃ —112.XLS
⑤ 120℃ Spreadsheet file saved as Syn_Pore_Evap_120.XLS

5. Ave_Pore Sample: adding SiO_2: 70.6 mg/L of SiO_2 ⇒ 1.175E-3 mol/L
① 101℃ Spreadsheet file saved as Ave_Pore_Evap_101.XLS
② 104℃ —104.XLS
③ 108℃ —108.XLS
④ 112℃ —112.XLS
⑤ 120℃ Spreadsheet file save as Ave_Pore_Evap_120.XLS

All files were printed out and filed in a binder.

Note: All files in Pages 19-20 are in Directory:

C:\work\J13_water

All Results are consolidated into one file, 6 sheets.

File name: J13_Water_Evaporation.xls.

See pages 21_26

L.Y. 09/27/00

J13_Water_Evaporation.xls Syn_J13 Page 1/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25°C						
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120	90oC, 85%RH
Ca	7.45E+00	6.76E+00	2.60E+01	4.94E+01	7.34E+01	1.17E+02	2.95E+01
Cl	6.90E+00	3.76E+03	1.48E+04	2.91E+04	4.21E+04	6.70E+04	1.73E+04
F	2.20E+00	1.20E+03	2.78E+03	3.55E+03	3.59E+03	2.32E+03	2.21E+03
HCO3	1.00E+02	1.01E+04	4.51E+04	7.25E+04	7.29E+04	2.44E+04	5.49E+04
K	6.17E+00	3.36E+03	1.32E+04	2.60E+04	3.76E+04	5.99E+04	1.54E+04
Mg	2.56E+00	-1.66E-01	-6.54E-01	-1.29E+00	-1.86E+00	-2.96E+00	-7.64E-01
Na	5.35E+01	2.92E+04	1.15E+05	1.80E+05	2.29E+05	2.88E+05	1.34E+05
NO3	4.60E+01	2.51E+04	9.87E+04	1.94E+05	2.80E+05	4.47E+05	1.15E+05
SO4	1.81E+01	9.87E+03	3.88E+04	1.30E+04	7.03E+03	6.40E+03	4.53E+04
Si	1.13E+01	6.16E+03	2.42E+04	4.76E+04	6.89E+04	1.10E+05	2.83E+04
pH after cooled to 25oC	8.09E+00	1.18E+01	1.21E+01	1.24E+01	1.27E+01	1.27E+01	1.19E+01
pH at T	8.09E+00	1.06E+01	1.08E+01	1.10E+01	1.10E+01	1.10E+01	1.09E+01
Sum of salt (mg/L)	2.54E+02	8.87E+04	3.52E+05	5.66E+05	7.41E+05	1.00E+06	4.13E+05
Dens at T (kg/m^3)	9.97E-01	1.03E+00	1.22E+00	1.36E+00	1.48E+00	1.65E+00	1.27E+00
Dens at 25oC (kg/m^3)	9.97E-01	1.07E+00	1.29E+00	1.47E+00	1.61E+00	1.83E+00	1.34E+00
V of liquid at 25oC (m^3)	1.00E-03	1.83E-06	4.66E-07	2.37E-07	1.64E-07	1.03E-07	3.99E-07
V fraction remaining	1.00E+00	1.83E-03	4.65E-04	2.37E-04	1.63E-04	1.03E-04	3.98E-04

1.27 t/m³
see page 15
L.Y.
12/04/00

File location: C:\work\J13_water\

Should be t/m³, see page 15.

L.Y. 12/04/00

J. Yang
8/19/02

J13_Water_Evaporation.xls Ave_J13 Page 2/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C						
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120	90oC, 85%RH
Ca	1.33E+01	1.33E+01	5.38E+01	1.04E+02	1.56E+02	4.79E+02	6.31E+01
Cl	6.70E+00	3.91E+03	1.63E+04	3.19E+04	4.81E+04	1.29E+05	1.94E+04
F	4.40E+00	5.39E+02	1.68E+03	2.84E+03	3.63E+03	2.66E+03	1.61E+03
HCO3	1.39E+02	1.20E+03	1.37E+04	3.69E+04	5.59E+04	2.51E+04	2.37E+04
K	5.22E+00	3.04E+03	1.27E+04	2.49E+04	3.75E+04	1.15E+05	1.51E+04
Mg	2.11E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-7.54E-01
Na	5.11E+01	2.98E+04	1.25E+05	2.14E+05	2,84E+05	2.91E+05	1.48E+05
NO3	8.80E+00	5.13E+03	2.15E+04	4.19E+04	6.32E+04	1.93E+05	2.55E+04
SO4	1.70E+01	9.91E+03	4.15E+04	2.07E+04	7.50E+03	2.38E+03	4.92E+04
Si	5.73E+01	2.57E+04	9.93E+04	1.85E+05	2.46E+05	2.20E+05	1.11E+05
pH after cooled to 25oC	7.92E+00	1.09E+01	1.12E+01	1.15E+01	1.16E+01	1.16E+01	1.13E+01
pH at T	7.92E+00	1.00E+01	1.05E+01	1.07E+01	1.09E+01	1.10E+01	1.07E+01
Sum of salt (mg/L)	3.05E+02	7.92E+04	3.31E+05	5.59E+05	7.47E+05	9.78E+05	3.93E+05
Dens at T (kg/m^3)	9.97E-01	1.05E+00	1.33E+00	1.61E+00	1.81E+00	1.86E+00	1.40E+00
Dens at 25oC (kg/m^3)	9.97E-01	1.10E+00	1.41E+00	1.73E+00	1.98E+00	2.04E+00	1.48E+00
V of liquid at 25oC(m^3)	1.00E-03	1.72E-06	4.10E-07	2.10E-07	1.39E-07	4.55E-08	3.46E-07
V fraction remaining	1.00E+00	1.71E-03	4.09E-04	2.09E-04	1.39E-04	4.54E-05	3.45E-04

File location: c:\work\J_13_water

t/m³. see page 21

J.Y. 12/04/00

J Yang

8/14/02

J13_Water_Evaporation.xls Syn_Pore Page 3/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C						
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120	90oC, 85%RH
Ca	6.01E+01	1.17E+04	3.60E+04	6.22E+04	8.03E+04	1.24E+05	3.94E+04
Cl	7.66E+01	3.87E+04	1.18E+05	1.89E+05	2.44E+05	3.25E+05	1.31E+05
F	2.16E+00	1.42E+00	7.31E-01	1.42E+00	3.31E+00	1.09E+01	-1.25E-01
HCO3	2.03E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-2.41E+00
K	4.22E+00	2.13E+03	6.47E+03	1.04E+04	1.35E+04	2.07E+04	7.22E+03
Mg	1.25E+01	4.25E+03	1.24E+04	1.73E+04	2.24E+04	3.38E+04	1.44E+04
Na	9.03E+00	4.56E+03	1.39E+04	2.23E+04	2.88E+04	4.44E+04	1.55E+04
NO3	1.07E+01	5.40E+03	1.64E+04	2.64E+04	3.41E+04	5.26E+04	1.83E+04
SO4	8.39E+01	4.24E+04	1.29E+05	2.07E+05	2.67E+05	4.12E+05	1.44E+05
SiO2	2.22E+01	8.35E+02	4.75E+02	2.93E+02	2.01E+02	1.29E+02	3.41E+02
pH after cooled to 25oC	7.82E+00	8.26E+00	7.86E+00	7.70E+00	7.55E+00	7.55E+00	7.88E+00
pH at T	7.82E+00	7.07E+00	6.60E+00	6.23E+00	5.93E+00	5.50E+00	6.80E+00
Sum of salt (mg/L)	3.02E+02	1.10E+05	3.32E+05	5.35E+05	6.91E+05	1.01E+06	3.70E+05
Dens at T (kg/m^3)	9.97E-01	1.01E+00	1.10E+00	1.17E+00	1.23E+00	1.31E+00	1.12E+00
Dens at 25oC (kg/m^3)	9.97E-01	1.05E+00	1.15E+00	1.23E+00	1.30E+00	1.39E+00	1.16E+00
V of liquid at 25oC(m^3)	1.00E-03	1.98E-06	6.52E-07	4.05E-07	3.14E-07	2.03E-07	5.84E-07
V fraction remaining	1.00E+00	1.97E-03	6.50E-04	4.04E-04	3.13E-04	2.03E-04	5.83E-04

File location ~~J13~~ c:\work\J13_water J.Y. 09/28/00

t/m³, see Page 21

J.Y. 12/04/00

J13_Water_Evaporation.xls Ave_Pore Page 4/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C						
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120	90oC, 85%RH
Ca	1.01E+02	3.41E+03	1.11E+04	1.85E+04	9.31E+04	2.53E+05	1.21E+04
Cl	1.17E+02	3.47E+04	1.17E+05	1.91E+05	2.55E+05	3.60E+05	1.31E+05
F	8.60E-01	2.33E+00	1.11E+00	1.53E+00	2.46E+00	2.39E+01	5.56E-01
HCO3	2.07E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.04E+02
K	8.00E+00	2.38E+03	7.98E+03	1.30E+04	6.37E+04	1.72E+05	8.95E+03
Mg	1.70E+01	2.95E+02	5.93E+02	5.97E+02	1.09E+03	1.03E+03	1.12E+03
Na	6.13E+01	1.82E+04	6.11E+04	9.99E+04	4.88E+05	1.32E+06	6.86E+04
NO3	1.00E+01	2.97E+03	9.97E+03	1.63E+04	7.96E+04	2.15E+05	1.12E+04
SO4	1.16E+02	3.45E+04	1.16E+05	1.89E+05	9.24E+05	2.49E+06	1.30E+05
SiO2	7.06E+01	1.05E+03	6.19E+02	3.60E+02	2.58E+02	3.62E+02	4.72E+02
pH after cooled to 25oC	7.32E+00	8.39E+00	7.86E+00	7.59E+00	7.86E+00	8.05E+00	7.86E+00
pH at T	7.32E+00	7.60E+00	7.18E+00	6.84E+00	6.37E+00	5.84E+00	7.28E+00
Sum of salt (mg/L)	7.09E+02	9.75E+04	3.24E+05	5.29E+05	1.90E+06	4.81E+06	3.63E+05
Dens at T (kg/m^3)	9.97E-01	1.00E+00	1.08E+00	1.15E+00	1.28E+00	1.49E+00	1.11E+00
Dens at 25oC (kg/m^3)	9.97E-01	1.04E+00	1.14E+00	1.22E+00	1.35E+00	1.58E+00	1.15E+00
V of liquid at 25oC(m^3)	1.00E-03	3.37E-06	1.00E-06	6.13E-07	1.26E-07	4.65E-08	8.94E-07
V fraction remaining	1.00E+00	3.36E-03	1.00E-03	6.11E-04	1.25E-04	4.64E-05	8.91E-04

File location: C:\work\J13_water\

t/m³, see page 21. J.Y. 12/04/00

J13_Water_Evaporation.xls Table16 Page 5/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C							Back to calculate again		good
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH			
Temperature °C	25	101	104	108	112	120	90oC, 85%RH	110	111	112, 09/27
Ca	6.00E+00	3.62E-01	-2.67E+00	-6.58E+00	-3.89E+01	-3.66E+01		-10.8389	-39.2772	-38.9486
Cl	7.27E+02	7.39E+02	2.30E+04	5.62E+04	5.40E+04	5.48E+04		92498.92	53973.61	53985.89
F	2.09E+02	2.13E+02	6.44E+03	1.57E+04	8.12E+04	8.16E+04		25909.74	81528.84	81154.49
HCO3	7.37E+03	7.45E+03	1.09E+05	1.39E+05	5.41E+04	2.70E+04		73492.5	58667.99	54122.61
K	5.33E+02	5.42E+02	1.69E+04	4.12E+04	4.59E+04	4.91E+04		67806.53	45601.28	45909.76
Mg	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00		0	0	0
Na	4.35E+03	4.42E+03	1.37E+05	3.36E+05	7.04E+05	6.49E+05		150894	712212.9	703523.2
NO3	8.44E+02	8.57E+02	2.67E+04	6.52E+04	3.86E+05	3.63E+05		107345.5	388991.3	385737.1
SO4	1.79E+03	1.81E+03	5.64E+04	1.38E+05	8.16E+05	7.67E+05		894.3439	822884	816000
Si	1.30E+01	1.32E+01	4.11E+02	1.00E+03	1.82E+03	1.77E+03		1653.818	1828.242	1818.21
pH after cooled to 25oC	7.98E+00	8.01E+00	1.01E+01	1.02E+01	1.01E+01	1.05E+01		10.094	9.98492	10.0571
pH at T	7.98E+00	7.89E+00	1.01E+01	1.02E+01	1.04E+01	1.04E+01		10.1871	10.3856	10.3898
Sum of salt (mg/L)	1.58E+04	1.60E+04	3.77E+05	7.92E+05	2.14E+06	1.99E+06		520484.5	2165649	2142212
Dens at T (kg/m^3)	9.97E-01	9.69E-01	1.18E+00	1.27E+00	3.87E+00	4.60E+00		1.260839	3.785547	3.873148
Dens at 25oC (kg/m^3)	9.97E-01	1.01E+00	1.26E+00	1.37E+00	3.09E+00	2.90E+00		1.378877	3.12606	3.09445
V of liquid at 25oC(m^3)	1.01E-03	9.84E-04	3.16E-05	1.29E-05	2.19E-06	2.33E-06		7.86E-06	2.17E-06	2.19E-06
V fraction remaining	1.00E+00	9.74E-01	3.13E-02	1.28E-02	2.16E-03	2.30E-03				

* Density(112oC) =3.87>Density(25oC)=3.09?, Right column shows 110oC no problem, 111oC problem started

File location: C:\work\J13_water\

t/m³, see page 21, J.Y. 12/04/00

J13_Water_Evaporation.xls Table17 Page 6/6 9/28/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C						
	Input	Evaporation under Boiling Condition (1 atm)					Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120	90oC, 85%RH
Ca							-2.56E+00
Cl							2.97E+04
F							4.66E+03
HCO3							1.27E+05
K							2.09E+04
Mg							-1.17E+00
Na							1.64E+05
NO3							2.98E+04
SO4							6.65E+04
Si							0.00E+00
pH after cooled to 25oC							1.03E+01
pH at T							1.02E+01
Sum of salt (mg/L)							4.43E+05
Dens at T (kg/m^3)							1.22E+00
Dens at 25oC (kg/m^3)							1.30E+00
V of liquid at 25oC(m^3)	1.01E-03						2.45E-05
V fraction remaining	1.00E+00						2.42E-02

t/m³, see page 21
L.y. 12/04/00

File location: c:\work\J13_Water

L. Yang 09/28/00

OLI Comments:

In the process Building stage, I specified

Flow (water) = 55.5087 mols/hr

Flow (total) = 55.8188 mols/hr

Everytime the program ran, the output flow rate is changed slightly? Why? (ie: total = ~~55.6995~~ = 55.8597 ; H_2O = 55.6955 ;

See below: L.y. 09/28/00

Table16_Evap_101.xls Data_sheet Page 1/2 9/28/00

Stream	Table16	V_Syn_J13	L_Syn_J13	S_Syn_J13	Out
Phase	Mixed	Vapor	Aqueous	Solid	Mixed
Temperature, C	25	101	101	101	25
Pressure, atm	1	1	1	1	1
pH	7.98174		7.88851		8.01333
Total mol/hr	55.8597	1.45609	54.3972	1.41E-04	54.4033
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.6955	1.45566	54.2338		54.2396
H2F2	5.11E-03	5.58E-24	5.26E-03		0.00523388
CO2	3.69E-02	0.00042869	3.01E-02		3.63E-02
H2SO4					
HCL	0.0208576	2.19E-17	2.06E-02		2.09E-02
HF	1.19E-07	1.23E-11	6.48E-07		1.13E-07
HNO3	1.38E-02	4.47E-16	1.38E-02		0.0138379
SICL4	9.051E-06	1.9139E-28	6.8184E-05		9.6158E-06
SIF4					

L.y. 09/28/00

Nov. 20/00.

Plotting results for J-13 Average Water

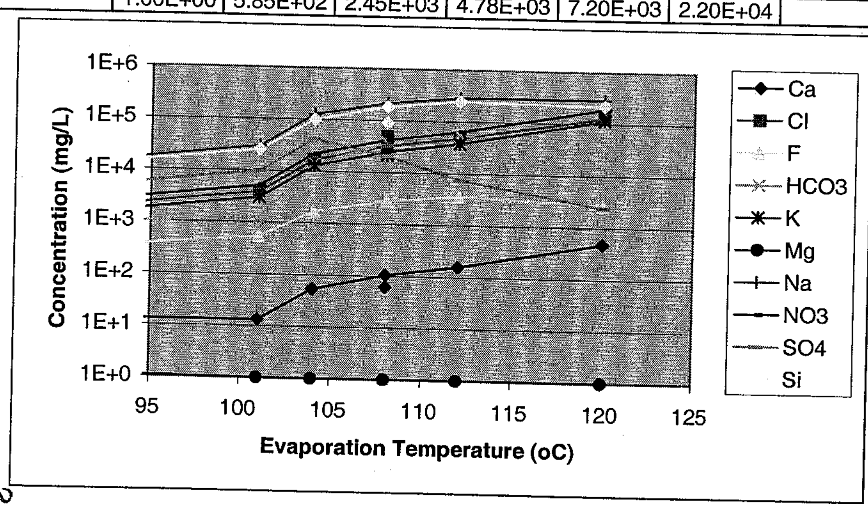
J13_Water_Evaporation_bobby.xls Ave_J13 Page 1/1 11/20/00

	Conc of species (mg/L) in liquid if sampled at high temperature and analyzed at 25 °C								
	Input	Evaporation under Boiling Condition (1 atm)						Table 16 DOE Report	Evaporation at Const T and RH
Temperature °C	25	101	104	108	112	120		108	90oC, 85%RH
Ca	1.33E+01	1.33E+01	5.38E+01	1.04E+02	1.56E+02	4.79E+02		6.20E+01	6.31E+01
Cl	6.70E+00	3.91E+03	1.63E+04	3.19E+04	4.81E+04	1.29E+05		4.98E+04	1.94E+04
F	4.40E+00	5.39E+02	1.68E+03	2.84E+03	3.63E+03	2.66E+03		1.00E+00	1.61E+03
HCO3	1.39E+02	1.20E+03	1.37E+04	3.69E+04	5.59E+04	2.51E+04		9.16E+04	2.37E+04
K	5.22E+00	3.04E+03	1.27E+04	2.49E+04	3.75E+04	1.15E+05		2.15E+04	1.51E+04
Mg	2.11E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00		1.00E+00	-7.54E-01
Na	5.11E+01	2.98E+04	1.25E+05	2.14E+05	2.84E+05	2.91E+05		1.91E+05	1.48E+05
NO3	8.80E+00	5.13E+03	2.15E+04	4.19E+04	6.32E+04	1.93E+05		5.04E+04	2.55E+04
SO4	1.70E+01	9.91E+03	4.15E+04	2.07E+04	7.50E+03	2.38E+03		3.29E+04	4.92E+04
Si	5.73E+01	2.57E+04	9.93E+04	1.85E+05	2.46E+05	2.20E+05		9.07E+04	1.11E+05
pH after cooled to 25oC	7.92E+00	1.09E+01	1.12E+01	1.15E+01	1.16E+01	1.16E+01			1.13E+01
pH at T	7.92E+00	1.00E+01	1.05E+01	1.07E+01	1.09E+01	1.10E+01			1.07E+01
Sum of salt (mg/L)	3.05E+02	7.92E+04	3.31E+05	5.59E+05	7.47E+05	9.78E+05			3.93E+05
Dens at T (kg/m^3)	9.97E-01	1.05E+00	1.33E+00	1.61E+00	1.81E+00	1.86E+00			1.40E+00
Dens at 25oC (kg/m^3)	9.97E-01	1.10E+00	1.41E+00	1.73E+00	1.98E+00	2.04E+00			1.48E+00
V of liquid at 25oC(m^3)	1.00E-03	1.72E-06	4.10E-07	2.10E-07	1.39E-07	4.55E-08			3.46E-07
Volume Factor	1.00E+00	5.85E+02	2.45E+03	4.78E+03	7.20E+03	2.20E+04			2.90E+03

t/m³

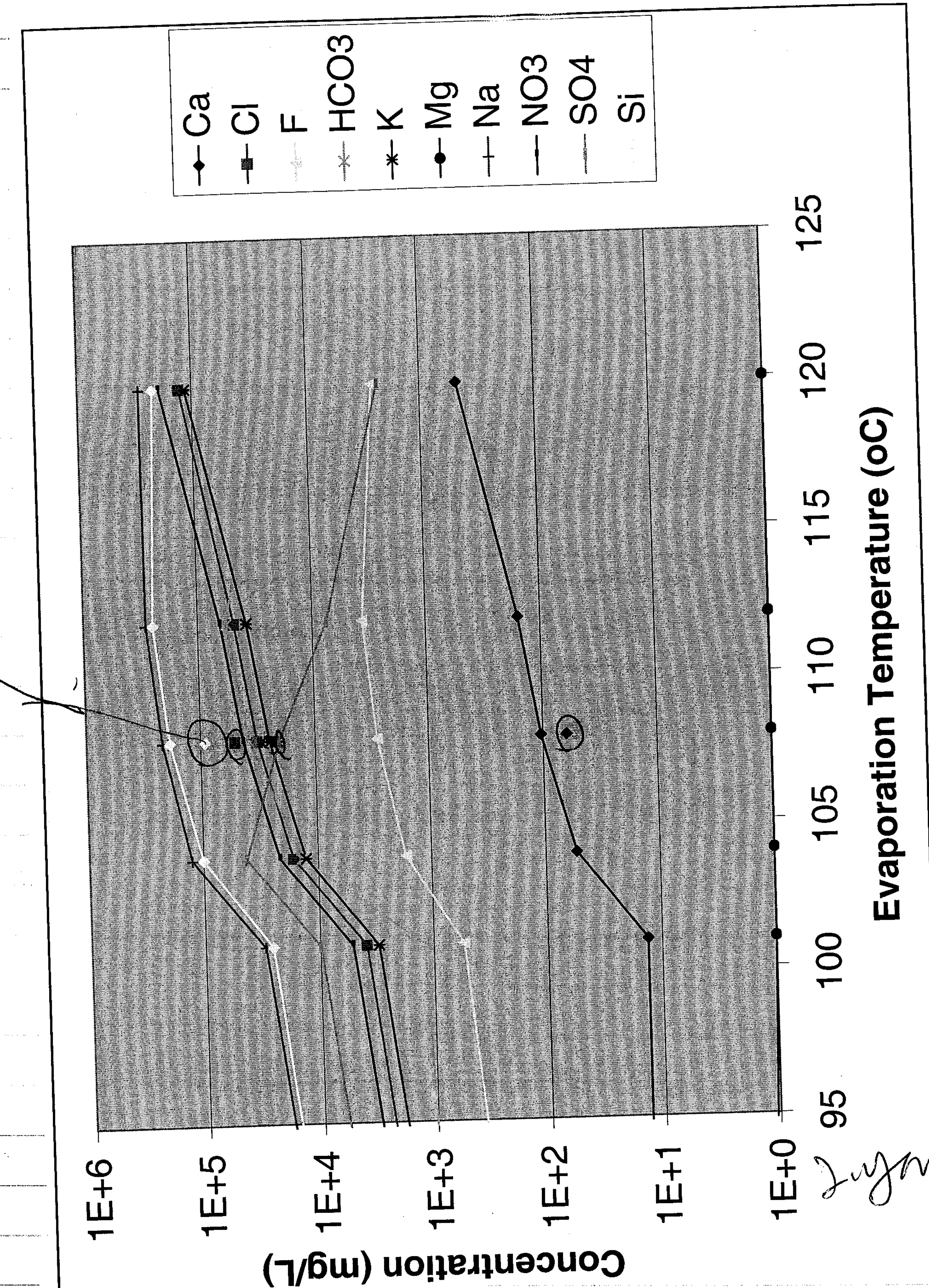
See page 21

J.Y. 12/4/00



DOE Results are similar. They are similar with our results.

J.Y. 11/20/00



J.Y. 8/19/02

Installation Test of OLI Software ESP V6.2e/CSP V2.0e

Date: November 29, 2000
Prepared by: Lietai Yang

In accordance with TOP-018, 5.6.3, the OLI Software ESP V6.2e/CSP V2.0e was tested by N. Sridhar on 11/29/00. Page A-1 to A-3 present the results obtained from ESP V6.2e/V2.0e and Page B-1 to B-2 present the results from Scientific Notebook #135 (page 10 and 11). The results in Page B-1 to B-2 were obtained from ESP V6.0. The two sets of results compares well.

This documentation is recorded in Scientific Notebook #430 (pages 30 through 35).

L. Yang 11/29/00


```
================================================================================

        O   O   O            L                   I I I I
      O           O          L                      I
    O               O        L                      I
   O                 O       L                      I
   O                 O       L                      I
   O                 O       L                      I
    O               O        L                      I
      O           O          L                      I
        O   O   O            L L L L L L L       I I I I

   E N V I R O N M E N T A L   S I M U L A T I O N   P R O G R A M

                    V - 6.2   July 1, 1999

                          SURVEY: FECL2
                 CHEMISTRY MODEL: FECL2
                  THIS FILE NAME: FECL2.LIS
                            DATE: 11/29/2000

================================================================================
```

TABLE OF CONTENTS

Page A-2

CRIIICL3IN moles	PH	CRIIICLION moles	CRIIIION moles	CRIIICL2ION moles	CROH3AQ moles
0.0000	0.4163	0.0000	0.0000	0.0000	0.0000
0.2500	0.4104	0.7557E-01	0.1728	0.1660E-02	0.2121E-19
0.5000	0.3542	0.1832	0.3118	0.4979E-02	0.1556E-19
0.7500	0.2899	0.3276	0.4120	0.1041E-01	0.1051E-19
1.000	0.2254	0.5074	0.4745	0.1811E-01	0.7111E-20
1.250	0.1629	0.7168	0.5053	0.2792E-01	0.4872E-20
1.500	0.1027	0.9488	0.5117	0.3947E-01	0.3377E-20
1.750	0.4449E-01	1.197	0.5002	0.5236E-01	0.2360E-20
2.000	-0.1211E-01	1.457	0.4764	0.6622E-01	0.1658E-20
2.250	-0.6741E-01	1.725	0.4444	0.8075E-01	0.1168E-20
2.500	-0.1217	1.997	0.4075	0.9575E-01	0.8224E-21
2.750	-0.1752	2.271	0.3682	0.1111	0.5786E-21
3.000	-0.2280	2.545	0.3284	0.1267	0.4062E-21
3.250	-0.2802	2.818	0.2896	0.1425	0.2844E-21
3.500	-0.3318	3.089	0.2528	0.1586	0.1985E-21
3.750	-0.3829	3.356	0.2188	0.1750	0.1382E-21
4.000	-0.4334	3.620	0.1880	0.1917	0.9605E-22
4.250	-0.4831	3.881	0.1606	0.2088	0.6667E-22
4.500	-0.5321	4.137	0.1367	0.2263	0.4627E-22
4.750	-0.5803	4.390	0.1160	0.2442	0.3215E-22
5.000	-0.6274	4.639	0.9834E-01	0.2627	0.2240E-22
5.250	-0.6735	4.885	0.8344E-01	0.2817	0.1567E-22
5.500	-0.7184	5.128	0.7097E-01	0.3013	0.1102E-22
5.750	-0.7621	5.368	0.6060E-01	0.3214	0.7795E-23
6.000	-0.8043	5.606	0.5203E-01	0.3421	0.5557E-23
6.250	-0.8452	5.842	0.4496E-01	0.3633	0.3996E-23
6.500	-0.8845	6.076	0.3917E-01	0.3851	0.2900E-23
6.750	-0.9222	6.308	0.3445E-01	0.4074	0.2126E-23
7.000	-0.9582	6.539	0.3060E-01	0.4303	0.1575E-23
7.250	-0.9926	6.769	0.2750E-01	0.4536	0.1181E-23
7.500	-1.025	6.998	0.2502E-01	0.4775	0.8959E-24
7.750	-1.056	7.225	0.2307E-01	0.5018	0.6881E-24
8.000	-1.085	7.452	0.2158E-01	0.5266	0.5354E-24

Page A-3

From Notebook #135

9/17/98 ~~9/18/98~~

Speciation modeling of simulated pit solutions

Objective: The objective is to understand the speciation in concentrated chloride solutions in pits of stainless steel and Ni-base alloys. Such an understanding will aid in an understanding of repassivation mechanisms in pits and in understanding the analyses performed

Approach: Used ESP version 6.0 from OLI Systems, Inc. to determine speciation in $CrCl_3$, $FeCl_2$ and $NiCl_2$ and mixtures.

Chemistry Model: $FeCl_2$

Specified Inflows:

H_2O	$FeBr_2$ / $FeCl_2$	H_2SO_4
HCl	$FeSO_4$	NaCl
NaOH		
$NiCl_2$	$FeCO_3$	$CrCl_3$

$Fe^{II}Cl_2$ = 0

$Ni^{II}Cl_2$ = 0

$Cr^{III}Cl_3$ = variable.

HCl = 0.5M

Temp: 25°C

Output of survey: $FeCl_2$.lis saved as excel file $crcl_3$sur.txt.

No precipitation was noted for $CrCl_3$ up to ~~8m~~. Hence the conc. was increased to 15m. No ~~0.5~~ HCl. No precipitation was seen even in this case. Output saved as $crcl_3$sur2.txt

J. [signature] 3/14/02

N. Sridhar 9/~~18~~17/98

From Notebook #135

9/17/98 ~~9/18/98~~

$CrCl_3$ + 0.5M HCl Survey

SURVEY: CrCl3
CHEMISTRY MODEL: FECL2
THIS FILE NAME: FECL2.LIS
DATE: 9/17/98

ESP V-6.0 SURVEY-VA 9/17/98 PAGE 2

CRIIICL3IN moles	PH moles	CRIIICLION moles	CRIIIION moles	CRIIICL2ION moles	CROH3AQ
0	0.4163	0	0	0	0
0.25	0.4103	7.56E-02	0.1728	1.66E-03	2.12E-20
0.5	0.354	0.1832	0.3118	4.98E-03	1.55E-20
0.75	0.2896	0.3277	0.4119	1.04E-02	1.05E-20
1	0.2251	0.5076	0.4742	1.81E-02	7.09E-21
1.25	0.1626	0.7172	0.5049	2.80E-02	4.86E-21
1.5	0.1023	0.9494	0.5111	3.95E-02	3.37E-21
1.75	4.40E-02	1.198	0.4996	5.24E-02	2.35E-21
2	-1.26E-02	1.458	0.4757	6.63E-02	1.65E-21
2.25	-6.80E-02	1.726	0.4436	8.08E-02	1.16E-21
2.5	-0.1223	1.998	0.4066	9.58E-02	8.18E-22
2.75	-0.1759	2.272	0.3673	0.1112	5.76E-22
3	-0.2287	2.546	0.3276	0.1268	4.04E-22
3.25	-0.281	2.819	0.2888	0.1426	2.83E-22
3.5	-0.3327	3.089	0.252	0.1587	1.97E-22
3.75	-0.3838	3.357	0.2181	0.1751	1.37E-22
4	-0.4343	3.621	0.1873	0.1918	9.53E-23
4.25	-0.4841	3.881	0.16	0.2089	6.61E-23
4.5	-0.5331	4.138	0.1361	0.2264	4.59E-23
4.75	-0.5813	4.39	0.1155	0.2444	3.19E-23
5	-0.6285	4.639	9.79E-02	0.2629	2.22E-23
5.25	-0.6746	4.885	8.31E-02	0.282	1.55E-23
5.5	-0.7195	5.128	7.06E-02	0.3015	1.09E-23
5.75	-0.7632	5.368	6.03E-02	0.3217	7.72E-24
6	-0.8055	5.606	5.18E-02	0.3424	5.50E-24
6.25	-0.8463	5.842	4.48E-02	0.3636	3.96E-24
6.5	-0.8856	6.076	3.90E-02	0.3854	2.87E-24
6.75	-0.9233	6.308	3.43E-02	0.4077	2.10E-24
7	-0.9594	6.539	3.05E-02	0.4306	1.56E-24
7.25	-0.9937	6.769	2.74E-02	0.454	1.17E-24
7.5	-1.026	6.997	2.49E-02	0.4778	8.87E-25
7.75	-1.057	7.225	2.30E-02	0.5022	6.81E-25
8	-1.086	7.451	2.15E-02	0.527	5.30E-25

J. [signature] 3/14/02

N. Sridhar 9/~~18~~17/98

Syn J13 Water evaporation. at Higher temp.

① 160°C. using OLI (OLI Esp 6.2e)

Note OLI only good for $X_{H_2O} > 0.65$

$0 < I < 30$.

The following Calculation may not be valid

Syn_J13_Evap_160.xls Summary_sheet Page 1 12/8/00

	input 25oC	Amount lost during evapor.	Amout left after evap	C of liquid after evap at 160oC	C of liquid if analyzed at 25oC
	mg/L	mg	mg	mg/L	mg/L
Ca	7.446	6.0852	1.3608	1.34E+02	1.02E+03
Cl	6.9	685.68428	-678.7843	-6.69E+04	-5.09E+05
F	2.2	9.2587004	-7.0587	-6.96E+02	-5.30E+03
HCO3	100	7500.2245	-7400.225	-7.30E+05	-5.55E+06
K	6.16657	221.94705	-215.7805	-2.13E+04	-1.62E+05
Mg	2.5597	0	2.5597	2.52E+02	1.92E+03
Na	53.5215	4004.3069	-3950.785	-3.90E+05	-2.96E+06
NO3	46	0.0001035	45.9999	4.54E+03	3.45E+04
SO4	18.1	1808.1024	-1790.002	-1.76E+05	-1.34E+06
Si	11.3	6.2275824	5.072418	5.00E+02	3.81E+03
pH	7.98174			10.3622	10.0623
Sum (mg/L)	2.54E+02			-1.38E+06	-1.05E+07
Density (kg/m^3)	1.008353			0.2412601	1.8358794
Volume of liquid (m^3/hr or m^3)				1.01E-05	1.33E-06

Note: pH= 8.205 (Before SiO2 introduced)

8/19/00

Result are negative. This back substraction method may not work. However look page 37 and 38. There is still water and conductivity still high.

Syn_J13_Evap_160.xls Data_sheet Page 1/2 12/8/00

Stream	Table16	V_Syn_J13	L_Syn_J13	S_Syn_J13	Out
Phase	Mixed	Vapor	Aqueous	Solid	Mixed
Temperature, C	25	160	160	160	25
Pressure, atm	1	1	1	1	1
pH	7.98174		10.3622		10.0623
Total mol/hr	55.8597	55.7517	0.0566408	9.99E-02	0.0567026
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.6955	55.69	0.0301065		0.0301645
H2F2	5.11E-03	1.18E-11	5.62E-05		
CO2	3.69E-02	[redacted]	1.87E-10		1.86E-10
H2SO4					
HCL	0.0208575	1.10E-10			8.66E-06
HF	1.19E-07	1.83E-04			4.30E-14
HNO3	1.38E-02	1.67E-09	1.45E-11		4.0901E-16
SICL4	9.0522E-06				
SIF4		4.1229E-16			
SO3					
H2SIO3	2.04E-04		1.68E-08		1.92E-07
KCL	1.14E-06		1.58E-03	0.00569095	9.84E-04
KHSO4	6.8059E-13		7.78E-17		
MGCO3					
MGH2SIO4					
MGSO4					
NAF	7.16E-04		8.23E-03	0	1.07E-02
NAHCO3	4.31E-03		8.21E-06		2.85E-06
NAHSIO3	4.48E-05		1.89E-04		2.34E-04
NANO3	2.25E-05		9.79E-03		6.63E-03
CASO4	2.16E-07				3.44E-16
CAH2SIO4	5.21E-13			0	5.42E-16
SIO2	2.05E-04		1.22E-06	0.00022178	6.88E-06
CACO3	3.30E-07		8.46E-16	0.00E+00	6.72E-14
H2CO3					
H6F6					
KMGCL3					
KOH			0.0000529		
NA3HSO42				0	
NA6SO42CO3	9.47E-03		5.01E-05	0	2.04E-05
MGOH2				0.00E+00	
NAOH					4.76E-07
CAOH2					
CA2CL2O.2H2O					
CACL2.1H2O					
CACL2.2H2O					
CACL2.4H2O					
CACL2.6H2O					
CACL2					1.12E-13
CAF2	0.00014938			1.52E-04	
CANO32.3H2O					
CANO32.4H2O					
CANO32	2.20E-06		1.7957E-13		
CASO4.2H2O				0	
K2CO3.1.5H2O					
K2CO3	6.95E-03		0.000048596		
K2SO4.1H2O					
K2SO4					

Species	FW	amount to vapour mole	amount to Solid mole	Total lost in Evapora mg
Ca	40		1.52E-04	6.0852
CL	35.5	1.10E-10	1.93E-02	685.684279
F	19	1.83E-04	3.04E-04	9.25870045
HCO3	61	[redacted]	6.14E-02	7500.2245
K	39		0.005691	221.94705
Mg	24.3		0.00E+00	0
Na	23		0.1741003	4004.3069
NO3	62	1.67E-09		0.00010345
SO4	96		0.0188344	1808.1024
Si	28.1		0.0002218	6.2275824

8/19/00

Syn_J13_Evap_160.xls Data_sheet Page 2/2 12/8/00

Aqueous.

K3NASO42					
KF.2H2O					
KF.4H2O					
KF			0.0024061		
KHCO3					
KMGCL3.2H2O					
KNO3			0.00407775		0.00722989
KOH.1H2O					
KOH.2H2O					
MGCL2.2H2O					
MGCL2.4H2O					
MGCL2.6H2O					
MGCL2					
MGCLOH					
MGCO3.3H2O					
MGF2				0	
MGNO32.2H2O					
MGNO32.6H2O					
MGNO32					
MGSO4.1H2O					
MGSO4.6H2O					
MGSO4.7H2O					
MGSO4OH.0.5H2O					
MGSO4OH					
NA2CO3.10H2O					
NA2CO3.1H2O				0	
NA2CO3.7H2O					
NA2CO3	6.54E-02			0.0614037	8.37E-05
NA2SIO3.5H2O					
NA2SIO3.6H2O					
NA2SIO3.9H2O					
NA2SIO3			5.13E-05		4.68E-07
NA2SO4.10H2O					
NA2SO4				0.0188344	
NA3FSO4					5.94E-05
NACL				0.0136241	5.87E-04
NAHF2				0	
NAHSO4					
NAOH.1H2O					
Total g/hr	1018.86	1005.98	2.44686	10.4291	2.44686
Volume, m3/hr	0.00101042	1.97066	1.01E-05	4.16E-06	1.33E-06
Enthalpy, cal/hr	-3.84E+06	-3.16E+06	-5264.61	-24483.1	-5409.63
Vapor fraction		1			
Solid fraction	2.6742E-06			1	3.42E-01
Organic fraction					
Osmotic Pres, atm	8.1305		464.935		623.402
Redox Pot, volts					
E-Con, 1/ohm-cm	1.59E-02		0.490378		0.241999
E-Con, cm2/ohm-mol	51.7807		30.2837		7.02455
Abs Visc, cP	0.951581		20165.7		3.43607
Rel Visc	1.06833		118360		3.85764
Ionic Strength	0.21882		33.8754		13.0215

J. Yang 3/19/02

Water 0.0301 mol/hr = 0.5418

Total total 2.44 g/hr

H_2O %wt = $\frac{0.5418}{2.44}$ = 22.2% in the aqueous phase

This number may not be correct. because OLI does not work at x_{H_2O} ~~x~~ < 0.65. J.Y. 12/08/00.

J.Y. 12/08/00

Does DOE have real measurement on ~~a~~ the H_2O %wt — temperature relationship

J.Y. 12/08/00

may be hard to measure. ~~Pr~~ Perhaps use conductivity probe.

A Review of past day showed.

J.Y. 12/08/00

~~S...~~	Total mol/hr	H_2O mol/hr	Total g/hr	E. Cond. 1/ohm-cm	x_{H_2O}	I
Syn_J13_Evap_120	0.005004	0.0036033	0.188176	0.6907	0.72	16.9
Syn_J13_Evap_108	0.01274	0.0108865	0.3498	0.5489	0.86	9.608
Syn_J13_Evap_104 (J.Y. 12/08/00)	0.02500	~~0.0208~~ 0.02327	~~0.5786~~ 0.603	~~0.3039~~ 0.460		~~3.925~~ 6.17
Syn_J13_Evap_101	0.1010	0.09928	1.470	0.2114		1.465
Syn_J13_Evap_160	0.03664	0.03010	2.446	0.4903	0.531	33.87

J. Yang 3/19/02

J. Yang
2/14/02

Jan. 26/01

Vapor pressure of saturated salts. using OLI Esp 6.2

① NaCl, KNO3 + NaNO3 (16.39°C) (289.39°K)

P_{H_2O} = 0.1216 atm (see page 42).

$P^{\circ}_{H_2O}$ (290°K) = 0.01917 Bar. (Handbook value)

$P^{\circ}_{(H_2O)}$ (t = 16.39) = 0.018473 atm (OLI), close Handbook value.

so Rel. Hum. = $\frac{0.1216}{0.018473}$ = 0.658 %

Note: Hand book value: CRC, 54th edition Page E46.
Rel. Hum = 30.49%.

② Pure water.

P_{H_2O} (16.39°C) = 0.018473 atm.

③ KCl pure salt

P_{H_2O} = 0.0158259 atm, RH = $\frac{0.0158259}{0.018473}$ = 0.8566

④ NaCl simple salt

P_{H_2O} = 0.0139816 atm, RH = $\frac{0.01398}{0.01847}$ = 0.7569

J. Yang
2/14/02

ESP V-6.2 PROCESS:EVAP_CTP 01/26/2001 PAGE 5

(1) NaCl, KNO3 + NaNO3

STREAM: Solid
TO :
FROM : NaKClNO3

Phases----------->	Aqueous	Solid	Vapor	Organic
Temperature, C	16.39	16.39	16.39	16.39
Pressure, atm	0.0121635	0.0121635	0.0121635	0.0121635
pH	0.0			
Total mol/hr	0.0	6.99772	0.0	0.0
-----------------	mol/hr	mol/hr	mol/hr	mol/hr
H2O	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0
HCL	0.0	0.0	0.0	0.0
HNO3	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0
NANO3	0.0	1.95626	0.0	0.0
KCL	0.0	0.0	0.0	0.0
NACL	0.0	2.2946	0.0	0.0
KNO3	0.0	2.74686	0.0	0.0
KOH.1H2O	0.0	0.0	0.0	0.0
KOH.2H2O	0.0	0.0	0.0	0.0
KOH	0.0	0.0	0.0	0.0
NAOH.1H2O	0.0	0.0	0.0	0.0
NAOH	0.0	0.0	0.0	0.0
	=============	=============	=============	=============
Total g/hr	0.0	578.092	0.0	0.0
Volume, m3/hr	0.0	2.6734E-04	0.0	0.0
Enthalpy, cal/hr	0.0	-7.6968E+05	0.0	0.0
Density, g/m3		2.1624E+06		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, atm	0.0			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	0.0			
E-Con, cm2/ohm-mol	0.0			
Abs Visc, cP	0.0			
Rel Visc	0.0			
Ionic Strength	0.0			

$P_{mix} = 0.01216$

$RH = \frac{0.01216}{0.018473} = 0.658$

See (2)

Hand book = 30.49 %

J. Yang 2/19/02

(5) $NaNO_3$, 16.39°C

$P = 0.0136496$ atm, $RH = \frac{0.0136496}{0.018473} = 0.739\%$

(6) KNO_3 16.39°C

$P = 0.0173728$ atm $RH = \frac{0.01737}{0.018473} = 0.9405$ ~~atm~~ %

J.Y. 1/31/01

Therefore, all P of simple salts are higher than their mixed salt. Both from handbook. and from OLI simulation.

At 60°C

(7) KNO_3 solid, 60°C

$P_{H_2O} = 0.1707$ atm, $RH = \frac{0.1707}{0.1965^*} = 0.866\%$

* 0.19695 atm is for pure water obtained using OLI.

J.Y. 1/31/01

Note that Handbook value is 82%, see ~~handbook~~ note book (page 41).

(8) pure water $P^\circ = 0.4673$ atm , T = 80°C

(9) pure water $P^\circ = 0.19695$ atm, T = 60°C

J. Yang 2/19/02

(10): NaNO3 at 30℃

$P = 0.26463$; $RH = \frac{0.26463}{0.4673} = 0.567$

close to handbook value, 65.6% (CRC book, see Page 41 Notebook.)

(11) NaCl at 30℃

$P = 0.3487$; $RH = \frac{0.3487}{0.4673} = 0.7462$

Handbook value = 76.4% (CRC book, see page 41 of Notebook)

(12) Input 4 salts, sometimes get two solid

See page 45.

[signature] 3/14/01

ESP V-6.2 PROCESS:EVAP_CTP 01/26/2001 PAGE 5

(12) Input 4 species.
NaCl + NaNO3 + KNO3 + KCl.

STREAM: Solid
TO :
FROM : NaKClNO3

Phases----------->	Aqueous	Solid	Vapor	Organic
Temperature, C	16.39	16.39	16.39	16.39
Pressure, atm	0.0129979	0.0129979	0.0129979	0.0129979
pH	0.0			
Total mol/hr	0.0	22.4145	0.0	0.0
------------------	mol/hr	mol/hr	mol/hr	mol/hr
H2O	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0
HCL	0.0	0.0	0.0	0.0
HNO3	0.0	0.0	0.0	0.0
O2	0.0	0.0	0.0	0.0
NANO3	0.0	0.0	0.0	0.0
KCL	0.0	0.0	0.0	0.0
NACL	0.0	10.4796	0.0	0.0
KNO3	0.0	11.9349	0.0	0.0
KOH.1H2O	0.0	0.0	0.0	0.0
KOH.2H2O	0.0	0.0	0.0	0.0
KOH	0.0	0.0	0.0	0.0
NAOH.1H2O	0.0	0.0	0.0	0.0
NAOH	0.0	0.0	0.0	0.0
	============	============	============	============
Total g/hr	0.0	1819.11	0.0	0.0
Volume, m3/hr	0.0	8.5521E-04	0.0	0.0
Enthalpy, cal/hr	0.0	-2.4426E+06	0.0	0.0
Density, g/m3		2.1271E+06		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, atm	0.0			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	0.0			
E-Con, cm2/ohm-mol	0.0			
Abs Visc, cP	0.0			
Rel Visc	0.0			
Ionic Strength	0.0			

end up (NACL 10.4796, KNO3 11.9349 circled)

[signature] 3/14/01

Solubility Calculations

① NaF at 100°C.

using ESP V-6.2.

Volume = 0.104895 × 10 L

F (NaF) = 1.19307 mol/hr

F (H2O) = 55.5 mol/hr

solubility: $\frac{1.193}{\frac{55.5}{1000} * 18} = 1.19$ molal

See attached sheet on Page 47

J. Yang 2/14/02

ESP V-6.2 PROCESS:EVAP_CTP 01/29/2001 PAGE 3

STREAM: L
TO :
FROM : Sept

print out for liquid stream of separator

Solubility ① NaF.

Phases----------->	Aqueous	Solid	Vapor	Organic
Temperature, C	100.	100.	100.	100.
Pressure, atm	1.	1.	1.	1.
pH	7.86975			
Total mol/hr	56.6932	0.0	0.0	0.0
------------------	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.5	0.0	0.0	0.0
H2F2	5.9887E-13	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0
H2SO4	0.0	0.0	0.0	0.0
HF	4.0722E-05	0.0	0.0	0.0
HNO3	0.0	0.0	0.0	0.0
SO3	0.0	0.0	0.0	0.0
NAF	1.19307	0.0	0.0	0.0
NAHCO3	0.0	0.0	0.0	0.0
NANO3	0.0	0.0	0.0	0.0
KHSO4	0.0	0.0	0.0	0.0
KNO3	0.0	0.0	0.0	0.0
K2SO4	0.0	0.0	0.0	0.0
NA2SO4	0.0	0.0	0.0	0.0
KF	0.0	0.0	0.0	0.0
K2CO3	0.0	0.0	0.0	0.0
NA2CO3	0.0	0.0	0.0	0.0
K2CO3.1.5H2O	0.0	0.0	0.0	0.0
K2SO4.1H2O	0.0	0.0	0.0	0.0
K3NASO42	0.0	0.0	0.0	0.0
KF.2H2O	0.0	0.0	0.0	0.0
KF.4H2O	0.0	0.0	0.0	0.0
KHCO3	0.0	0.0	0.0	0.0
KOH.1H2O	0.0	0.0	0.0	0.0
KOH.2H2O	0.0	0.0	0.0	0.0
KOH	0.0	0.0	0.0	0.0
NA2CO3.10H2O	0.0	0.0	0.0	0.0
NA2CO3.1H2O	0.0	0.0	0.0	0.0
NA2CO3.7H2O	0.0	0.0	0.0	0.0
NA2SO4.10H2O	0.0	0.0	0.0	0.0
NA3FSO4	0.0	0.0	0.0	0.0
NA3HSO42	0.0	0.0	0.0	0.0
NA6SO42CO3	0.0	0.0	0.0	0.0
NAHF2	0.0	0.0	0.0	0.0
NAHSO4	0.0	0.0	0.0	0.0
NAOH.1H2O	0.0	0.0	0.0	0.0
NAOH	4.0722E-05	0.0	0.0	0.0
H2CO3	0.0	0.0	0.0	0.0
H6F6	0.0	0.0	0.0	0.0
	============	============	============	============
Total g/hr	1049.95	0.0	0.0	0.0
Volume, m3/hr	0.00104895	0.0	0.0	0.0
Enthalpy, cal/hr	-3.8804E+06	0.0	0.0	0.0
Density, g/m3	1.0010E+06			
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	0.0	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, atm	58.9172			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	0.178208			
E-Con, cm2/ohm-mol	93.4643			
Abs Visc, cP	0.400901			

$\frac{1.1930}{1.04895} = 1.137$ M. ✓

$\frac{1.193}{\frac{55.5}{1000} * 0.018} = 1.19$ molal

On page 4, print out for solid stream shows 0.80689 of NaF. J.Y. 1/31/01

Page 4 of the print out is not included in the notebook. J.Y. 1/31/01

I = 0.98.

J. Yang 2/14/02

② solubility of K_2SO_4, 100°C

$$S = \frac{1.1329 \text{ mol/hr}}{\frac{48 \times 18}{1000}} = 1.34 \text{ molal}$$

I (strength) = 2.76.

③ KNO_3, 100°C

$$S = \frac{9.033 \text{ mol/hr}}{\frac{20 \times 18}{1000}} = 25.09 \text{ molal}$$

I = ~~0.966~~ 25.07
J.Y. 1/31/01

Water fraction $= \frac{20}{29.033} = 0.68887$.

This is within OLI limit.

④ Solubility of $NaNO_3$ at 100°C

$$S = \frac{7.685 \text{ mol/hr}}{\frac{20 \times 18}{1000}} = 21.3 \text{ molal}$$

I = 21.1178

$$X_{H_2O} = \frac{20}{27.6857} = 0.722$$

o.k.

[signature] 3/1/01

Note: the results are not printed. It is easy to do the calculation with OLI.

StreamAnalyzer Version 1.01 is a new release of the OLI software. It is window based it is very user friendly.

Due to the approaching release date of another version of the software, QA paper work will be done after the new release is received.

The results obtained with StreamAnalyzer should only be used as non-decision making information only.

J.Y. April 12/01

J.Y. 04/11/01

Calculate the water activity at 25 °C for NaCl + $NaNO_3$ system.

(0.1 mol)

Do equilibrium calculation given vapour amount, giving temperature (25 °C). The software calculate the water activity, vapour pressure of salt solution. The results are as follows (Note print out not attached. The result can be easily obtained in a second if give the input (The results from one run are given in pages 52, 53, 54)

[NaCl_NaNO3_Activity.xls] [Date] J.Y. 02/12/01 OLI_Simulation_Results

T=25 oC

Run #	Input Water	Input NaCl	Input NaNO3	Output liquid Water	Output liquid NaCl	Output liquid NaNO3	x(Water)	I	Solid NaCl	Solid NaNO3	Vapour Water	P(H2O)	a(H2O)
1	55.508	10	10	55.408	3.716	6.8202	0.840226	10.46	6.284	3.1798	0.1	0.020865	0.66491
2	55.508	8	10	55.408	3.716	6.8202	0.840226	10.46	4.284	3.1798	0.1	0.020865	0.66491
3	55.508	3.8	10	55.408	3.716	6.8202	0.840226	10.46	0.084	3.1798	0.1	0.020865	0.66491
4	55.508	3.8	6.83	55.408	3.716	6.8202	0.840226	10.46	0.084	0.0098	0.1	0.020865	0.66491
In the above, the both solid salts are present, the solution composition are the same (Eutonic), water activity are the same													
5	55.508	3	6.8	55.408	3	6.8	0.849712	9.7522	0	0	0.1	0.021767	0.69365
above not saturated													
6	55.508	3	12	55.408	3	7.5103	0.840556	10.425	0	4.4897	0.1	0.021237	0.67677
7	55.508	3	7.6	55.408	3	7.5103	0.840556	10.425	0	0.0897	0.1	0.021237	0.67677
8	55.508	2	12	55.408	2	8.5509	0.840038	10.452	0	3.4491	0.1	0.021707	0.69175
9	55.508	0	12	55.408	0	10.888	0.835767	10.761	0	1.112	0.1	0.022251	0.71717
10	55.508	0.1	12	55.408	0.1	10.763	0.836082	10.738	0	1.237	0.1	0.022469	0.71602
11	55.508	0.5	12	55.408	0.5	10.273	0.837219	10.653	0	1.727	0.1	0.02232	0.71129
12	55.508	1	12	55.408	1	9.6781	0.838421	10.565	0	2.3219	0.1	0.022127	0.70512
13	55.508	1.5	12	55.408	1.5	9.1039	0.839364	10.498	0	2.8961	0.1	0.021923	0.69862
The above shows the solubility of NaNO3 and the activity of water as a function of NaCl													
14	55.508	10	0	55.408	6.14	0	0.90024	6.1511	3.86	0	0.1	0.023744	0.75662
15	55.508	10	0.1	55.408	6.0983	0.1	0.899389	6.2082	3.9017	0	0.1	0.023699	0.7552
16	55.508	6.1	0.1	55.408	6.0983	0.1	0.899389	6.2082	0.0017	0	0.1	0.023699	0.7552
17	55.508	10	0.5	55.408	5.9336	0.5	0.895966	6.4381	4.0664	0	0.1	0.023521	0.74954
18	55.508	10	1	55.408	5.7319	1	0.891665	6.7297	4.2681	0	0.1	0.023301	0.74253
19	55.508	10	2	55.408	5.3423	2	0.882992	7.3269	4.6577	0	0.1	0.022868	0.72872
20	55.508	10	4	55.408	4.6177	4	0.865402	8.576	5.3823	0	0.1	0.022022	0.70179
21	55.508	10	5	55.408	4.2821	5	0.856514	9.2277	5.7179	0	0.1	0.021608	0.6886
22	55.508	10	6	55.408	3.964	6	0.84758	9.8972	6.036	0	0.1	0.021198	0.67555
23	55.508	10	6.5	55.408	3.8114	6.5	0.8431	10.239	6.1886	0	0.1	0.020995	0.66906
24	55.508	10	6.8	55.408	3.722	6.8	0.840406	10.446	6.278	0	0.1	0.020873	0.66518
25	55.508	10	7	55.408	3.716	6.8202	0.840226	10.46	6.284	0.1798	0.1	0.020865	0.66491
26	55.508	10	17	55.408	3.716	6.8202	0.840226	10.46	6.284	10.1798	0.1	0.020865	0.66491
The above shows the solubility of NaCl and the activity of water as a function of NaNO3													
27	55.508	0	0	55.408	0	0		1.00E-07	0	0	0.1	0.031385	1

Numbers in the table are in Moles

I and x(water) are all within the limits (30, 0.65)

Example output

Calculation Summary

Run #1 (1)

SinglePoint1 Calculation for Stream1

Automatic Chemistry Model
Public Databank

Vapor Amount Calculation — 0.1 mol in vapour.

Temperature	25.000	C
Pressure	0.020865	atm

Stream Parameters

Stream Amount	75.508	mol
Temperature	25.000	C
Pressure	0.020865	atm
pH	6.9902	
Osmotic Pressure	582.32	atm
Ionic Strength	10.460	mol/kg H2O
WaterActivity	0.66491	Activity
Electrical Cond, specific	0.23231	1/Ohm
Electrical Cond, molar	15.213	cm2/ohm-mol
Viscosity, absolute	2.6681	cP
Viscosity, relative	2.9955	cP/cP H2O

	Units	Total	Aqueous	Vapor	Solid	Organic
Density	g/ml	n/a	1.3706	1.5368e-5	2.2023	0.0
Enthalpy	cal	-5.8522e6	-4.8733e6	-5779.8	-9.7312e5	0.0

Stream Inflows

	Input	Final	
Water	55.508		mol
Sodium chloride	10.0000	10.000	mol
Sodium nitrate	10.000		mol

Scaling Tendencies

solids within temperature range

Sodium nitrate	1.0000
Sodium chloride	1.0000
Sodium hydroxide monohydrate	1.2129e-11

J.-Y.
02/12/01

Total and Phase Flows

	Units	Total	Aqueous	Vapor	Solid	Organic
Molar flow	mol	75.508	76.385	0.100000	9.4638	0.0
Mass flow	g	2434.4	1795.0	1.8015	637.52	0.0
Volumetric flow	L	118.82	1.3097	117.22	0.28948	0.0

Species Output

	Total	Aqueous	Vapor	Solid	Organic
	mol	mol	mol	mol	n/a
H2O	55.508	55.408	0.100000	0.0	0.0
NaCl	6.2840	0.0	0.0	6.2840	0.0
NaNO3	3.2753	0.095508	0.0	3.1798	0.0
HCl	1.8997e-12	1.0306e-13	1.7967e-12	0.0	0.0
HNO3	9.0409e-10	9.0104e-10	3.0480e-12	0.0	0.0
H+1	2.0482e-8	2.0482e-8	0.0	0.0	0.0
OH-1	2.1388e-8	2.1388e-8	0.0	0.0	0.0
Na+1	10.441	10.441	0.0	0.0	0.0
Cl-1	3.7160	3.7160	0.0	0.0	0.0
NO3-1	6.7248	6.7248	0.0	0.0	0.0

Molecular Output

solubility

	Total	Aqueous	Vapor	Solid	Organic
	mol	mol	mol	mol	n/a
H2O	55.508	55.408	0.100000	0.0	0.0
NaCl	10.000	3.7160	0.0	6.2840	0.0
NaNO3	10.000	6.8202	0.0	3.1798	0.0
HCl	1.8997e-12	1.0306e-13	1.7967e-12	0.0	0.0
NaOH	9.0598e-10	9.0598e-10	0.0	0.0	0.0
HNO3	9.0408e-10	9.0104e-10	3.0480e-12	0.0	0.0

Elements

	Aqueous	Vapor	Solid	Organic
	mol	mol	mol	n/a
CL(-1)	3.7160	1.7967e-12	6.2840	0.0
H(+1)	110.82	0.20000	0.0	0.0
N(+5)	6.8203	3.0480e-12	3.1798	0.0
NA(+1)	10.536	0.0	9.4638	0.0
O(-2)	75.869	0.10000	9.5394	0.0

Speciation Summary

J.-Y.
02/12/01

SinglePoint1 Results
2/9/01 3:21:03 PM

StreamAnalyzer

OLI Systems, Inc.

User Inflows	Related Inflows	Aqueous Species	Vapor Species	Solid Species	Organic Species
H2O	NaOH.1H2O	H2O	H2O - Vap	NaOH.1H2O	
NaCl	HCl	HCl - Aq	HCl - Vap	NaCl - Solid	
NaNO3	NaOH	NaNO3 - Aq	HNO3 - Vap	NaOH - Solid	
	HNO3	HNO3 - Aq		NaNO3 - Solid	
		H+1			
		OH-1			
		Na+1			
		Cl-1			
		NO3-1			

J. Y. 02/12/01

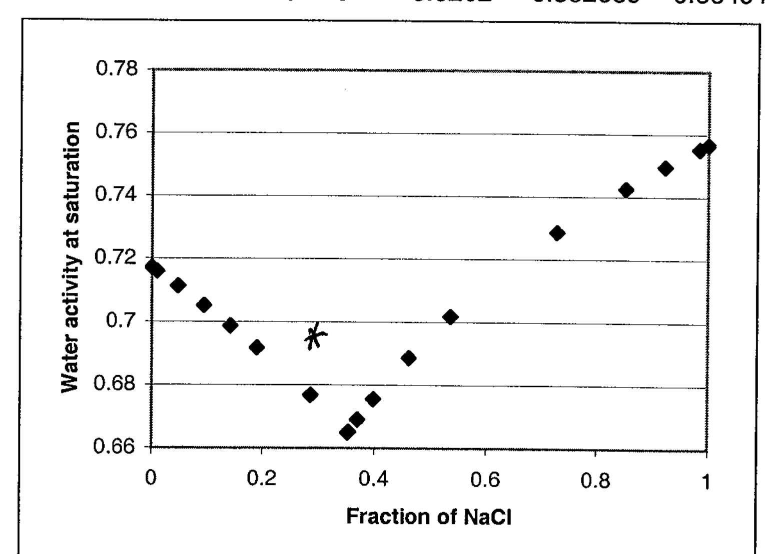
NaCl_NaNO3_Activity.xls 2/12/01 Water_Activity_at_Saturation

T=25 oC

Simulation	Liquid, composition moles Water	NaCl	NaNO3	Fraction	Activity a(H2O)
1	55.408	3.716	6.8202	0.352689	0.66491
2	55.408	3.716	6.8202	0.352689	0.66491
3	55.408	3.716	6.8202	0.352689	0.66491
4	55.408	3.716	6.8202	0.352689	0.66491
5	This run is non saturated	3	6.80	0.3063	0.6937
6	55.408	3	7.5103	0.285434	0.67677
7	55.408	3	7.5103	0.285434	0.67677
8	55.408	2	8.5509	0.189557	0.69175
9	55.408	0	10.888	0	0.71717
10	55.408	0.1	10.763	0.009206	0.71602
11	55.408	0.5	10.273	0.046412	0.71129
12	55.408	1	9.6781	0.09365	0.70512
13	55.408	1.5	9.1039	0.141457	0.69862
14	55.408	6.14	0	1	0.75662
15	55.408	6.0983	0.1	0.983867	0.7552
16	55.408	6.0983	0.1	0.983867	0.7552
17	55.408	5.9336	0.5	0.922283	0.74954
18	55.408	5.7319	1	0.851454	0.74253
19	55.408	5.3423	2	0.727606	0.72872
20	55.408	4.6177	4	0.535839	0.70179
21	55.408	4.2821	5	0.461329	0.6886
22	55.408	3.964	6	0.397832	0.67555
23	55.408	3.8114	6.5	0.36963	0.66906
24	55.408	3.722	6.8	0.353735	0.66518
25	55.408	3.716	6.8202	0.352689	0.66491
26	55.408	3.716	6.8202	0.352689	0.66491

J. Y.

02/12/01



very close to published result. see page 56.

* would be for run 5.

176 J. Phys. Chem. A, Vol. 102, No. 1, 1998 Ge et al.

Information potentially subject to copyright protection was redacted from this location. The redacted material was a n article published in the journal mentioned above.

published Results.

J.Y. 02/12/01

02/14/01

Comparision of OLI Results with Published Results

This work is postponed until a full release of OLI StreamAnalyzer is received.

J.Y. 04/11/01

J.Y. 04/11/01

Calculation of the Chemistry Lead containing salts using OLI ESP 6.2e
April 11, 2001

The objective is to know the speciations of of lead in NaCl, LiCl solutions at 80, ~~1000~~ 100, and 120 °C. The background is given in the e-mail attached:

— J. Yang 04/10/01

J. Yang 03/31/06

-----Original Message-----
From: Gustavo Cragnolino [mailto:gcragnolino@gargol.cnwra.swri.edu]
Sent: Monday, April 09, 2001 8:42 AM
To: nsridhar@gargol.cnwra.swri.edu; ddunn@gargol.cnwra.swri.edu; 'Vijay Jain (vjain)'; 'Gustavo Cragnolino'; 'Yi-ming Pan (ypan)'; 'Sean Brossia (sbrossia)'; 'Lietai Yang'
Subject: RE: Augmented work

I agree with Sridhar. Let's do NaCl with the test matrix Darrell suggested and later decide depending upon the results. Rather than go the LiCl route I prefer to evaluate the overall set of anions and evaluate other potential detrimental cations within ranges of concentrations that are achievable.

-----Original Message-----
From: Narasi Sridhar [mailto:nsridhar@gargol.cnwra.swri.edu]
Sent: Friday, April 06, 2001 4:58 PM
To: ddunn@gargol.cnwra.swri.edu; 'Vijay Jain (vjain)'; 'Gustavo Cragnolino'; 'Yi-ming Pan (ypan)'; 'Sean Brossia (sbrossia)'; 'Lietai Yang'
Subject: RE: Augmented work

I don't think we should go the route of Catholic in terms of using HCl. I think this is unrealistic and we would be subject to the same criticsms that they have been. I would lean towards using NaCl solutions with lead chloride. But maybe Lietai can do different simulations and find

J. Yang 7/16/02

out what is best.

-----Original Message-----
From: Darrell Dunn [mailto:ddunn@gargol.cnwra.swri.edu]
Sent: Friday, April 06, 2001 4:48 PM
To: Vijay Jain (vjain); Gustavo Cragnolino; Yi-ming Pan (ypan); Narasi Sridhar (nsridhar); Sean Brossia (sbrossia); Lietai Yang
Subject: Augmented work

Augmented work: the effect of trace elements

As we have discussed it is desirable to break this into two sections Localized corrosion and Stress corrosion cracking. If this division is used then the localized corrosion should be completed first and the results used as input for SCC tests.

Previously we have used NaCl solutions MgCl2 solutions and LiCl solutions for testing of Alloy 22. The Catholic University tests were performed in HCl solutions where lead was added as lead acetate.

I suggest the following solutions be evaluated using the OLI software. What is needed is a determination of the free chloride concentration, the concentration of dissolved lead as well as an assessment of the type and concentration of lead complexes. Also if you feel that the suggested solution are not appropriate then please provide your input. Statistical design should be considered if we do not have to wait 2 months for an answer.

NaCl Solutions - Tested to compare the results obtained in such solutions without lead.

Cl concentrations: 0.5, 1.0, 4.0 molar

Temperatures: 80 and 100 C

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lead concentration: 1, 100, 1600 (or maximum) ppm as lead chloride, lead acetate or possibly another soluble lead salt but not lead nitrate

The strategy would be to look at the most aggressive conditions first. If there is no effect in the Cl solutions at 100 C with 1600 ppm lead then there is probably not a need to look at lower lead concentrations.

Number of tests 3 for initial screening, 18 for total matrix.

LiCl solution - used to look at high Cl concentrations

Cl concentrations: 6 and 9 molal

Temperatures: 80, 100 and 120 C (6 molal LiCl boiling point?)

lead concentration: 1, 100, 1600 (or maximum) ppm

HCl solutions - used for direct comparison to Catholic University tests

Cl concentrations: 1 and 5 molar

Temperatures: 80 and 100 and

lead concentration: 1, 100, 1600 (or maximum) ppm.

For the initial calculations it is desirable to know how much lead we can have dissolved as Pb2+ in the chloride solutions considering the limited solubility of lead chloride and the possible formation of lead chloride complexes.

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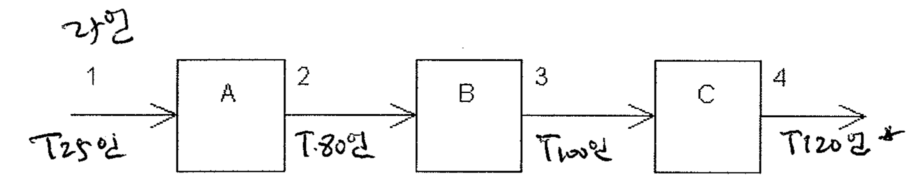
[Streams | Output Device | Exit]

Using OLI 6.2e.

3 conventional mixers. to get 3 temperature at one shot.



T25인, T80인, T100인 T120인 are the stream names.

Use isotherm calculation.

Process Name: Darrell.

Chemistry Name: Darrell1: { H2O, NaCl, PbCl2, PbAcet2, PbSO4, LiCl, HCl }

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~~Results: File Name: Darrell-Pb-Chem.xls~~ in c:\work\CSLT\ directory.

Results from ESP V6.2e, April 10, 2001

Pb MW=	207.2	mg (ppm)	1	100	1600
		mM	0.0048263	0.482625	7.722008

(1)

Inputs	Case 1, 0.5 M NaCl, No solid above 80 oC				
H2O (mol)	55.5				
NaCl (mol)	0.5				
LiCl (mol)	0				
HCl (mol)	0				
PbCl2 (mol)	4.00E-03				
Pb(CH3CO2)2 (mol)	0.004				
PbSO4 (mol)	0.001				
Total Pb (ppm)	**1808.6943**				
Stream	T25oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Solid	Aqueous	Aqueous	Aqueous
Temperature, C	25	25	80	100	120
Pressure, atm	1	1	1	1	2
pH	6.78395		6.04375	5.89688	5.78944
Total mol/hr	56.5068	0.0027333	56.5096	56.5088	56.508
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.4997		55.4994	55.4993	55.4992
ACETACID	4.03E-05		2.53E-04	3.79E-04	5.26E-04
ACET2	2.78E-17		5.06E-15	1.67E-14	4.41E-14
H2SO4	8.78E-27		1.15E-24	3.85E-24	1.10E-23
HCL	2.99E-14		3.81E-12	1.34E-11	3.76E-11
SO3	1.16E-30		4.16E-28	2.33E-27	1.17E-26
LIOH					
NAACET	0.001077		0.0012685	0.001437	0.001634
PBACET2	7.99E-06		2.39E-05	3.30E-05	4.44E-05
PBCL2	0.0018636	0.0025077	0.003267	0.003451	0.003593
PBO	6.05E-08		5.32E-07	9.25E-07	1.49E-06
LIACET					
OHION	8.44E-08		4.12E-07	6.82E-07	1.08E-06
CLION	0.493561		0.49393	0.493463	0.492971
HION	2.15E-07		1.25E-06	1.80E-06	2.37E-06
HPBO2ION	6.50E-12		1.10E-10	2.40E-10	4.73E-10
HSO4ION	2.21E-09		6.84E-08	1.69E-07	3.78E-07
LIION					
LISO4ION					
NAION	0.498868		0.498656	0.498495	0.498307
NASO4ION	5.25E-05		7.25E-05	6.59E-05	5.63E-05
ACETATEION	0.0065306		0.0060438	0.005752	0.0054
PBACET3ION	4.98E-06		1.07E-05	1.61E-05	2.46E-05
PBACETION	3.21E-04		3.54E-04	3.18E-04	2.78E-04
PBCL3ION	4.94E-04		8.37E-04	9.23E-04	0.001023
PBCL4ION	4.42E-04		4.50E-04	4.73E-04	5.24E-04
PBCLION	0.0024445		0.0032239	0.002971	0.002673
PBION	6.48E-04		5.80E-04	4.35E-04	3.13E-04
PBOHION	4.03E-05		2.53E-04	3.78E-04	5.24E-04
SO4ION	7.22E-04		9.27E-04	9.34E-04	9.43E-04
PBSO4		2.26E-04			
NACL					
LICL					
LI2SO4.1H2O					
LI2SO4					
LIACET.2H2O					
LICL.1H2O					
LICL.2H2O					
LIOH.1H2O					
NA2SO4.10H2O					
NA2SO4					
NA3HSO42					
NAACET.3H2O					
NAHSO4					
NAOH.1H2O					
NAOH					
PBHSO42					
PBOH2					
Total g/hr	1031.02	0.76581	1031.78	1031.78	1031.78
Volume, m3/hr	0.0010123	1.30E-07	0.0010391	0.001053	0.00107
Enthalpy, cal/hr	-3.84E+06	-265.003	-3.79E+06	-3.77E+06	########
Density, g/m3	1.02E+06	5.89E+06	9.93E+05	9.80E+05	9.64E+05
Vapor fraction					
Solid fraction		1			
Organic fraction					
Osmotic Pres, atm	22.8623		26.0598	26.9772	27.7647
Redox Pot, volts					
E-Con, 1/ohm-cm	0.0462659		0.0998507	0.11922	0.138152
E-Con, cm2/ohm-mol	92.0167		204.141	247.075	290.735
Abs Visc, cP	0.933946		0.377935	0.301039	0.248232
Rel Visc	1.04853		1.06707	1.06912	1.07
Ionic Strength	0.504865		0.50569	0.504961	0.504279

Inputs	Case 2, 1 M NaCl, No solid above 80 oC				
H2O (mol)	55.5				
NaCl (mol)	1				
LiCl (mol)	0				
HCl (mol)	0				
PbCl2 (mol)	4.00E-03				
Pb(CH3CO2)2 (mol)	0.004				
PbSO4 (mol)	0.001				
Total Pb (ppm)	**1774.34395**				
Stream	T25oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Solid	Aqueous	Aqueous	Aqueous
Temperature, C	25	25	80	100	120
Pressure, atm	1	1	1	1	2
pH	7.02567		6.28311	6.14	6.03875
Total mol/hr	56.9907	0.002272	56.9927	56.9922	56.9913
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.0086		55.0085	55.0085	55.0084
ACETACID	1.89E-05		1.20E-04	1.76E-04	2.40E-04
ACET2	6.78E-18		1.25E-15	4.01E-15	1.02E-14
H2SO4	1.99E-27		1.88E-25	6.00E-25	1.61E-24
HCL	3.00E-14		3.79E-12	1.32E-11	3.63E-11
SO3			6.93E-29	3.69E-28	1.74E-27
LIOH					
NAACET	0.00170985		0.001997	0.002241	0.002526
PBACET2	1.58E-06		4.76E-06	6.32E-06	8.09E-06
PBCL2	0.00167755	0.002272	0.002876	0.002931	0.002909
PBO	4.33E-08		3.78E-07	6.50E-07	1.04E-06
LIACET					
OHION	1.42E-07		7.20E-07	1.22E-06	1.99E-06
CLION	0.977239		0.977376	0.977084	0.976599
HION	1.15E-07		6.86E-07	9.83E-07	1.28E-06
HPBO2ION	9.05E-12		1.53E-10	3.34E-10	6.64E-10
HSO4ION	9.91E-10		2.23E-08	5.30E-08	1.13E-07
LIION					
LISO4ION					
NAION	0.989354		0.989069	0.988835	0.988562
NASO4ION	8.25E-05		8.07E-05	7.07E-05	5.81E-05
ACETATEION	0.00610914		0.0057	0.005406	0.005061
PBACET3ION	1.09E-06		2.39E-06	3.44E-06	5.05E-06
PBACETION	8.49E-05		9.52E-05	8.31E-05	7.01E-05
PBCL3ION	9.77E-04		0.001619	0.001724	0.001824
PBCL4ION	0.00243066		0.002349	0.002359	0.002468
PBCLION	0.00128365		0.001696	0.00152	0.001316
PBION	1.73E-04		1.59E-04	1.17E-04	8.21E-05
PBOHION	1.88E-05		1.19E-04	1.75E-04	2.38E-04
SO4ION	9.09E-04		9.10E-04	9.20E-04	9.33E-04
PBSO4					
NACL					
LICL					
LI2SO4.1H2O					
LI2SO4					
LIACET.2H2O					
LICL.1H2O					
LICL.2H2O					
LIOH.1H2O					
NA2SO4.10H2O					
NA2SO4					
NA3HSO42					
NAACET.3H2O					
NAHSO4					
NAOH.1H2O					
NAOH					
PBHSO42					
PBOH2					
Total g/hr	1050.98	0.631813	1051.62	1051.62	1051.62
Volume, m3/hr	0.0010129	1.08E-07	0.001041	0.001055	0.001071
Enthalpy, cal/hr	-3.86E+06	-195.149	-3.80E+06	-3.78E+06	-3.76E+06
Density, g/m3	1.04E+06	5.85E+06	1.01E+06	9.97E+05	9.82E+05
Vapor fraction					
Solid fraction		1			
Organic fraction					
Osmotic Pres, atm	46.6328		52.9188	54.8012	56.4493
Redox Pot, volts					
E-Con, 1/ohm-cm	0.0836697		0.179759	0.215077	0.249256
E-Con, cm2/ohm-mol	84.7429		187.297	227.053	267.06
Abs Visc, cP	0.97815		0.4002	0.319175	0.263346
Rel Visc	1.09816		1.12993	1.13352	1.13515
Ionic Strength	1.00364		1.00376	1.00329	1.00287

Inputs	Case 3, 4 M NaCl, No solid above25 oC			
H2O (mol)	55.5			
NaCl (mol)	4			
LiCl (mol)	0			
HCl (mol)	0			
PbCl2 (mol)	4.00E-03			
Pb(CH3CO2)2 (mol)	0.004			
PbSO4 (mol)	0.001			
Total Pb (ppm)	**1602.585**			
Stream	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80	100	120
Pressure, atm	1	1	1	2
pH	7.95701	7.18945	7.0032	6.85401
Total mol/hr	59.7523	59.7523	59.7521	59.7519
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr
H2O	52.2355	52.2355	52.2355	52.2355
ACETACID	9.34E-07	6.09E-06	9.60E-06	1.41E-05
ACET2	3.13E-20	6.11E-18	2.24E-17	6.63E-17
H2SO4	3.42E-30	2.74E-28	9.47E-28	2.77E-27
HCL	9.15E-15	1.18E-12	4.50E-12	1.38E-11
SO3				3.39E-30
LIOH				
NAACET	0.0035208	0.003855	0.004154	0.004485
PBACET2	1.28E-09	4.68E-09	6.30E-09	7.82E-09
PBCL2	5.19E-05	1.07E-04	1.16E-04	1.18E-04
PBO	3.57E-09	3.57E-08	5.45E-08	7.26E-08
LIACET				
OHION	6.67E-07	3.94E-06	6.48E-06	1.01E-05
CLION	3.73873	3.73909	3.73916	3.73921
HION	6.00E-09	4.47E-08	7.44E-08	1.14E-07
HPBO2ION	8.23E-12	1.57E-10	2.77E-10	4.15E-10
HSO4ION	2.13E-11	3.98E-10	9.35E-10	1.97E-09
LIION				
LISO4ION				
NAION	3.76111	3.7608	3.76052	3.7602
NASO4ION	8.87E-05	6.33E-05	4.85E-05	3.43E-05
ACETATEION	0.0040076	0.003668	0.003366	0.00303
PBACET3ION	1.53E-09	4.03E-09	5.77E-09	8.02E-09
PBACETION	1.89E-07	2.70E-07	2.49E-07	2.14E-07
PBCL3ION	2.18E-04	4.33E-04	4.90E-04	5.33E-04
PBCL4ION	0.0081882	0.007908	0.007841	0.007798
PBCLION	1.19E-05	2.01E-05	1.95E-05	1.76E-05
PBION	1.66E-07	2.04E-07	1.62E-07	1.18E-07
PBOHION	2.66E-07	2.12E-06	3.09E-06	3.94E-06
SO4ION	8.52E-04	8.78E-04	8.93E-04	9.07E-04
PBSO4				
NACL				
LICL				
LI2SO4.1H2O				
LI2SO4				
LIACET.2H2O				
LICL.1H2O				
LICL.2H2O				
LIOH.1H2O				
NA2SO4.10H2O				
NA2SO4				
NA3HSO42				
NAACET.3H2O				
NAHSO4				
NAOH.1H2O				
NAOH				
PBHSO42				
PBOH2				
Total g/hr	1163.62	1163.62	1163.62	1163.62
Volume, m3/hr	0.0010204	0.001059	0.001071	0.001083
Enthalpy, cal/hr	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06
Density, g/m3	1.14E+06	1.10E+06	1.09E+06	1.07E+06
Vapor fraction				
Solid fraction				
Organic fraction				
Osmotic Pres, atm	231.494	258.729	268.568	278.325
Redox Pot, volts				
E-Con, 1/ohm-cm	0.218002	0.474041	0.574753	0.677594
E-Con, cm2/ohm-mol	58.9564	133.018	163.196	194.602
Abs Visc, cP	1.37419	0.569755	0.458327	0.38248
Rel Visc	1.54279	1.60865	1.62771	1.64867
Ionic Strength	4.00641	4.00582	4.00547	4.0051

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(2)

	Case 4, 9M NaCl, No solid above 25 oC for Pb, but for NaCl							
H2O (mol)	55.5							
NaCl (mol)	9							
LiCl (mol)	0							
HCl (mol)	0							
PbCl2 (mol)	4.00E-03							
Pb(CH3CO2)2 (mol)	0.004							
PbSO4 (mol)	0.001							
Total Pb (ppm)	**1575.6654**							
Stream	T25oC	T25oC	T80oC	T80oC	T100oC	T100oC	T120oC	T120oC
Phase	Aqueous	Solid	Aqueous	Solid	Aqueous	Solid	Aqueous	Solid
Temperature, C	25	25	80	80	100	100	120	120
Pressure, atm	1	1	1	1	1	1	2	2
pH	8.03016		7.25043		7.041		6.86298	
Total mol/hr	58.8869	2.4577	59.5056	2.14827	59.8216	1.99015	60.1793	1.81114
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	48.1868		48.1868		48.1868		48.1868	
ACETACID	4.63E-07		2.85E-06		4.52E-06		6.70E-06	
ACET2	1.27E-20		2.38E-18		9.10E-18		2.86E-17	
H2SO4			5.02E-29		1.61E-28		4.28E-28	
HCL	8.97E-15		1.19E-12		4.78E-12		1.56E-11	
SO3								
LIOH								
NAACET	0.00394584		0.004251		0.004522		0.004813	
PBACET2	4.10E-11		1.13E-10		1.29E-10		1.32E-10	
PBCL2	6.51E-06		1.19E-05		1.20E-05		1.14E-05	
PBO	1.52E-10		1.10E-09		1.29E-09		1.28E-09	
LIACET								
OHION	4.53E-07		2.80E-06		4.47E-06		6.67E-06	
CLION	5.33215		5.64166		5.79979		5.97881	
HION	2.52E-09		2.13E-08		3.89E-08		6.63E-08	
HPBO2ION	4.52E-13		6.30E-12		8.32E-12		8.81E-12	
HSO4ION	7.53E-12		1.10E-10		2.32E-10		4.27E-10	
LIION								
LISO4ION								
NAION	5.35235		5.66151		5.81937		5.9981	
NASO4ION	8.07E-05		4.65E-05		3.15E-05		1.90E-05	
ACETATEION	0.00299953		0.002692		0.002419		0.002126	
PBACET3ION	7.63E-11		1.63E-10		2.03E-10		2.40E-10	
PBACETION	1.00E-08		1.19E-08		9.85E-09		7.46E-09	
PBCL3ION	6.44E-05		1.28E-04		1.45E-04		1.57E-04	
PBCL4ION	0.0077422		0.007672		0.007656		0.007645	
PBCLION	9.53E-07		1.42E-06		1.28E-06		1.05E-06	
PBION	3.50E-09		3.13E-09		2.07E-09		1.22E-09	
PBOHION	1.17E-08		7.37E-08		8.98E-08		9.34E-08	
SO4ION	7.88E-04		8.22E-04		8.37E-04		8.49E-04	
PBSO4								
NACL		2.4577		2.14827		1.99015		1.81114
LICL								
LI2SO4.1H2O								
LI2SO4								
LIACET.2H2O								
LICL.1H2O								
LICL.2H2O								
LIOH.1H2O								
NA2SO4.10H2O								
NA2SO4								
NA3HSO42								
NAACET.3H2O								
NAHSO4								
NAOH.1H2O								
NAOH								
PBHSO42								
PBOH2								
Total g/hr	1183.5	143.635	1201.59	125.551	1210.83	116.311	1221.29	105.848
Volume, m3/hr	9.83E-04	6.64E-05	0.001036	5.80E-05	0.001052	5.38E-05	0.001066	4.89E-05
Enthalpy, cal/hr	-3.81E+06	-2.42E+05	-3.80E+06	-2.10E+05	-3.80E+06	-1.94E+05	-3.80E+06	-1.76E+05
Density, g/m3	1.20E+06	2.16E+06	1.16E+06	2.16E+06	1.15E+06	2.16E+06	1.15E+06	2.16E+06
Vapor fraction								
Solid fraction		1		1		1		1
Organic fraction								
Osmotic Pres, atm	409.048		485.639		522.087		563.583	
Redox Pot, volts								
E-Con, 1/ohm-cm	0.254902		0.571254		0.707486		0.856789	
E-Con, cm2/ohm-mol	32.0321		75.6519		95.1479		116.807	
Abs Visc, cP	1.79839		0.775384		0.648454		0.570609	
Rel Visc	2.01903		2.18923		2.30293		2.45959	
Ionic Strength	6.17546		6.53155		6.71339		6.91929	

	Case 5, 6 M LiCl, No solid above25 oC			
H2O (mol)	55.5	Boiling at		
NaCl (mol)	0	110.47 oC		
LiCl (mol)	6			
HCl (mol)	0			
PbCl2 (mol)	4.00E-03			
Pb(CH3CO2)2 (mol)	0.004			
PbSO4 (mol)	0.001			
Total Pb (ppm)	**1629.31509**			
Stream	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80	100	120
Pressure, atm	1	1	1	2
pH	7.09538	6.44181	6.25503	6.09412
Total mol/hr	61.4485	61.4488	61.4487	61.4486
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr
H2O	50.537	50.537	50.537	50.537
ACETACID	8.27E-07	6.00E-06	1.02E-05	1.65E-05
ACET2	5.53E-20	1.34E-17	5.73E-17	2.05E-16
H2SO4	1.40E-28	9.46E-27	3.66E-26	1.26E-25
HCL	1.61E-13	1.36E-11	4.90E-11	1.45E-10
SO3		4.85E-30	3.09E-29	1.87E-28
LIOH	6.66E-07	5.14E-06	9.04E-06	1.50E-05
NAACET				
PBACET2	4.07E-14	4.31E-13	7.31E-13	1.09E-12
PBCL2	6.51E-07	1.34E-06	1.39E-06	1.33E-06
PBO	2.29E-14	5.47E-13	9.02E-13	1.20E-12
LIACET	0.00585005	0.005469	0.005515	0.005613
OHION	1.85E-07	1.03E-06	1.50E-06	2.02E-06
CLION	5.43803	5.43807	5.43808	5.43807
HION	2.38E-08	1.60E-07	2.81E-07	4.64E-07
HPBO2ION	2.37E-17	1.41E-15	2.74E-15	4.08E-15
HSO4ION	2.14E-10	4.48E-09	1.18E-08	2.87E-08
LIION	5.45705	5.45734	5.45725	5.45711
LISO4ION	5.65E-04	6.46E-04	6.86E-04	7.25E-04
NAION				
NASO4ION				
ACETATEION	0.00143374	0.001809	0.001759	0.001655
PBACET3ION	3.05E-14	3.39E-13	6.62E-13	1.18E-12
PBACETION	5.01E-11	1.44E-10	1.56E-10	1.50E-10
PBCL3ION	6.05E-05	1.02E-04	1.05E-04	1.02E-04
PBCL4ION	0.00813398	0.008092	0.008089	0.008092
PBCLION	4.87E-08	9.94E-08	9.84E-08	8.82E-08
PBION	6.66E-11	1.15E-10	9.84E-11	7.44E-11
PBOHION	2.21E-11	3.31E-10	5.23E-10	6.91E-10
SO4ION	3.46E-04	2.65E-04	2.24E-04	1.86E-04
PBSO4				
NACL				
LICL				
LI2SO4.1H2O				
LI2SO4				
LIACET.2H2O				
LICL.1H2O				
LICL.2H2O				
LIOH.1H2O				
NA2SO4.10H2O				
NA2SO4				
NA3HSO42				
NAACET.3H2O				
NAHSO4				
NAOH.1H2O				
NAOH				
PBHSO42				
PBOH2				
Total g/hr	1144.53	1144.53	1144.53	1144.53
Volume, m3/hr	0.00101885	0.001045	0.001053	0.001053
Enthalpy, cal/hr	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06
Density, g/m3	1.12E+06	1.10E+06	1.09E+06	1.09E+06
Vapor fraction				
Solid fraction				
Organic fraction				
Osmotic Pres, atm	564.387	614.008	630.547	650.486
Redox Pot, volts				
E-Con, 1/ohm-cm	0.181633	0.40845	0.501116	0.600299
E-Con, cm2/ohm-mol	33.8208	78.0279	96.4221	115.491
Abs Visc, cP	1.94168	0.719375	0.516263	0.329371
Rel Visc	2.1799	2.03109	1.83347	1.41974
Ionic Strength	6.00321	6.0034	6.00325	6.00306

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(3)

	Case 6, 9 M LiCl, No solid above25 oC					Case 7, 4 M NaCl, Pb Acetate only				Case 8, 4 M NaCl, Pb Acetate only			
H2O (mol)	55.5	Boiling at				55.5				55.5			
NaCl (mol)	0	118.8 oC				4				4			
LiCl (mol)	9					0				0			
HCl (mol)	0					0				0			
PbCl2 (mol)	4.00E-03					0.00E+00				0.00E+00			
Pb(CH3CO2)2 (m	0.004					0.000004826				0.0004826			
PbSO4 (mol)	0.001					0				0			
Total Pb (ppm)	**1551.76288**					**0.861102959**				**86.100657**			
Stream	T25oC	T80oC	T100oC		T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous		Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80		100	120	25	80	100	120	25	80	100	120
Pressure, atm	1	1		1	2	1	1	1	2	1	1	1	2
pH	6.84331	6.22504		6.04877	5.89815	6.96995	6.24848	6.06334	5.90814	7.57726	6.83093	6.63678	6.47545
Total mol/hr	63.7995	63.7999		63.7999	63.7998	59.774	59.774	59.774	59.774	59.7727	59.7726	59.7726	59.7726
Flow Units	mol/hr	mol/hr	mol/hr		mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	48.1868	48.1868		48.1868	48.1868	52.2434	52.2434	52.2434	52.2434	52.243	52.243	52.243	52.243
ACETACID	4.55E-07	3.39E-06		5.80E-06	9.35E-06	1.09E-08	6.35E-08	9.95E-08	1.47E-07	2.69E-07	1.67E-06	2.68E-06	4.04E-06
ACET2	3.81E-20	9.70E-18		4.19E-17	1.50E-16	4.27E-24	6.67E-22	2.41E-21	7.29E-21	2.61E-21	4.61E-19	1.75E-18	5.47E-18
H2SO4	1.03E-28	5.94E-27		2.17E-26	7.15E-26								
HCL	4.24E-13	2.97E-11		1.00E-10	2.80E-10	8.92E-14	1.04E-11	3.94E-11	1.22E-10	2.20E-14	2.71E-12	1.05E-11	3.30E-11
SO3		4.09E-30		2.44E-29	1.39E-28								
LIOH	3.96E-07	3.07E-06		5.38E-06	8.89E-06								
NAACET						4.25E-06	4.63E-06	4.97E-06	5.34E-06	4.25E-04	4.65E-04	5.01E-04	5.40E-04
PBACET2	5.74E-17	1.14E-15		2.34E-15	4.17E-15	9.67E-19	3.49E-18	4.68E-18	5.75E-18	9.71E-13	3.54E-12	4.76E-12	5.90E-12
PBCL2	2.11E-08	5.29E-08		5.84E-08	5.90E-08	2.74E-08	5.64E-08	6.11E-08	6.23E-08	2.74E-06	5.64E-06	6.11E-06	6.23E-06
PBO	1.49E-17	6.47E-16		1.30E-15	2.10E-15	1.96E-14	2.44E-13	3.74E-13	4.84E-13	3.23E-11	3.57E-10	5.25E-10	6.61E-10
LIACET	0.00603542	0.005651		0.00564555	0.005684								
OHION	7.57E-08	4.59E-07		6.87E-07	9.50E-07	6.86E-08	4.50E-07	7.43E-07	1.14E-06	2.78E-07	1.72E-06	2.78E-06	4.22E-06
CLION	7.78978	7.78979		7.7898	7.7898	3.76527	3.76527	3.76527	3.76527	3.76346	3.76348	3.76348	3.76349
HION	1.74E-08	1.39E-07		2.63E-07	4.65E-07	5.77E-08	3.87E-07	6.43E-07	9.97E-07	1.43E-08	1.01E-07	1.72E-07	2.70E-07
HPBO2ION	1.42E-20	1.73E-18		4.23E-18	7.91E-18	4.67E-18	1.22E-16	2.18E-16	3.14E-16	3.11E-14	6.86E-13	1.15E-12	1.58E-12
HSO4ION	1.42E-10	2.85E-09		7.35E-09	1.76E-08								
LIION	7.80733	7.80767		7.80765	7.80759								
LISO4ION	7.08E-04	7.52E-04		7.73E-04	7.93E-04								
NAION						3.76529	3.76529	3.76529	3.76529	3.76483	3.7648	3.76476	3.76472
NASO4ION													
ACETATEION	9.10E-04	0.001292		0.0012945	0.001252	4.82E-06	4.39E-06	4.02E-06	3.60E-06	4.83E-04	4.42E-04	4.05E-04	3.64E-04
PBACET3ION	6.88E-17	1.60E-15		3.91E-15	8.61E-15	1.40E-21	3.62E-21	5.13E-21	7.03E-21	1.40E-13	3.68E-13	5.27E-13	7.30E-13
PBACETION	2.30E-13	1.12E-12		1.42E-12	1.61E-12	1.19E-13	1.69E-13	1.55E-13	1.33E-13	1.19E-09	1.70E-09	1.57E-09	1.34E-09
PBCL3ION	1.50E-05	2.78E-05		2.95E-05	2.93E-05	1.16E-07	2.31E-07	2.61E-07	2.84E-07	1.16E-05	2.31E-05	2.62E-05	2.84E-05
PBCL4ION	0.00779905	0.007786		0.00778457	0.007785	4.39E-06	4.24E-06	4.21E-06	4.19E-06	4.39E-04	4.24E-04	4.21E-04	4.19E-04
PBCLION	7.55E-10	2.16E-09		2.39E-09	2.38E-09	6.23E-09	1.06E-08	1.03E-08	9.26E-09	6.24E-07	1.06E-06	1.03E-06	9.27E-07
PBION	1.13E-13	3.08E-13		3.04E-13	2.63E-13	8.52E-11	1.05E-10	8.36E-11	6.07E-11	8.54E-09	1.05E-08	8.38E-09	6.08E-09
PBOHION	4.13E-14	1.07E-12		2.04E-12	3.21E-12	1.42E-11	1.26E-10	1.84E-10	2.32E-10	5.76E-09	4.83E-08	6.91E-08	8.58E-08
SO4ION	1.60E-04	1.16E-04		9.49E-05	7.57E-05								
PBSO4													
NACL													
LICL													
LI2SO4.1H2O													
LI2SO4													
LIACET.2H2O													
LICL.1H2O													
LICL.2H2O													
LIOH.1H2O													
NA2SO4.10H2O													
NA2SO4													
NA3HSO42													
NAACET.3H2O													
NAHSO4													
NAOH.1H2O													
NAOH													
PBHSO42													
PBOH2													
Total g/hr	1201.73	1201.73		1201.73	1201.73	1161.24	1161.24	1161.24	1161.24	1161.37	1161.37	1161.37	1161.37
Volume, m3/hr	0.00102514	0.001055		0.00106023	0.001052	0.00102008	0.001058	0.001071	0.001083	0.00102011	0.001058	0.001071	0.001083
Enthalpy, cal/hr	-4.12E+06	-4.07E+06		-4.05E+06	-4.03E+06	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06
Density, g/m3	1.17E+06	1.14E+06		1.13E+06	1.14E+06	1.14E+06	1.10E+06	1.08E+06	1.07E+06	1.14E+06	1.10E+06	1.08E+06	1.07E+06
Vapor fraction													
Solid fraction													
Organic fraction													
Osmotic Pres, atm	1076.9	1150.44		1177.03	1215.68	232.718	260.04	269.919	279.72	232.643	259.959	269.835	279.632
Redox Pot, volts													
E-Con, 1/ohm-cm	0.172903	0.40698		0.507759	0.618284	0.218926	0.476031	0.577191	0.680508	0.218849	0.475863	0.576985	0.680261
E-Con, cm2/ohm-r	22.6607	54.892		68.8328	83.2	59.3104	133.781	164.142	195.743	59.285	133.722	164.069	195.655
Abs Visc, cP	2.99834	1.03343		0.70352	0.383514	1.35275	0.562206	0.452812	0.378359	1.35511	0.563014	0.453393	0.378785
Rel Visc	3.3662	2.91781		2.49849	1.65313	1.51872	1.58734	1.60812	1.63091	1.52137	1.58962	1.61019	1.63274
Ionic Strength	9.00281	9.00313		9.00309	9.00299	4.00063	4.00063	4.00063	4.00063	4.00064	4.00058	4.00054	4.0005

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	Case 9, 4 M NaCl, Pb Acetate only				Case 10, 4 M NaCl, PbCl2 only				Case 11, 4 M NaCl, PbCl2 only			
H2O (mol)	55.5				55.5				55.5			
NaCl (mol)	4				4				4			
LiCl (mol)	0				0				0			
HCl (mol)	0				0				0			
PbCl2 (mol)	0.00E+00				4.83E-06				4.83E-04			
Pb(CH3CO2)2 (m	0.007722				0				0			
PbSO4 (mol)	0				0				0			
Total Pb (ppm)	**1375.21887**				**0.86110296**				**86.109554**			
Stream	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80	100	120	25	80	100	120	25	80	100	120
Pressure, atm	1	1	1	2	1	1	1	2	1	1	1	2
pH	8.10747	7.34166	7.15458	7.00416	6.93241	6.21549	6.0321	5.87818	6.93201	6.21494	6.03162	5.87779
Total mol/hr	59.7525	59.7521	59.7516	59.751	59.774	59.774	59.774	59.774	59.7739	59.7739	59.7739	59.7739
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	52.2366	52.2366	52.2366	52.2366	52.2434	52.2434	52.2434	52.2434	52.2434	52.2434	52.2434	52.2434
ACETACID	1.28E-06	8.28E-06	1.31E-05	1.93E-05								
ACET2	5.84E-20	1.13E-17	4.16E-17	1.24E-16								
H2SO4												
HCL	6.47E-15	8.33E-13	3.18E-12	9.74E-12	9.73E-14	1.12E-11	4.23E-11	1.31E-10	9.74E-14	1.12E-11	4.24E-11	1.31E-10
SO3												
LIOH												
NAACET	0.00679641	0.007444	0.00802	0.008662								
PBACET2	4.12E-09	1.50E-08	2.03E-08	2.51E-08								
PBCL2	4.47E-05	9.19E-05	9.96E-05	1.02E-04	2.74E-08	5.64E-08	6.11E-08	6.23E-08	2.74E-07	5.64E-07	6.11E-07	6.23E-07
PBO	6.15E-09	6.21E-08	9.44E-08	1.25E-07	1.65E-14	2.09E-13	3.23E-13	4.22E-13	1.65E-13	2.09E-12	3.23E-12	4.21E-12
LIACET												
OHION	9.44E-07	5.59E-06	9.18E-06	1.43E-05	6.29E-08	4.17E-07	6.91E-07	1.07E-06	6.29E-08	4.17E-07	6.91E-07	1.07E-06
CLION	3.73605	3.73636	3.73643	3.73647	3.76528	3.76528	3.76528	3.76528	3.7652	3.7652	3.7652	3.7652
HION	4.24E-09	3.15E-08	5.25E-08	8.05E-08	6.29E-08	4.18E-07	6.91E-07	1.07E-06	6.30E-08	4.18E-07	6.92E-07	1.07E-06
HPBO2ION	2.00E-11	3.86E-10	6.79E-10	1.01E-09	3.60E-18	9.74E-17	1.76E-16	2.55E-16	3.60E-17	9.71E-16	1.75E-15	2.55E-15
HSO4ION												
LIION												
LISO4ION												
NAION	3.75801	3.75736	3.75678	3.75614	3.76529	3.76529	3.76529	3.76529	3.76529	3.76529	3.76529	3.76529
NASO4ION												
ACETATEION	0.0077341	0.00708	0.006498	0.00585								
PBACET3ION	9.49E-09	2.50E-08	3.58E-08	4.97E-08								
PBACETION	3.14E-07	4.48E-07	4.14E-07	3.55E-07								
PBCL3ION	1.87E-04	3.72E-04	4.21E-04	4.58E-04	1.16E-07	2.31E-07	2.61E-07	2.84E-07	1.16E-06	2.31E-06	2.61E-06	2.84E-06
PBCL4ION	0.00702297	0.006781	0.006724	0.006686	4.39E-06	4.24E-06	4.21E-06	4.19E-06	4.39E-05	4.24E-05	4.21E-05	4.19E-05
PBCLION	1.02E-05	1.73E-05	1.68E-05	1.51E-05	6.23E-09	1.06E-08	1.03E-08	9.26E-09	6.23E-08	1.06E-07	1.03E-07	9.26E-08
PBION	1.43E-07	1.75E-07	1.39E-07	1.01E-07	8.52E-11	1.05E-10	8.36E-11	6.07E-11	8.52E-10	1.05E-09	8.36E-10	6.07E-10
PBOHION	3.24E-07	2.59E-06	3.77E-06	4.80E-06	1.30E-11	1.17E-10	1.71E-10	2.16E-10	1.30E-10	1.17E-09	1.71E-09	2.16E-09
SO4ION												
PBSO4												
NACL												
LICL												
LI2SO4.1H2O												
LI2SO4												
LIACET.2H2O												
LICL.1H2O												
LICL.2H2O												
LIOH.1H2O												
NA2SO4.10H2O												
NA2SO4												
NA3HSO42												
NAACET.3H2O												
NAHSO4												
NAOH.1H2O												
NAOH												
PBHSO42												
PBOH2												
Total g/hr	1163.45	1163.45	1163.45	1163.45	1161.24	1161.24	1161.24	1161.24	1161.25	1161.25	1161.25	1161.25
Volume, m3/hr	0.0010206	0.001059	0.001071	0.001084	0.00102008	0.001058	0.001071	0.001083	0.0010201	0.001058	0.001071	0.001083
Enthalpy, cal/hr	-3.94E+06	-3.89E+06	-3.87E+06	-3.85E+06	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06
Density, g/m3	1.14E+06	1.10E+06	1.09E+06	1.07E+06	1.14E+06	1.10E+06	1.08E+06	1.07E+06	1.14E+06	1.10E+06	1.08E+06	1.07E+06
Vapor fraction												
Solid fraction												
Organic fraction												
Osmotic Pres, atm	231.503	258.736	268.563	278.304	232.719	260.041	269.92	279.72	232.714	260.036	269.915	279.716
Redox Pot, volts												
E-Con, 1/ohm-cm	0.217848	0.473557	0.574194	0.676964	0.218926	0.476032	0.577192	0.680509	0.218922	0.476024	0.577182	0.680497
E-Con, cm2/ohm-r	58.9424	132.908	163.069	194.459	59.3105	133.781	164.142	195.743	59.309	133.777	164.137	195.738
Abs Visc, cP	1.3911	0.575331	0.462264	0.385288	1.35273	0.562198	0.452806	0.378355	1.35274	0.562204	0.452811	0.378359
Rel Visc	1.56177	1.6244	1.64169	1.66077	1.51869	1.58732	1.6081	1.63089	1.5187	1.58733	1.60812	1.63091
Ionic Strength	4.00088	3.99994	3.99927	3.99855	4.00063	4.00063	4.00063	4.00063	4.00067	4.00067	4.00067	4.00067

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	Case 12, 4 M NaCl, PbCl2 only				Case 13, 6 M LiCl, Pb Acetate only				Case 14, 6 M LiCl, Pb Acetate only			
H2O (mol)	55.5				55.5				55.5			
NaCl (mol)	4				6 [handwritten arrow]				6 [handwritten arrow]			
LiCl (mol)	0				0				0			
HCl (mol)	0				0				0			
PbCl2 (mol)	7.72E-03				0.00E+00				0.00E+00			
Pb(CH3CO2)2 (mo	0				0.000004826				0.0004826			
PbSO4 (mol)	0				0				0			
Total Pb (ppm)	**1375.6209**				**0.875434195**				**87.5334571**			
Stream	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80	100	120	25	80	100	120	25	80	100	120
Pressure, atm	1	1	1	2	1	1	1	2	1	1	1	2
pH	6.87026	6.13473	5.95933	5.81709	6.32527	5.65566	5.47513	5.31952	6.67407	6.01768	5.83175	5.67144
Total mol/hr	59.7592	59.7595	59.7596	59.7596	61.4729	61.4729	61.4729	61.4729	61.4713	61.4714	61.4713	61.4713
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	52.2366	52.2366	52.2366	52.2366	50.5444	50.5444	50.5444	50.5444	50.544	50.544	50.544	50.544
ACETACID					5.83E-09	4.38E-08	7.34E-08	1.16E-07	2.61E-07	1.91E-06	3.25E-06	5.21E-06
ACET2					2.75E-24	7.12E-22	2.95E-21	1.02E-20	5.53E-21	1.35E-18	5.78E-18	2.05E-17
H2SO4												
HCL	1.12E-13	1.35E-11	4.99E-11	1.50E-10	9.52E-13	8.37E-11	2.96E-10	8.65E-10	4.26E-13	3.63E-11	1.30E-10	3.85E-10
SO3												
LIOH					1.14E-07	8.44E-07	1.51E-06	2.52E-06	2.54E-07	1.94E-06	3.42E-06	5.67E-06
NAACET												
PBACET2					3.04E-23	3.21E-22	5.42E-22	7.99E-22	3.05E-17	3.24E-16	5.48E-16	8.13E-16
PBCL2	4.42E-05	9.09E-05	9.85E-05	1.00E-04	3.43E-10	7.09E-10	7.35E-10	6.99E-10	3.43E-08	7.10E-08	7.36E-08	7.00E-08
PBO	2.02E-11	2.35E-10	3.76E-10	5.18E-10	3.42E-19	7.60E-18	1.29E-17	1.77E-17	1.71E-16	4.04E-15	6.69E-15	8.95E-15
LIACET					7.06E-06	6.58E-06	6.62E-06	6.71E-06	7.07E-04	6.60E-04	6.65E-04	6.76E-04
OHION	5.46E-08	3.47E-07	5.85E-07	9.28E-07	3.14E-08	1.68E-07	2.48E-07	3.39E-07	7.01E-08	3.86E-07	5.64E-07	7.63E-07
CLION	3.75057	3.75087	3.75093	3.75097	5.46425	5.46425	5.46425	5.46425	5.46247	5.46247	5.46247	5.46247
HION	7.30E-08	5.05E-07	8.21E-07	1.24E-06	1.39E-07	9.68E-07	1.68E-06	2.75E-06	6.24E-08	4.21E-07	7.39E-07	1.22E-06
HPBO2ION	3.82E-15	9.07E-14	1.73E-13	2.72E-13	6.01E-23	3.22E-21	6.51E-21	1.01E-20	6.71E-20	3.93E-18	7.66E-18	1.15E-17
HSO4ION												
LIION					5.46426	5.46426	5.46425	5.46425	5.46351	5.46356	5.46355	5.46354 [handwritten check]
LISO4ION												
NAION	3.7648	3.7648	3.7648	3.7648								
NASO4ION												
ACETATEION					1.72E-06	2.16E-06	2.10E-06	1.97E-06	1.72E-04	2.17E-04	2.11E-04	1.98E-04
PBACET3ION					2.74E-26	3.03E-25	5.88E-25	1.04E-24	2.76E-18	3.07E-17	5.98E-17	1.06E-16
PBACETION					3.14E-17	9.02E-17	9.71E-17	9.33E-17	3.14E-13	9.07E-13	9.77E-13	9.42E-13
PBCL3ION	1.86E-04	3.70E-04	4.19E-04	4.56E-04	3.22E-08	5.44E-08	5.59E-08	5.41E-08	3.23E-06	5.44E-06	5.60E-06	5.41E-06
PBCL4ION	0.0070273	0.006789	0.006733	0.006696	4.36E-06	4.34E-06	4.34E-06	4.34E-06	4.36E-04	4.34E-04	4.34E-04	4.34E-04
PBCLION	1.01E-05	1.71E-05	1.65E-05	1.49E-05	2.56E-11	5.24E-11	5.18E-11	4.65E-11	2.56E-09	5.25E-09	5.19E-09	4.66E-09
PBION	1.40E-07	1.71E-07	1.37E-07	9.90E-08	3.42E-14	5.93E-14	5.08E-14	3.84E-14	3.43E-12	5.94E-12	5.09E-12	3.85E-12
PBOHION	1.84E-08	1.58E-07	2.36E-07	3.06E-07	1.95E-15	2.81E-14	4.51E-14	6.03E-14	4.36E-13	6.48E-12	1.03E-11	1.36E-11
SO4ION												
PBSO4												
NACL												
LICL												
LI2SO4.1H2O												
LI2SO4												
LIACET.2H2O												
LICL.1H2O												
LICL.2H2O												
LIOH.1H2O												
NA2SO4.10H2O												
NA2SO4												
NA3HSO42												
NAACET.3H2O												
NAHSO4												
NAOH.1H2O												
NAOH												
PBHSO42												
PBOH2												
Total g/hr	1163.11	1163.11	1163.11	1163.11	1142.23	1142.23	1142.23	1142.23	1142.36	1142.36	1142.36	1142.36
Volume, m3/hr	0.0010202	0.001058	0.001071	0.001083	0.00101844	0.001045	0.001052	0.001052	0.00101848	0.001045	0.001052	0.001052
Enthalpy, cal/hr	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06
Density, g/m3	1.14E+06	1.10E+06	1.09E+06	1.07E+06	1.12E+06	1.09E+06	1.09E+06	1.09E+06	1.12E+06	1.09E+06	1.09E+06	1.09E+06
Vapor fraction												
Solid fraction												
Organic fraction												
Osmotic Pres, atm	231.966	259.261	269.134	278.93	567.921	617.824	634.471	654.6	567.679	617.567	634.207	654.325
Redox Pot, volts												
E-Con, 1/ohm-cm	0.218487	0.475058	0.576001	0.679089	0.182314	0.410143	0.503262	0.602976	0.182293	0.410085	0.503187	0.60288
E-Con, cm2/ohm-m	59.0917	133.282	163.525	195.002	33.9801	78.4096	96.9063	116.08	33.9749	78.3957	96.8884	116.058
Abs Visc, cP	1.35464	0.563187	0.453629	0.379061	1.93856	0.718057	0.515182	0.328416	1.93876	0.718137	0.515252	0.328486
Rel Visc	1.52084	1.59011	1.61103	1.63393	2.1764	2.02737	1.82963	1.41563	2.17662	2.02759	1.82987	1.41593
Ionic Strength	4.0081	4.00786	4.0078	4.00776	6.00094	6.00094	6.00094	6.00094	6.00064	6.00069	6.00068	6.00067

wrong. should be LiCl. J.Y. 04/11/01

J. Young 08/19/02

	Case 15, 6 M LiCl, Pb Acetate only				Case 16, 6 M LiCl, PbCl2 only				Case 17, 6 M LiCl, PbCl2 only				Case 18, 6 M LiCl, PbCl2 only			
H2O (mol)	55.5				55.5				55.5				55.5			
NaCl (mol)	6 [handwritten arrow] J.Y.				6 [handwritten arrow] J.Y.				6 [handwritten arrow] J.Y.				6 [handwritten arrow] J.Y.			
LiCl (mol)	0				0				0				0			
HCl (mol)	0				0				0				0			
PbCl2 (mol)	0.00E+00				4.83E-06				4.83E-04				7.72E-03			
Pb(CH3CO2)2 (m	0.007722				0				0				0			
PbSO4 (mol)	0				0				0				0			
Total Pb (ppm)	**1398.1478**				**0.8754342**				**87.53499**				**1398.5511**			
Stream	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	80	100	120	25	80	100	120	25	80	100	120	25	80	100	120
Pressure, atm	1	1	1	2	1	1	1	2	1	1	1	2	1	1	1	2
pH	7.23557	6.58211	6.39518	6.23411	6.31636	5.64606	5.46585	5.31051	6.31646	5.64615	5.46593	5.31059	6.31788	5.64744	5.4672	5.31185
Total mol/hr	61.447	61.4478	61.4477	61.4475	61.4729	61.4729	61.4729	61.4729	61.472	61.472	61.472	61.472	61.4583	61.4583	61.4583	61.4583
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	50.5381	50.5381	50.5381	50.5381	50.5444	50.5444	50.5444	50.5444	50.544	50.544	50.544	50.544	50.5381	50.5381	50.5381	50.5381
ACETACID	1.16E-06	8.40E-06	1.43E-05	2.31E-05												
ACET2	1.08E-19	2.61E-17	1.12E-16	4.01E-16												
H2SO4																
HCL	1.17E-13	9.87E-12	3.55E-11	1.05E-10	9.72E-13	8.55E-11	3.02E-10	8.83E-10	9.71E-13	8.55E-11	3.02E-10	8.83E-10	9.67E-13	8.51E-11	3.01E-10	8.79E-10
SO3																
LIOH	9.20E-07	7.10E-06	1.25E-05	2.07E-05	1.11E-07	8.26E-07	1.47E-06	2.47E-06	1.11E-07	8.26E-07	1.47E-06	2.47E-06	1.11E-07	8.27E-07	1.48E-06	2.47E-06
NAACET																
PBACET2	1.31E-13	1.39E-12	2.36E-12	3.51E-12												
PBCL2	5.61E-07	1.16E-06	1.20E-06	1.14E-06	3.43E-10	7.09E-10	7.35E-10	6.99E-10	3.43E-08	7.09E-08	7.35E-08	6.99E-08	5.52E-07	1.14E-06	1.18E-06	1.13E-06
PBO	3.78E-14	9.03E-13	1.49E-12	1.98E-12	3.28E-19	7.27E-18	1.24E-17	1.69E-17	3.28E-17	7.28E-16	1.24E-15	1.70E-15	5.36E-16	1.19E-14	2.02E-14	2.77E-14
LIACET	0.0112932	0.010561	0.010651	0.010843												
OHION	2.56E-07	1.42E-06	2.07E-06	2.79E-06	3.07E-08	1.64E-07	2.43E-07	3.32E-07	3.08E-08	1.64E-07	2.43E-07	3.32E-07	3.09E-08	1.65E-07	2.44E-07	3.34E-07
CLION	5.4355	5.43554	5.43554	5.43554	5.46425	5.46425	5.46425	5.46425	5.46334	5.46335	5.46335	5.46335	5.44957	5.4496	5.44961	5.4496
HION	1.73E-08	1.16E-07	2.03E-07	3.36E-07	1.42E-07	9.90E-07	1.72E-06	2.80E-06	1.42E-07	9.90E-07	1.72E-06	2.80E-06	1.42E-07	9.91E-07	1.72E-06	2.81E-06
HPBO2ION	5.39E-17	3.22E-15	6.22E-15	9.27E-15	5.65E-23	3.01E-21	6.11E-21	9.47E-21	5.66E-21	3.02E-19	6.11E-19	9.48E-19	9.27E-20	4.93E-18	1.00E-17	1.55E-17
HSO4ION																
LIION	5.45228	5.45301	5.45291	5.45271	5.46426	5.46426	5.46426	5.46426	5.46422	5.46422	5.46422	5.46422	5.46358	5.46358	5.46358	5.46357
LISO4ION																
NAION																
NASO4ION																
ACETATEION	0.0027689	0.003494	0.003398	0.003198												
PBACET3ION	1.90E-13	2.11E-12	4.12E-12	7.35E-12												
PBACETION	8.36E-11	2.41E-10	2.60E-10	2.51E-10												
PBCL3ION	5.20E-05	8.77E-05	9.02E-05	8.73E-05	3.22E-08	5.44E-08	5.59E-08	5.41E-08	3.22E-06	5.44E-06	5.59E-06	5.41E-06	5.17E-05	8.72E-05	8.97E-05	8.68E-05
PBCL4ION	0.006979	0.006943	0.00694	0.006943	4.36E-06	4.34E-06	4.34E-06	4.34E-06	4.36E-04	4.34E-04	4.34E-04	4.34E-04	0.0069793	0.006943	0.006941	0.006944
PBCLION	4.20E-08	8.58E-08	8.49E-08	7.61E-08	2.56E-11	5.24E-11	5.18E-11	4.65E-11	2.56E-09	5.24E-09	5.19E-09	4.65E-09	4.12E-08	8.42E-08	8.34E-08	7.48E-08
PBION	5.75E-11	9.92E-11	8.49E-11	6.43E-11	3.42E-14	5.93E-14	5.08E-14	3.84E-14	3.43E-12	5.93E-12	5.08E-12	3.85E-12	5.58E-11	9.66E-11	8.27E-11	6.26E-11
PBOHION	2.64E-11	3.95E-10	6.24E-10	8.24E-10	1.91E-15	2.75E-14	4.42E-14	5.91E-14	1.91E-13	2.75E-12	4.42E-12	5.92E-12	3.11E-12	4.48E-11	7.20E-11	9.62E-11
SO4ION																
PBSO4																
NACL																
LICL																
LI2SO4.1H2O																
LI2SO4																
LIACET.2H2O																
LICL.1H2O																
LICL.2H2O																
LIOH.1H2O																
NA2SO4.10H2O																
NA2SO4																
NA3HSO42																
NAACET.3H2O																
NAHSO4																
NAOH.1H2O																
NAOH																
PBHSO42																
PBOH2																
Total g/hr	1144.37	1144.37	1144.37	1144.37	1142.23	1142.23	1142.23	1142.23	1142.34	1142.34	1142.34	1142.34	1144.04	1144.04	1144.04	1144.04
Volume, m3/hr	0.001019	0.001045	0.001053	0.001053	0.0010184	0.001045	0.001052	0.001052	0.0010185	0.001045	0.001052	0.001052	0.0010186	0.001045	0.001052	0.001052
Enthalpy, cal/hr	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06	-4.03E+06	-3.98E+06	-3.96E+06	-3.94E+06
Density, g/m3	1.12E+06	1.09E+06	1.09E+06	1.09E+06	1.12E+06	1.09E+06	1.09E+06	1.09E+06	1.12E+06	1.09E+06	1.09E+06	1.09E+06	1.12E+06	1.10E+06	1.09E+06	1.09E+06
Vapor fraction																
Solid fraction																
Organic fraction																
Osmotic Pres, atr	564.015	613.677	630.215	650.159	567.923	617.826	634.472	654.602	567.796	617.685	634.327	654.45	565.878	615.562	632.136	652.159
Redox Pot, volts																
E-Con, 1/ohm-cm	0.181704	0.408573	0.501255	0.600458	0.182314	0.410143	0.503262	0.602976	0.182298	0.410104	0.503213	0.602915	0.181787	0.408878	0.501673	0.601011
E-Con, cm2/ohm	33.8454	78.0637	96.4644	115.538	33.9801	78.4096	96.9063	116.08	33.975	78.3974	96.8909	116.062	33.8475	78.0911	96.5057	115.593
Abs Visc, cP	1.94179	0.719344	0.516304	0.329537	1.93856	0.718057	0.515182	0.328416	1.93869	0.718117	0.515226	0.328445	1.94071	0.719027	0.515899	0.328893
Rel Visc	2.18003	2.031	1.83361	1.42046	2.1764	2.02737	1.82962	1.41563	2.17655	2.02754	1.82978	1.41575	2.17881	2.03011	1.83217	1.41768
Ionic Strength	5.9962	5.99696	5.99685	5.99664	6.00094	6.00094	6.00094	6.00094	6.00142	6.00142	6.00142	6.00142	6.0086	6.00856	6.00856	6.00857

J.Y. 04/10/01

Continued on page 93.

J. Young 8/19/02

Page 1 through 68

are submitted for Printing (photo copying)

on

~~April 04/11/01~~ 04/11/01.

J. Yang

04/11/01

April. 19/01

Conductivity Calculation to know if

Conductivity method would allow the

~~Measurement of Deliquescence point~~

for mixtures of salt.

J. Yang

8/19/02

J. Y. 04/19/01

File Name: NaNO3_NaCl_Conductivity_Weight.xls, Directory: NoteBook#430
OLI 6.2d simulation, April 18, 2001
Dependence of electrical conductivity, weight loss on relative humidity at 25oC
Chemistry Model H2O +NaCl +NaNO3

RH *	0.6937	RH	**0.6989**	**0.7039**	**0.7181**	**0.7391**
E-Con, 1/ohm-cm	**0.2272**	Conductivity	**0.2271**	**0.2269**	**0.2263**	**0.2246**
H2O total (Mol/h)	**55.408008**		**56.408008**	**57.408008**	**60.408008**	**65.408008**
H2O total (g/h)	**997.34414**	H2O Weight	**1015.3441**	**1033.3441**	**1087.3441**	**1177.3441**
Total g/hr	**1751.4847**	Total Weight	**1769.5028**	**1787.5208**	**1841.5648**	**1931.6349**
Fraction (NaCl/NaNO3)	0.3061224		0.3061224	0.3061224	0.3061224	0.3061224

* Note: 0.6937 is from Notebook #430 page 55

	Case 1			Case 2			Case 3			Case 4			Case 5	
Stream	In	out	out	In	out	out	In	out	out	In	out	out	In	out
Phase	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous
Temperature, C	25	25	25	25	25	25	25	25	25	25	25	25	25	25
Pressure, atm	1	0.0217784	0.021778	1	0.0219417	0.021942	1	0.0220999	0.0221	1	0.0225457	0.022546	1	0.0232045
pH	7.00101	7.00123		7.00116	7.00138		7.0013	7.00152		7.00167	7.00188		7.00215	7.00237
Total mol/hr	65.208	65.1428	0.065208	66.208	66.1418	0.066208	67.208	67.1408	0.067208	70.208	70.1378	0.070208	75.208	75.1328
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.408	55.3428	0.065208	56.408	56.3418	0.066208	57.408	57.3408	0.067208	60.408	60.3378	0.070208	65.408	65.3328
H2			5.88E-28			5.95E-28			6.03E-28			6.26E-28		
HCL	8.70E-14	8.69E-14	8.25E-13	8.72E-14	8.71E-14	8.02E-13	8.73E-14	8.73E-14	7.81E-13	8.77E-14	8.77E-14	7.26E-13	8.83E-14	8.82E-14
HNO3	1.13E-09	1.13E-09	1.87E-12	1.18E-09	1.18E-09	1.86E-12	1.24E-09	1.23E-09	1.84E-12	1.40E-09	1.39E-09	1.80E-12	1.68E-09	1.67E-09
O2			2.94E-28			2.98E-28			3.01E-28			3.13E-28		
NANO3	6.8	6.8		6.8	6.8		6.8	6.8		6.8	6.8		6.8	6.8
NACL	3	3		3	3		3	3		3	3		3	3
NAOH.1H2O														
NAOH	1.13E-09	1.13E-09		1.18E-09	1.18E-09		1.24E-09	1.24E-09		1.40E-09	1.40E-09		1.68E-09	1.68E-09
Total g/hr	1751.49	1750.31	1.17474	1769.5	1768.31	1.19276	1787.52	1786.31	1.21077	1841.56	1840.3	1.26482	1931.64	1930.28
Volume, m3/hr	0.001292	0.0012907	0.073232	0.00131	0.0013084	0.073801	0.001327	0.0013261	0.07438	0.001381	0.0013793	0.076163	0.001469	0.0014681
Enthalpy, cal/hr	-4.80E+06	-4.80E+06	-3768.91	-4.87E+06	-4.87E+06	-3826.71	-4.94E+06	-4.93E+06	-3884.51	-5.14E+06	-5.14E+06	-4057.9	-5.49E+06	-5.48E+06
Density, g/m3	1.36E+06	1.36E+06	16.0414	1.35E+06	1.35E+06	16.1618	1.35E+06	1.35E+06	16.2783	1.33E+06	1.33E+06	16.6068	1.31E+06	1.31E+06
Vapor fraction			1			1			1			1		
Solid fraction														
Organic fraction														
Osmotic Pres, atm	517.429	518.126		506.664	507.343		496.316	496.979		467.556	468.175		426.116	426.671
Redox Pot, volts	0.403347	0.407497		0.403274	0.407424		0.403205	0.407355		0.403012	0.407162		0.402737	0.406887
E-Con, 1/ohm-cm	0.227158	0.227163		0.22705	0.227058		0.226902	0.226913		0.226249	0.226267		0.224582	0.22461
E-Con, cm2/ohm-mol	29.9436	29.9187		30.3398	30.3149		30.7307	30.7057		31.8715	31.8464		33.6739	33.6488
Abs Visc, cP	2.46794	2.47063		2.42583	2.42844		2.38565	2.38818		2.27266	2.27508		2.11083	2.11293
Rel Visc	2.77073	2.77375		2.72346	2.72638		2.67835	2.68118		2.55148	2.5542		2.3698	2.37216
Ionic Strength	9.72259	9.73405		9.55022	9.56144		9.38388	9.39487		8.918	8.92837		8.23676	8.24623

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		0.6883			**0.6828**			**0.6770**			**0.6759**			**0.6750**	
		0.2272			**0.2272**			**0.2272**			**0.2272**			**0.2272**	
		54.408008			**53.408008**			**52.408008**			**52.208008**			**52.057958**	
		979.34414			**961.34414**			**943.34414**			**939.74414**			**937.04324**	
		1733.4667			**1715.4587**			**1697.4407**			**1693.8371**			**1691.1344**	
		0.3061224			0.3061224			0.3061224			0.3061224			0.3061224	
	Case 6			Case 7			Case 8			Case 9			Case 10		
out	In	out	out	In	out	out	In	out	out	In	out	out	In	out	out
Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor
25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25
0.023205	1	0.0216096	0.02161	1	0.0214352	0.021435	1	0.0212549	0.021255	1	0.0212181	0.021218	1	0.0211903	0.02119
	7.00086	7.00108		7.0007	7.00092		7.00052	7.00075		7.00049	7.00071		7.00046	7.00069	
0.075208	64.208	64.1438	0.064208	63.208	63.1448	0.063208	62.208	62.1458	0.062208	62.008	61.946	0.062008	61.858	61.7961	0.061858
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
0.075208	54.408	54.3438	0.064208	53.408	53.3448	0.063208	52.408	52.3458	0.062208	52.208	52.146	0.062008	52.058	51.9961	0.061858
6.64E-28			5.80E-28			5.73E-28			5.65E-28			5.64E-28			5.63E-28
6.51E-13	8.68E-14	8.68E-14	8.48E-13	8.66E-14	8.66E-14	8.74E-13	8.64E-14	8.64E-14	9.00E-13	8.64E-14	8.63E-14	9.06E-13	8.64E-14	8.63E-14	9.10E-13
1.75E-12	1.08E-09	1.07E-09	1.89E-12	1.03E-09	1.02E-09	1.90E-12	9.77E-10	9.73E-10	1.92E-12	9.66E-10	9.63E-10	1.93E-12	9.59E-10	9.55E-10	1.93E-12
3.32E-28			2.90E-28			2.86E-28			2.83E-28			2.82E-28			2.81E-28
	6.8	6.8		6.8	6.8		6.8	6.8		6.8	6.8		6.8	6.8	
	3	3		3	3		3	3		3	3		3	3	
	1.08E-09	1.08E-09		1.03E-09	1.03E-09		9.77E-10	9.76E-10		9.67E-10	9.66E-10		9.59E-10	9.58E-10	
1.35489	1733.47	1732.31	1.15673	1715.46	1714.32	1.13871	1697.44	1696.32	1.1207	1693.84	1692.72	1.11709	1691.13	1690.02	1.11439
0.07927	0.001274	0.001273	0.072672	0.001256	0.0012553	0.072123	0.001239	0.0012377	0.071584	0.001235	0.0012341	0.071478	0.001233	0.0012315	0.071398
-4346.89	-4.73E+06	-4.73E+06	-3711.11	-4.67E+06	-4.66E+06	-3653.31	-4.60E+06	-4.59E+06	-3595.51	-4.58E+06	-4.58E+06	-3583.95	-4.57E+06	-4.57E+06	-3575.28
17.0922	1.36E+06	1.36E+06	15.9171	1.37E+06	1.37E+06	15.7886	1.37E+06	1.37E+06	15.6557	1.37E+06	1.37E+06	15.6286	1.37E+06	1.37E+06	15.6081
1			1			1			1			1			1
	528.637	529.352		540.315	541.048		552.49	553.243		554.988	555.744		556.875	557.634	
	0.403422	0.407572		0.403501	0.407651		0.403584	0.407734		0.4036	0.407751		0.403613	0.407763	
	0.227225	0.227227		0.227247	0.227246		0.227221	0.227218		0.22721	0.227206		0.2272	0.227196	
	29.5417	29.5169		29.1342	29.1094		28.7208	28.6961		28.6374	28.6127		28.5747	28.55	
	2.51211	2.51489		2.5585	2.56138		2.60729	2.61026		2.61735	2.62035		2.62496	2.62798	
	2.82032	2.82344		2.8724	2.87563		2.92717	2.93051		2.93847	2.94183		2.94701	2.9504	
	9.90132	9.91302		10.0868	10.0987		10.2793	10.2916		10.3187	10.331		10.3485	10.3608	

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	0.6741			**0.6735**			**0.6729**					**0.6728**		
	0.2272			**0.2272**			**0.2272**					**0.2272**		
	51.908008			**51.808008**			**51.708008**					**51.608008**		
	934.34414			**932.54414**			**930.74414**					**928.94414**		
	1688.4317			**1686.6299**			**1684.8252**					**1683.0328**		
	0.3061224			0.3061224			0.3061362					0.3067249		
Case 11			Case 12			Case 13				Case 14				
In	out	out	In	out	out	In	out	out	out	In	In	out	out	out
Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Vapor	Aqueous	Aqueous	Solid	Vapor	Aqueous	Solid	Aqueous	Solid	Vapor
25	25	25	25	25	25	25	25	25	25	25	25	25	25	25
1	0.0211624	0.021162	1	0.0211437	0.021144	1	0.0211254	0.021125	0.021125	1	1	0.0211222	0.021122	0.021122
7.00044	7.00066		7.00042	7.00064		7.0004	7.00062			7.00033		7.00046		
61.708	61.6463	0.061708	61.608	61.5464	0.061608	61.508	61.4461	4.37E-04	0.061508	61.4003	0.007688	61.3274	0.019254	0.061408
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
51.908	51.8463	0.061708	51.808	51.7464	0.061608	51.708	51.6465		0.061508	51.608		51.5466		0.061408
		5.62E-28			5.61E-28				5.60E-28					5.59E-28
8.63E-14	8.63E-14	9.15E-13	8.63E-14	8.63E-14	9.18E-13	8.63E-14	8.62E-14		9.20E-13	8.63E-14		8.62E-14		9.21E-13
9.51E-10	9.48E-10	1.93E-12	9.46E-10	9.43E-10	1.93E-12	9.41E-10	9.38E-10		1.93E-12	9.37E-10		9.35E-10		1.93E-12
		2.81E-28			2.80E-28				2.80E-28					2.80E-28
6.8	6.8		6.8	6.8		6.8	6.79956	4.37E-04		6.79231	0.007688	6.78075	0.019254	
3	3		3	3		3	3			3		3		
9.52E-10	9.51E-10		9.47E-10	9.46E-10		9.42E-10	9.41E-10			9.34E-10		9.35E-10		
1688.43	1687.32	1.11169	1686.63	1685.52	1.10989	1684.83	1683.68	0.037137	1.10809	1682.37	0.653405	1680.29	1.63648	1.10628
0.00123	0.0012288	0.071319	0.001228	0.0012271	0.071266	0.001226	0.0012253	1.65E-08	0.071213	0.001224	2.90E-07	0.0012229	7.25E-07	0.071108
-4.56E+06	-4.56E+06	-3566.61	-4.56E+06	-4.55E+06	-3560.83	-4.55E+06	-4.54E+06	-48.8416	-3555.05	-4.54E+06	-859.34	-4.54E+06	-2152.25	-3549.27
1.37E+06	1.37E+06	15.5876	1.37E+06	1.37E+06	15.5738	1.37E+06	1.37E+06	2.26E+06	15.5602	1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.5579
		1			1				1					1
								1			1		1	
558.774	559.537		560.047	560.812		561.326	562.068			562.185		562.314		
0.403626	0.407776		0.403635	0.407785		0.403643	0.407794			0.403652		0.407805		
0.227189	0.227185		0.227181	0.227176		0.227173	0.227169			0.227194		0.227234		
28.5119	28.4872		28.4699	28.4452		28.4279	28.4031			28.3833		28.3548		
2.63264	2.63567		2.63779	2.64083		2.64296	2.6459			2.64614		2.64615		
2.95563	2.95903		2.96141	2.96483		2.96722	2.97052			2.97079		2.9708		
10.3784	10.3908		10.3984	10.4108		10.4186	10.4305			10.4306		10.4308		

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0.6726
0.2274
51.408008
925.34414
1679.427
0.3079096

Case 15				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0211157	0.021116	0.021116
7.00007		6.99954		
61.1627	0.045353	61.0899	0.056878	0.061208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
51.408		51.3468		0.061208
				5.58E-28
8.62E-14		8.63E-14		9.24E-13
9.31E-10		9.30E-10		1.93E-12
				2.79E-28
6.75465	0.045353	6.74312	0.056878	
3		3		
8.66E-10		8.68E-10		
1675.57	3.85479	1673.49	4.83432	1.10268
0.001219	1.71E-06	0.001218	2.14E-06	0.070898
-4.52E+06	-5069.72	-4.52E+06	-6357.97	-3537.71
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.5532
				1
	1		1	
562.678		562.808		
0.40367		0.407862		
0.227323		0.227363		
28.2866		28.2581		
2.64663		2.64664		
2.97134		2.97135		
10.4311		10.4312		

0.6721
0.2277
50.90801
916.3441
1670.418
0.310909

Case 16				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.021099	0.021099	0.021099
6.9994		6.99956		
60.5685	0.139459	60.4964	0.150879	0.060708
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
50.908		50.8473		0.060708
				5.53E-28
8.60E-14		8.59E-14		9.26E-13
9.16E-10		9.13E-10		1.90E-12
				2.77E-28
6.66054	0.139459	6.64912	0.150879	
3		3		
9.17E-10		9.17E-10		
1658.56	11.8533	1656.5	12.824	1.09367
0.001207	5.25E-06	0.001206	5.68E-06	0.070373
-4.48E+06	-15589.1	-4.47E+06	-16865.7	-3508.82
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.5411
				1
	1		1	
563.932		564.064		
0.403717		0.407867		
0.227652		0.227692		
28.0448		28.0166		
2.6479		2.64791		
2.97277		2.97278		
10.4323		10.4325		

0.6715
0.2280
50.408008
907.34414
1661.411
0.3139648

Case 17				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0210827	0.021083	0.021083
6.99872		6.99887		
59.9745	0.233479	59.903	0.244795	0.060208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
50.408		50.3478		0.060208
				5.49E-28
8.58E-14		8.57E-14		9.30E-13
9.00E-10		8.98E-10		1.88E-12
				2.74E-28
6.56652	0.233479	6.55521	0.244795	
3		3		
9.01E-10		9.01E-10		
1641.57	19.8445	1639.52	20.8063	1.08467
0.001195	8.79E-06	0.0011937	9.22E-06	0.069849
-4.44E+06	-26099	-4.43E+06	-27363.9	-3479.92
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.5288
				1
	1		1	
565.216		565.35		
0.403764		0.407914		
0.227986		0.228027		
27.8031		27.7752		
2.64922		2.64923		
2.97425		2.97426		
10.4337		10.4338		

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0.6693
0.2294
48.408008
871.34414
1625.3768
0.3267814

Case 18				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0210117	0.021012	0.021012
6.99586		6.99601		
57.5994	0.60865	57.5303	0.619546	0.058208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
48.408		48.3498		0.058208
				5.31E-28
8.50E-14		8.49E-14		9.46E-13
8.39E-10		8.37E-10		1.81E-12
				2.66E-28
6.19135	0.60865	6.18045	0.619546	
3		3		
8.39E-10		8.40E-10		
1573.65	51.7321	1571.67	52.6582	1.04863
0.001147	2.29E-05	0.0011451	2.33E-05	0.067757
-4.26E+06	-68036.7	-4.25E+06	-69254.7	-3364.32
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.4765
				1
	1		1	
570.683		570.827		
0.403962		0.408113		
0.229393		0.229436		
26.8369		26.8099		
2.65501		2.65504		
2.98074		2.98078		
10.4404		10.4406		

0.6668
0.2310
46.408008
835.34414
1589.3465
0.3406261

Case 19				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0209333	0.020933	0.020933
6.99276		6.99291		
55.2258	0.98222	55.1591	0.992693	0.056208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
46.408		46.3518		0.056208
				5.13E-28
8.41E-14		8.40E-14		9.65E-13
7.78E-10		7.76E-10		1.73E-12
				2.57E-28
5.81778	0.98222	5.80731	0.992693	
3		3		
7.78E-10		7.79E-10		
1505.86	83.4837	1503.96	84.3739	1.0126
0.001098	3.70E-05	0.0010966	3.74E-05	0.065674
-4.08E+06	-1.10E+05	-4.08E+06	-1.11E+05	-3248.72
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.4187
				1
	1		1	
576.741		576.896		
0.404177		0.408328		
0.230921		0.230965		
25.8715		25.8454		
2.66175		2.6618		
2.98831		2.98837		
10.4496		10.4499		

0.6654
0.2318
45.408008
817.34414
1571.3296
0.3479713

Case 20				
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208909	0.020891	0.020891
6.99111		6.99126		
54.0397	1.16834	53.9742	1.1786	0.055208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
45.408		45.3528		0.055208
				5.05E-28
8.36E-14		8.35E-14		9.74E-13
7.48E-10		7.46E-10		1.69E-12
				2.52E-28
5.63166	1.16834	5.6214	1.1786	
3		3		
7.48E-10		7.49E-10		
1472.03	99.3026	1470.16	100.175	0.994589
0.001074	4.40E-05	0.0010724	4.44E-05	0.064636
-3.99E+06	-1.31E+05	-3.99E+06	-1.32E+05	-3190.92
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.3875
				1
	1		1	
580.022		580.184		
0.404292		0.408443		
0.231734		0.23178		
25.3892		25.3636		
2.66554		2.6656		
2.99257		2.99264		
10.4554		10.4557		

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0.6652
0.2319
45.208008
813.74414
1567.731
0.349476

Case 21

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208822	0.020882	0.020882
6.99078		6.99093		
53.8025	1.2055	53.7373	1.21572	0.055008
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
45.208		45.153		0.055008
				5.03E-28
8.35E-14		8.34E-14		9.76E-13
7.42E-10		7.40E-10		1.68E-12
				2.51E-28
5.5945	1.2055	5.58428	1.21572	
3		3		
7.42E-10		7.43E-10		
1465.27	102.462	1463.41	103.33	0.990986
0.001069	4.54E-05	0.0010676	4.58E-05	0.064429
-3.98E+06	-1.35E+05	-3.97E+06	-1.36E+05	-3179.37
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.381
				1
	1		1	
580.7		580.863		
0.404315		0.408467		
0.231902		0.231948		
25.2927		25.2673		
2.66633		2.6664		
2.99346		2.99354		
10.4566		10.457		

0.6647
0.2322
44.908008
808.34414
1562.3256
0.3517564

Case 22

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208689	0.020869	0.020869
6.99027		6.99041		
53.4468	1.26121	53.3819	1.27137	0.054708
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
44.908		44.8533		0.054708
				5.00E-28
8.33E-14		8.33E-14		9.80E-13
7.33E-10		7.31E-10		1.67E-12
				2.50E-28
5.53879	1.26121	5.52863	1.27137	
3		3		
7.33E-10		7.34E-10		
1455.13	107.197	1453.28	108.06	0.985581
0.001062	4.75E-05	0.0010603	4.79E-05	0.064119
-3.95E+06	-1.41E+05	-3.95E+06	-1.42E+05	-3162.03
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.3712
				1
	1		1	
581.732		581.897		
0.404351		0.408502		
0.232155		0.232201		
25.1481		25.1228		
2.66755		2.66762		
2.99483		2.99491		
10.4585		10.4589		

0.6646
0.2323
44.408008
799.34414
1553.3196
0.352691

Case 23

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208634	0.020863	0.020863
6.98996		6.99021		
52.8525	1.35547	52.788	1.36579	0.054208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
44.408		44.3538		0.054208
				4.96E-28
8.27E-14		8.25E-14		9.74E-13
7.22E-10		7.21E-10		1.65E-12
				2.48E-28
5.46601	1.33399	5.45954	1.34046	
2.97852	0.02148	2.97467	0.02533	
7.23E-10		7.24E-10		
1438.68	114.638	1436.93	115.413	0.976573
0.00105	5.08E-05	0.0010484	5.12E-05	0.063549
-3.91E+06	-1.51E+05	-3.90E+06	-1.52E+05	-3133.13
1.37E+06	2.26E+06	1.37E+06	2.26E+06	15.3672
				1
	1		1	
582.358		582.322		
0.404372		0.408517		
0.232308		0.232306		
24.882		24.8525		
2.66829		2.66812		
2.99566		2.99547		
10.4597		10.4597		

J.Y. 04/19/01

0.6646
0.2323
40.408008
727.34414
1481.2565
0.3526909

Case 24

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208634	0.020863	0.020863
6.98996		6.99021		
48.0919	2.1161	48.0321	2.12566	0.050208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
40.408		40.3578		0.050208
				4.59E-28
7.52E-14		7.51E-14		9.02E-13
6.57E-10		6.56E-10		1.53E-12
				2.30E-28
4.97366	1.82633	4.96767	1.83233	
2.71023	0.289765	2.70667	0.293329	
6.58E-10		6.59E-10		
1309.09	172.164	1307.47	172.882	0.904512
9.55E-04	7.66E-05	9.54E-04	7.69E-05	0.05886
-3.55E+06	-2.33E+05	-3.55E+06	-2.34E+05	-2901.93
1.37E+06	2.25E+06	1.37E+06	2.25E+06	15.3672
				1
	1		1	
582.358		582.322		
0.404372		0.408516		
0.232308		0.232306		
22.6408		22.6134		
2.66829		2.66812		
2.99566		2.99547		
10.4597		10.4597		

0.6646
0.2323
35.408008
637.34414
1391.1834
0.3526909

Case 25

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208634	0.020863	0.020863
6.98996		6.99024		
42.1411	3.06689	42.0873	3.0755	0.045208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
35.408		35.3628		0.045208
				4.13E-28
6.59E-14		6.58E-14		8.12E-13
5.76E-10		5.75E-10		1.38E-12
				2.07E-28
4.35823	2.44177	4.35283	2.44717	
2.37488	0.625124	2.37167	0.628328	
5.78E-10		5.79E-10		
1147.11	244.072	1145.65	244.719	0.814436
8.37E-04	1.09E-04	8.36E-04	1.09E-04	0.052998
-3.11E+06	-3.34E+05	-3.11E+06	-3.35E+05	-2612.94
1.37E+06	2.24E+06	1.37E+06	2.24E+06	15.3672
				1
	1		1	
582.358		582.322		
0.404372		0.408515		
0.232308		0.232306		
19.8393		19.8146		
2.66829		2.66812		
2.99566		2.99547		
10.4597		10.4597		

0.6646
0.2323
25.408008
457.34414
1211.0263
0.3526909

Case 26

In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25
1	1	0.0208634	0.020863	0.020863
6.98996		6.99021		
30.2395	4.96847	30.1976	4.97517	0.035208
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
25.408		25.3728		0.035208
				3.22E-28
4.73E-14		4.72E-14		6.33E-13
4.13E-10		4.13E-10		1.07E-12
				1.61E-28
3.12737	3.67263	3.12315	3.67684	
1.70416	1.29584	1.70167	1.29833	
4.14E-10		4.15E-10		
823.139	387.888	822.001	388.391	0.634283
6.01E-04	1.73E-04	6.00E-04	1.74E-04	0.041275
-2.23E+06	-5.38E+05	-2.23E+06	-5.39E+05	-2034.96
1.37E+06	2.24E+06	1.37E+06	2.24E+06	15.3672
				1
	1		1	
582.358		582.322		
0.404372		0.408516		
0.232308		0.232306		
14.2362		14.217		
2.66829		2.66812		
2.99566		2.99547		
10.4597		10.4597		

J.Y. 04/19/01

0.6646	**0.6646**	**0.6646**
0.2323	**0.2323**	**0.2323**
15.408008	**5.407998**	**1.407998**
277.34414	**97.343964**	**25.343964**
1030.8741	**850.72098**	**778.65972**
0.3526918	0.3526914	0.3526913

Case 27					Case 28					Case 29					Case 30
In Aqueous	In Solid	out Aqueous	out Solid	out Vapor	In Aqueous	In Solid	out Aqueous	out Solid	out Vapor	In Aqueous	In Solid	out Aqueous	out Solid	out Vapor	In Aqueous
25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25
1	1	0.0208634	0.020863	0.020863	1	1	0.0208634	0.020863	0.020863	1	1	0.0208634	0.020863	0.020863	1
6.98996		6.99035			6.98996		6.99025			6.98996		6.99003			6.98996
18.338	6.87005	18.308	6.87485	0.025208	6.43637	8.77163	6.41827	8.77452	0.015208	1.67574	9.53226	1.6624	9.53439	0.011208	0.485584
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
15.408		15.3828		0.025208	5.408		5.39279		0.015208	1.408		1.39679		0.011208	0.408
				2.31E-28					1.39E-28					1.03E-28	
2.87E-14		2.86E-14		4.53E-13	1.01E-14		1.00E-14		2.73E-13	2.62E-15		2.60E-15		2.01E-13	7.59E-16
2.51E-10		2.50E-10		7.68E-13	8.80E-11		8.77E-11		4.64E-13	2.29E-11		2.27E-11		3.42E-13	6.64E-12
				1.15E-28					6.95E-29					5.13E-29	
1.89651	4.90349	1.89348	4.90653		0.66565	6.13435	0.663802	6.1362		0.173305	6.6267	0.171932	6.62807		0.050219
1.03344	1.96656	1.03168	1.96832		0.362724	2.63728	0.361678	2.63832		0.094437	2.90556	0.0936785	2.90632		0.027365
2.54E-10		2.55E-10			8.80E-11		8.84E-11			2.20E-11		2.24E-11			6.64E-12
499.171	531.703	498.356	532.064	0.45413	175.202	675.519	174.71	675.737	0.273977	45.6148	733.045	45.2518	733.206	0.201915	13.2179
3.64E-04	2.38E-04	3.64E-04	2.38E-04	0.029552	1.28E-04	3.02E-04	1.27E-04	3.02E-04	0.017829	3.33E-05	3.28E-04	3.30E-05	3.28E-04	0.013139	9.64E-06
-1.36E+06	-7.41E+05	-1.35E+06	-7.42E+05	-1456.98	-4.76E+05	-9.45E+05	-4.74E+05	-9.45E+05	-878.996	-1.24E+05	-1.03E+06	-1.23E+05	-1.03E+06	-647.803	-35884.6
1.37E+06	2.24E+06	1.37E+06	2.24E+06	15.3672	1.37E+06	2.24E+06	1.37E+06	2.24E+06	15.3672	1.37E+06	2.23E+06	1.37E+06	2.23E+06	15.3672	1.37E+06
				1					1					1	
	1		1			1		1			1		1		
582.358		582.322			582.358		582.322			582.358		582.322			582.358
0.404372		0.408508			0.404372		0.408514			0.404373		0.408527			0.404372
0.232308		0.232306			0.232308		0.232306			0.232308		0.232306			0.232308
8.63318		8.61933			3.03013		3.02171			0.788909		0.782655			0.228604
2.66829		2.66812			2.66829		2.66812			2.66829		2.66812			2.66829
2.99566		2.99547			2.99566		2.99547			2.99566		2.99547			2.99566
10.4597		10.4597			10.4597		10.4597			10.4597		10.4597			10.4597

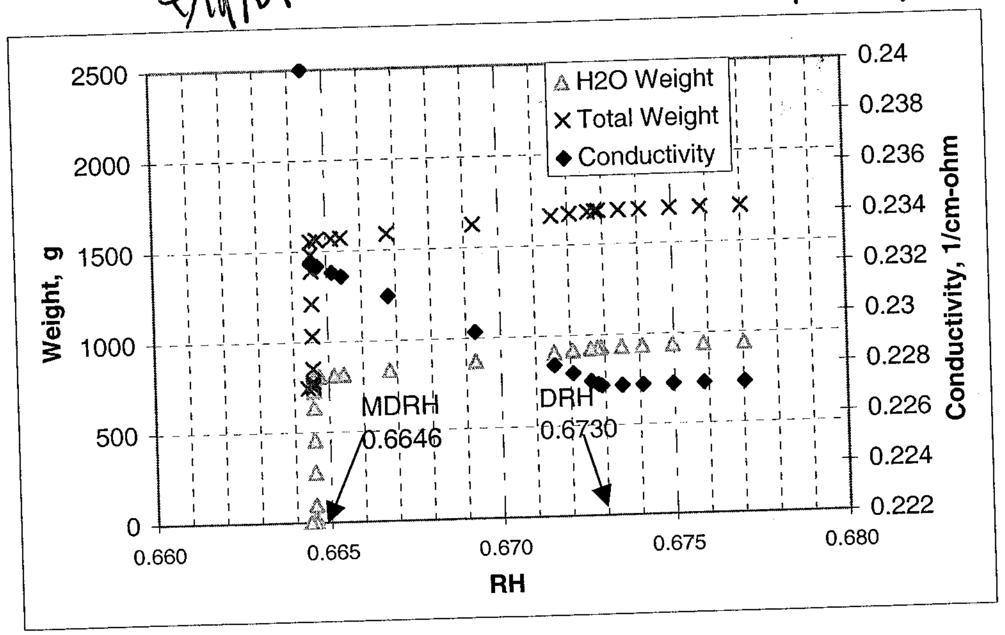
J.Y. 04/19/01

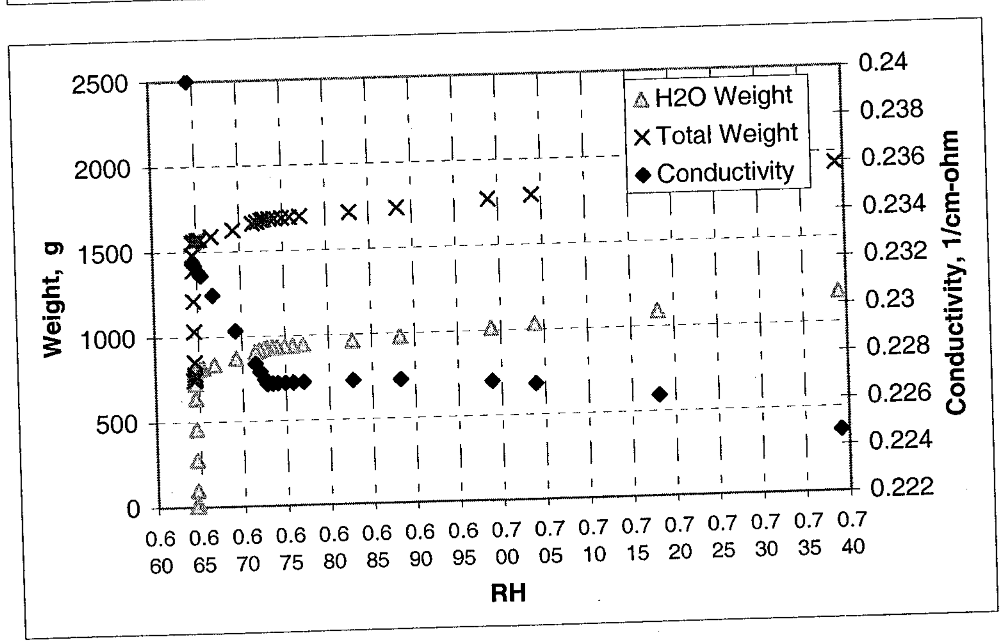
0.6646	**0.6646**	0.6645
0.2323	**0.2323**	**0.2400**
0.408	**0.10691**	
7.344	**1.92438**	0
760.6442	**747.6175**	**745.69312**
0.3526913	0.3526921	

				Case 31				
In Solid	out Aqueous	out Solid	out Vapor	In Aqueous	In Solid	out Aqueous	out Solid	out Vapor
25	25	25	25	25	25	25	25	25
1	0.0208634	0.020863	0.020863	1	1	0.0208634	0.020863	0.020863
	6.99087			6.98995		6.9929		
9.72242	0.473435	9.72436	0.010208	0.12724	9.68076	0.115567	9.68263	0.009808
mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
	0.397792		0.010208	0.10691		0.097102		0.009808
			9.34E-29					8.97E-29
	7.39E-16		1.83E-13	1.99E-16		1.80E-16		1.75E-13
	6.46E-12		3.11E-13	1.74E-12		1.57E-12		2.97E-13
			4.67E-29					4.49E-29
6.74979	0.0489645	6.75104		0.013159	6.71821	0.0119523	6.71942	
2.97263	0.0266787	2.97332		0.007171	2.96255	0.0065123	2.96321	
	6.95E-12			1.74E-12		2.04E-12		
747.427	12.8873	747.573	0.1839	3.46355	744.154	3.14581	744.295	0.176694
3.34E-04	9.40E-06	3.35E-04	0.011967	2.53E-06	3.33E-04	2.30E-06	3.33E-04	0.011498
-1.05E+06	-34986.7	-1.05E+06	-590.004	-9402.99	-1.04E+06	-8540.34	-1.04E+06	-566.885
2.23E+06	1.37E+06	2.23E+06	15.3672	1.37E+06	2.23E+06	1.37E+06	2.23E+06	15.3672
			1					1
1		1			1		1	
	582.322			582.358		582.322		
	0.408478			0.404373		0.408357		
	0.232306			0.232308		0.232306		
	0.222892			0.060513		0.0549632		
	2.66812			2.66829		2.66812		
	2.99547			2.99566		2.99547		
	10.4597			10.4597		10.4597		

J.Y. 4/19/01

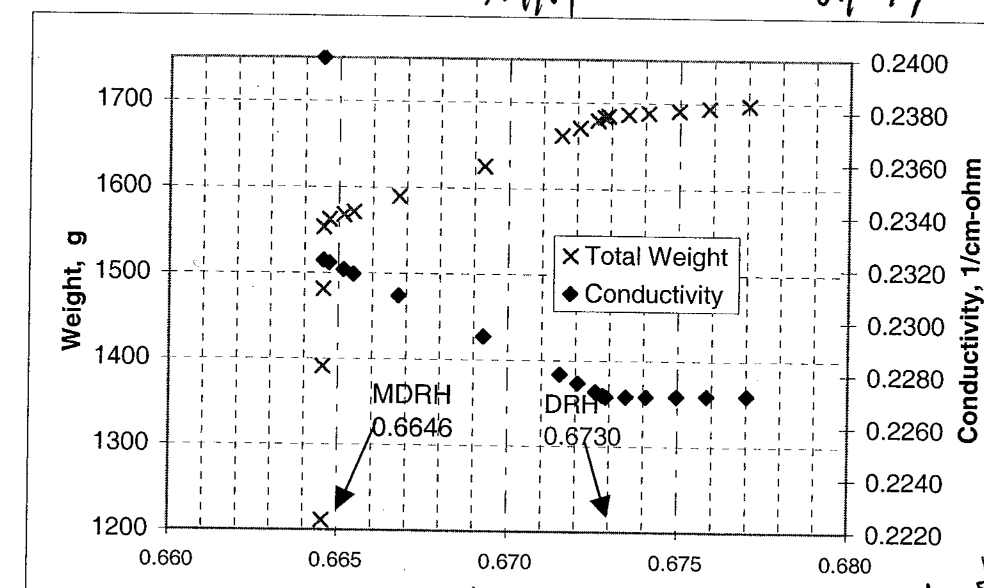
Results see pages 69–77



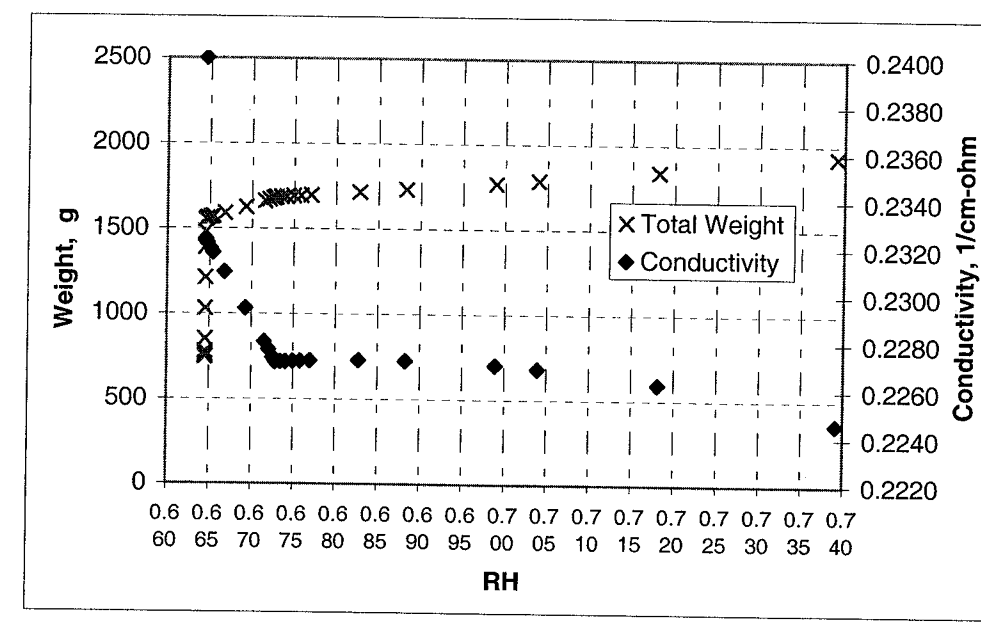


J.Y. 4/19/01

Results see pages 69–77



Note 75.6 g when completely dried. J.Y.



Compare Results on page 55.

YM Waters Evaporation

Lietai Yang

From: Lauren Browning [lbrowning@gargol.cnwra.swri.edu]
Sent: Wednesday, April 18, 2001 3:21 PM
To: Lietai Yang
Subject: waters

Lietai,

This should give you a start, anyway. You might try running these with different fixed values of CO2(g). I'd suggest fixing the log f CO2 to -3 and -3.5 to start. These are measured CO2 gas pressures in the matrix pores, and atmospheric. It would also be interesting at some point to try a closed system (i.e. don't fix the p CO2(g), but let it be consumed).

Species	units	Init.PoreWater	PERM-2	PERM-3	Infiltration
HCO3-	mg/L	200	200	200	216
redox	log f	-0.7706	-0.7706	-0.7706	
Mg++	mg/L	17	16.6	17.4	17
SiO2(aq)	mg/L	70.5	66	75	70.5
K+	mg/L	8	7	9	8
Al+++	mg/L	9.92E-07	9.92E-07	9.92E-07	2.64E-06
SO4--	mg/L	116	111	120	116
Ca++	mg/L	101	106	97	101
Fe++	mg/L	6.40E-08	6.46E-08	6.46E-08	2.88E-08
Na+	mg/L	61.3	61	62	61.3
Cl-	mg/L	117	110	123	118
pH		8.32	8.32	8.31	7.75
T =	°C	25	25	25	17
Reference:		1	1	1	1
NO3		6.5	3	10	6.5

m_{SiO_2} = 60
1.175 1.1 1.25 1.175 mmol/L
L.Y.

~~M_{AlCl_3} = 2~~ L.Y. 04/20/01

M_{Al} = 27
3.67E-8, 3.67E-8 3.67E-8, 9.78E-7 mmol/L

L.Y. 04/20/01

given by Lauren by phone.

References:
1)CRWMS M&O, Drift-Scale Coupled Processes (DST and THC Seepage) Models, MDL-NB
S-HS-000001, Revision 01 ICN 01, Las Vegas, NV, Office of Civilian Radioactive Waste Management S
System, Management and Operating Contractor, 2000.

L data there is no F-
L.Y.
5/18/01

L. Yang 3/19/02

April 20/01

Data Reconcile:

① Init. pore water

Template Reconcile Units LastResult Help

Lauren Study
J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	101.	100.999	CL-1	117.	116.998
K+1	8.	7.9999	F-1		
MG+2	17.	16.9998	HCO3-1	200.	212.949
NA+1	61.3	61.2992	NO3-1	6.5	6.49991
			SO4-2	116.	115.998

<PgDn>

added NO_3^-

File Name: L13_pore

Calc. pH: 7.33417

to add: SiO_2 and CO_2 later.
add $AlCl_3$ too.

L. Yang 3/19/02

04/23/01

(2) Perm-2 water

Template Reconcile Units LastResult Help

LAUREN Study
J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	106.	105.995	CL-1	110.	109.995
K+1	7.	6.99968	F-1		
MG+2	16.6	16.5992	HCO3-1	200.	245.642
NA+1	61.	60.9972	NO3-1	3.	2.99986
			SO4-2	111.	110.995

added J.Y.

<PgDn>

Calculate pH Reconcile pH Help

LAUREN Study
J13 Model
Sample LB_PM-2

Sample LB_PM-2

Measured pH: 0.0

Calculated pH: 7.25418

Sample: LB_PM-2

J. Yang 3/4/02

04/23/01

Template Reconcile Units LastResult Help

LAUREN Study
J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	97.	97.0002	CL-1	123.	123.
K+1	9.	8.99999	F-1		
MG+2	17.4	17.4	HCO3-1	187.346	187.346
NA+1	62.	61.9999	NO3-1	10.	10.
			SO4-2	120.	120.

Reduced from 200 mg/L. J.Y.

<PgDn>

Calculate pH Reconcile pH Help

LAUREN Study
J13 Model
Sample LB_PM_3

Sample LB_PM_3

Measured pH: 0.0

Calculated pH: 7.37052

J. Yang 3/4/02

Template Reconcile Units LastResult Help

LAUREN Study
J13 Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	101.	101.	CL-1	118.	118.
K+1	8.	7.99999	F-1		
MG+2	17.	17.	HCO3-1	211.228	211.229
NA+1	61.3	61.3	NO3-1	6.5	6.49997
			SO4-2	116.	116.

Reduced from 216 mg/L J.Y.

Calculate pH Reconcile pH Help

LAUREN Study
J13 Model
Sample LB_INFIL

Sample LB_INFIL

Measured pH: 0.0

Calculated pH: 7.3172

J. Y. 3/..../01

Simulation using OLI V6.2 e

using water reconciled on pages 81, 82, 83, 84.

Evaporate the waters in a mixer to ~~48%~~ J.Y. 04/23/01 98% of vapour.

File Config Parameters Units Process Check Memo Help

Mix: LB_mix

LB_WATER Process
LB_WATER Model
Define Mix

LB_Pore

(optional)

LB_Pore_out

Mix Equilibrium Calc

T, Vapor Fraction Equilibrium Calculation

Temperature	90.	C
Vapor Fraction	0.98	molar

Either enter the pressure or pressure drop when specifying a pressure.

Blank pressure defaults to inlet conditions.

J. Y. 3/..../01

During simulation, SiO_2, $AlCl_3$ as shown in page 80 were added

04/23/01

File: Lb_Waters.xls
Pore Water: Reconciled 04/21/01, Note Book Page 81
Additional: SiO2 70.5 mg, AlCl3 3.67E-8 molal, 9.92e-7 mg/L for Al

Case 1 Input CO2 = 0 (molal) = 0 (mg) logPCo2= -4.53114
Case 2 Input CO2 = 0.02 (molal) = 880 (mg) logPCo2= -3.56103
Case 3 Input CO2 = 0.065 (molal) = 2860 (mg) logPCo2= -3.07422

Stream	LB_Pore	LB_Pore	LB_Pore_c	LB_Pore_c	LB_Pore_out	LB_Pore	LB_Pore	LB_Pore	LB_Pore_c	LB_Pore_c	LB_Pore_out	LB_Pore	LB_Pore	LB_Pore	LB_Pore_c	LB_Pore_c	LB_Pore_out
Phase	Aqueous	Solid	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90
Pressure, atm	1	1	0.68715	0.68715	0.68715	1	1	1	0.687288	0.687288	0.687288	1	1	1	0.687867	0.687867	0.687867
pH	6.83245		7.93621			6.246			7.58009			6.24595			7.33786		
Total mol/hr	55.5198	8.03E-04	1.10845	0.003347	54.4102	55.4661	6.16E-05	0.053779	1.10998	0.003018	54.4095	55.3198	6.46E-05	0.200038	1.10999	0.003029	54.4095
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087		55.5087		0.999957	55.5087		0.69272	55.5087		0.9996	55.5087		0.692719	55.5087		0.998775
CO2	0.00222602		3.31E-07		4.28E-05	0.006064		3.07E-01	3.06E-06		4.00E-04	0.006064		0.307281	9.40E-06		0.001225
H2SO4					2.98E-29			1.08E-26			2.78E-28			1.08E-26			8.54E-28
H2					3.26E-22			2.25E-22			3.26E-22			2.25E-22			3.26E-22
HCL					3.34E-13			2.82E-13	6.84E-14		7.53E-13			2.82E-13	1.19E-13		1.31E-12
HNO3	4.91E-12		8.76E-12		2.04E-14	1.18E-11		1.83E-14	1.98E-11		4.65E-14	1.19E-11		1.84E-14	3.45E-11		8.11E-14
O2					1.63E-22			1.12E-22			1.63E-22			1.12E-22			1.63E-22
SICL4	8.15E-06					3.40E-06						3.40E-06					
SO3																	
[redacted]																	
ALOH3	3.84E-09		7.51E-09			8.07E-09			1.63E-08			8.08E-09			2.82E-08		
KCL	1.77E-08		2.46E-05			1.74E-06			2.28E-05			1.74E-08			2.28E-05		
KHSO4	1.0961E-12		8.17E-12			2.45E-12			3.14E-11			2.46E-12			5.51E-11		
MGCO3	7.70E-06		5.26E-07			3.39E-04			3.82E-06			3.39E-04			3.84E-06		
MGH2SIO4	6.51E-10		1.31E-05			1.05E-10			1.02E-05			1.05E-10			3.34E-06		
[redacted]																	
NAHCO3	6.45E-06		1.94E-06			1.13E-05			7.60E-06			1.13E-05			1.33E-05		
NAHSIO3	9.13E-08		8.24E-04			3.73E-08			3.46E-04			3.74E-08			1.98E-04		
[redacted]																	
CAH2SIO4	1.58E-10		4.54E-06			3.68E-11			4.82E-07			3.68E-11			1.57E-07		
[redacted]																	
CACO3	5.29E-06	1	5.08E-06	0.346977		4.59E-05	1		5.04E-06	0.572939		4.45E-05	1		5.04E-06	0.572292	
[redacted]																	
ALCL3	3.2854E-08																
CAOH2			9.52E-04														
H2CO3																	
MGOH2				0.164702					4.44E-04						2.55E-04		
[redacted]																	
NA6SO42CO3	4.44E-04		2.34E-05			4.43E-04			1.04E-04			4.44E-04			1.81E-04		
AL2SO43.16H2O																	
AL2SO43.6H2O																	
AL2SO43																	
ALCL3.6H2O																	
ALNO33.6H2O																	
ALNO33.8H2O																	
ALNO33.9H2O																	
ALOOH																	
CA2CL2O.2H2O	4.39E-04					8.18E-04						8.18E-04					
CACL2.1H2O																	
CACL2.2H2O																	
CACL2.4H2O																	
CACL2.6H2O																	
[redacted]																	
CANO32.3H2O																	
CANO32.4H2O																	
CANO32	5.24E-05					5.25E-05						5.26E-05					
CASO4.2H2O				0.239498						0.138748						0.136678	
K1ALSO4.12H2O																	
K1ALSO4																	
K2CO3.1.5H2O																	
K2CO3																	
K2SO4.1H2O																	
K2SO4																	
K3NASO42			0.001152														
KHCO3																	
KMGCL3.2H2O																	
KNO3																	
KOH.1H2O																	
KOH.2H2O																	
KOH																	
MGCL2.2H2O																	
MGCL2.4H2O																	
MGCL2.6H2O																	
[redacted]																	
MGCLOH																	
MGCO3.3H2O																	
MGNO32.2H2O																	
MGNO32.6H2O																	
MGNO32																	
MGSO4.1H2O																	
MGSO4.6H2O																	
MGSO4.7H2O																	
MGSO4OH.0.5H2O																	
MGSO4OH	1.20E-04					8.22E-05						8.24E-05					
NA2CO3.10H2O																	
NA2CO3.1H2O																	
NA2CO3.7H2O																	
NA2CO3																	
NA2SIO3.5H2O																	
NA2SIO3.6H2O																	
NA2SIO3.9H2O																	
NA2SIO3			0.002407						0.001087						6.22E-04		
NA2SO4.10H2O																	
[redacted]																	
NAALCO3OH2																	
NAALO22.2.5H2O						1.43E-08						1.44E-08					
NAALO2			1.84E-06						1.82E-06						1.81E-06		
[redacted]																	
NAHSO4																	
NAOH.1H2O																	
NAOH																	
Total g/hr	1000.72	0.080392	20.1905	0.336394	980.277	999.919	6.16E-03	1.39841	20.257	0.297414	980.769	997.283	6.47E-03	5.20158	20.2564	0.297718	981.937
Volume, m3/hr	0.00103588	2.97E-08	2.07E-05	1.32E-07	2.34504	0.001035	2.27E-09	1.59E-03	2.07E-05	1.15E-07	2.34454	0.001032	2.39E-09	5.92E-03	2.07E-05	1.16E-07	2.34257
Enthalpy, cal/hr	-3.73E+06	-230.203	-74767.9	-1018.35	-3.12E+06	-3.73E+06	-17.6417	-3678.67	-74977.8	-883.819	-3.12E+06	-3.72E+06	-18.5188	-13683.3	-74975.5	-885.231	-3.12E+06
Density, g/m3	9.66E+05	2.71E+06	9.76E+05	2.54E+06	418.021	9.66E+05	2.71E+06	8.78E+02	9.78E+05	2.58E+06	418.32	9.66E+05	2.71E+06	878.453	9.78E+05	2.58E+06	419.171
Vapor fraction					1			1			1			1			1
Solid fraction		1		1			1			1			1			1	
Organic fraction																	
Osmotic Pres, atm	0.333537		8.87972			0.464512			9.13374			0.464931			9.11836		
Redox Pot, volts	0.346839		0.260148			0.374751			0.28581			0.374755			0.303264		
E-Con, 1/ohm-cm	1.98E-03		0.045693			2.26E-03			0.049381			2.26E-03			0.049394		
E-Con, cm2/ohm-mol	186.074		143.808			75.3094			38.5055			30.6978			14.3153		
Abs Visc, cP	0.315178		0.325141			0.315467			0.32883			0.315468			0.328846		
Rel Visc	1.00306		1.03477			1.00398			1.0465			1.00398			1.04656		
Ionic Strength	0.0103817		0.249523			0.012315			0.306012			0.012329			0.305866		

J. Yang 2/14/02

04/23/01

File: Lb_Waters.xls
Perm-2: Reconciled 04/21/01, Note Book Page 82
Additional: SiO2 66 mg, AlCl3 3.67E-8 molal, 9.92e-7 mg/L for Al

Case 1 Input CO2 = 0 (molal) = 0 (mg) logPCo2= -4.482252
Case 2 Input CO2 = 0.02 (molal) = 880 (mg) logPCo2= -3.555147
Case 3 Input CO2 = 0.065 (molal) = 2860 (mg) logPCo2= -3.072221

Stream	LB_PM-2	LB_PM-2	LB_PM-2_c	LB_PM-2_c	LB_PM-2_out	LB_PM-2	LB_PM-2	LB_PM-2_c	LB_PM-2_c	LB_PM-2_out	LB_PM-2	LB_PM-2	LB_PM-2	LB_PM-2_c	LB_PM-2_c	LB_PM-2_out
Phase	Aqueous	Solid	Aqueous	Solid	Vapor	Aqueous	Solid	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	25	25	90	90	90	25	25	90	90	90	25	25	25	90	90	90
Pressure, atm	1	1	0.687334	0.687334	0.687334	1	1	0.68746	0.68746	0.68746	1	1	1	0.688038	0.688038	0.688038
pH	7.24704		7.94064			5.58174		7.59829			5.37278			7.35799		
Total mol/hr	55.5214	3.23E-04	1.10947	0.003447	54.4113	55.5214	3.10E-08	1.11069	0.003094	54.411	55.4878	2.66E-08	0.033645	1.11071	0.003106	54.411
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087		55.5087		0.999952	55.5087		55.5087		0.999595	55.5087		0.031772	55.5087		0.998769
CO2	0.002903		3.70E-07		4.79E-05	0.023074		3.11E-06		4.05E-04	0.03546		0.968228	9.44E-06		0.001231
H2SO4					3.34E-29					2.82E-28			1.16E-28			8.57E-28
H2					3.26E-22					3.26E-22			2.51E-28			3.25E-22
HCL					3.11E-13			6.16E-14		6.78E-13			7.52E-15	1.07E-13		1.18E-12
HNO3	1.21E-13		4.03E-12		9.38E-15	5.56E-12		8.78E-12		2.06E-14	9.00E-12		4.39E-16	1.53E-11		3.58E-14
O2					1.63E-22					1.63E-22			1.24E-28			1.63E-22
SICL4	4.43E-06					9.65E-08					5.97E-08					
SO3																
[redacted]																
ALOH3	2.40E-09	6.92E-05	7.49E-09			2.40E-09	1	1.57E-08			2.40E-09	1		2.71E-08		
KCL	3.66E-09		2.03E-05			3.63E-09		1.87E-05			3.62E-09			1.87E-05		
KHSO4			8.10E-12			4.76E-13		2.90E-11			7.70E-13			5.07E-11		
MGCO3	2.73E-04		5.89E-07			2.89E-04		4.06E-06			2.89E-04			4.08E-06		
MGH2SIO4	4.12E-10		1.31E-05			1.88E-13		1.07E-05			7.19E-14			3.54E-06		
[redacted]																
NAHCO3	2.87E-06		2.19E-06			3.42E-06		8.00E-06			3.42E-06			1.40E-05		
NAHSIO3	3.99E-07		8.31E-04			8.64E-09		3.60E-04			5.35E-09			2.07E-04		
[redacted]																
CAH2SIO4	1.48E-10		4.06E-06			7.79E-14		4.77E-07						1.57E-07		
[redacted]																
CACO3	1.08E-04	0.999931	5.09E-06	0.418707		2.41E-04		5.05E-06	0.645183		2.40E-04			5.05E-06	0.644249	
[redacted]																
ALCL3																
CAOH2			9.60E-04													
H2CO3																
MGOH2				0.155833				4.62E-04						2.66E-04		
[redacted]																
NA6SO42CO3	4.42E-04		2.60E-05			4.42E-04		1.08E-04			4.42E-04			1.89E-04		
AL2SO43.16H2O																
AL2SO43.6H2O																
AL2SO43																
ALCL3.6H2O																
ALNO33.6H2O																
ALNO33.8H2O																
ALNO33.9H2O																
ALOOH																
CA2CL2O.2H2O	8.04E-04					9.74E-04					9.75E-04					
CACL2.1H2O																
CACL2.2H2O																
CACL2.4H2O																
CACL2.6H2O																
[redacted]																
CANO32.3H2O																
CANO32.4H2O																
CANO32	2.42E-05					2.42E-05					2.42E-05					
CASO4.2H2O				0.206002					0.098438						0.096467	
K1ALSO4.12H2O																
K1ALSO4																
K2CO3.1.5H2O																
K2CO3																
K2SO4.1H2O																
K2SO4																
K3NASO42			0.000791													
KHCO3																
KMGCL3.2H2O																
KNO3																
KOH.1H2O																
KOH.2H2O																
KOH																
MGCL2.2H2O																
MGCL2.4H2O																
MGCL2.6H2O																
[redacted]																
MGCLOH																
MGCO3.3H2O																
MGNO32.2H2O																
MGNO32.6H2O																
MGNO32																
MGSO4.1H2O																
MGSO4.6H2O																
MGSO4.7H2O																
MGSO4OH.0.5H2O																
MGSO4OH	1.43E-04					1.33E-04					1.33E-04					
NA2CO3.10H2O																
NA2CO3.1H2O																
NA2CO3.7H2O																
NA2CO3																
NA2SIO3.5H2O																
NA2SIO3.6H2O																
NA2SIO3.9H2O																
NA2SIO3			0.002424					0.001132						6.51E-04		
NA2SO4.10H2O																
[redacted]																
NAALCO3OH2																
NAALO22.2.5H2O	5.99E-09					1.62E-09					3.85E-09					
NAALO2			1.83E-06					1.82E-06						1.81E-06		
[redacted]																
NAHSO4																
NAOH.1H2O																
NAOH																
Total g/hr	1000.82	0.032278	20.2009	0.343462	980.304	1001.37	2.42E-06	20.2645	0.299922	980.803	1001.08	2.07E-06	1.45292	20.264	0.300206	981.971
Volume, m3/hr	0.001003	1.19E-08	2.07E-05	1.34E-07	2.34446	0.001004	9.92E-13	2.07E-05	1.16E-07	2.34402	0.001003	8.49E-13	8.19E-04	2.07E-05	1.16E-07	2.34205
Enthalpy, cal/hr	-3.79E+06	-92.8745	-74833.2	-1035.67	-3.12E+06	-3.79E+06	-0.009597	-75028.3	-889.071	-3.12E+06	-3.79E+06	-0.008215	-3125.92	-75026.3	-890.45	-3.12E+06
Density, g/m3	9.97E+05	2.71E+06	9.76E+05	2.56E+06	418.136	9.98E+05	2.44E+06	9.77E+05	2.59E+06	418.428	9.98E+05	2.44E+06	1774.39	9.77E+05	2.59E+06	419.279
Vapor fraction					1					1			1			1
Solid fraction		1		1			1		1			1			1	
Organic fraction																
Osmotic Pres, atm	0.308679		8.46119			0.808665		8.74496			1.11085			8.73		
Redox Pot, volts	0.385671		0.259826			0.484191		0.284496			0.498511			0.301811		
E-Con, 1/ohm-cm	8.80E-04		0.043707			9.31E-04		0.04767			9.31E-04			0.047688		
E-Con, cm2/ohm-mol	77.6969		131.124			29.8003		36.7414			12.2432			13.7662		
Abs Visc, cP	0.89396		0.324818			0.894302		0.328721			0.894302			0.328741		
Rel Visc	1.00364		1.03374			1.00402		1.04816			1.00402			1.04622		
Ionic Strength	0.01227		0.238899			0.013169		0.298902			0.013171			0.298805		

J. Yang 2/14/02

04/23/01

File: Lb_Waters.xls
Perm-3: Reconciled 04/21/01, Note Book Page 83
Additional: SiO2 75 mg, AlCl3 3.67E-8 molal, 9.92e-7 mg/L for Al

	Case 1	Input CO2 =		0 (molal) =		0 (mg)	Case 2	Input CO2 =		0.02 (molal) =		880 (mg)	Case 3	Input CO2 =		0.065 (molal) =		2860 (mg)
					logPCo2=	-4.569272					logPCo2=	-3.565348					logPCo2=	-3.075684
Stream	LB_PM_3	LB_PM_3		LB_PM_3_	LB_PM_3_	LB_PM_3_out	LB_PM_3	LB_PM_3		LB_PM_3_	LB_PM_3_	LB_PM_3_out	LB_PM_3	LB_PM_3	LB_PM_3	LB_PM_3_	LB_PM_3_	LB_PM_3_out
Phase	Aqueous	Solid		Aqueous	Solid	Vapor	Aqueous	Solid		Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	25	25		90	90	90	25	25		90	90	90	25	25	25	90	90	90
Pressure, atm	1	1		0.68698	0.68698	0.68698	1	1		0.687125	0.687125	0.687125	1	1	1	0.687703	0.687703	0.687703
pH	7.36867			7.93384			5.4655			7.56561			5.25615			7.32196		
Total mol/hr	55.5203	1.96E-04		1.10917	0.003278	54.4101	55.5203	2.92E-08		1.11013	0.002968	54.4099	55.4866	2.07E-08	0.033618	1.11014	0.002979	54.4099
Flow Units	molality	molality		molality	molality	molality	molality	molality		molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087			55.5087		0.999961	55.5087			55.5087		0.999604	55.5087		0.031772	55.5087		0.998778
CO2	0.00224			3.03E-07		3.92E-05	0.022354			3.03E-06		3.96E-04	0.034767		0.968228	9.36E-06		0.001222
H2SO4						2.73E-29						2.76E-28			2.18E-28			8.51E-28
H2						3.26E-22						3.26E-22			2.51E-28			3.26E-22
HCL						3.53E-13				7.42E-14		8.19E-13			1.10E-14	1.30E-13		1.43E-12
HNO3	3.04E-13			1.34E-11		3.14E-14	2.43E-11			3.13E-11		7.38E-14	3.93E-11		1.92E-15	5.49E-11		1.29E-13
O2						1.63E-22						1.63E-22			1.24E-28			1.63E-22
SICL4	6.65E-06						8.38E-08						5.17E-08					
SO3																		
[redacted]																		
ALOH3	2.40E-09	9.41E-05		7.50E-09			2.40E-09	1		1.68E-08			2.40E-09	1		2.91E-08		
KCL	5.26E-09			2.89E-05			5.23E-09			2.70E-05			5.22E-09			2.69E-05		
KHSO4				8.33E-12			8.76E-13			3.38E-11			1.42E-12			5.96E-11		
MGCO3	1.44E-04			4.81E-07			1.55E-04			3.65E-06			1.55E-04			3.67E-06		
MGH2SIO4	8.69E-10			1.31E-05			1.34E-13			9.83E-06						3.20E-06		
[redacted]																		
NAHCO3	2.30E-06			1.77E-06			2.66E-06			7.34E-06			2.67E-06			1.29E-05		
NAHSIO3	6.09E-07			8.24E-04			7.65E-09			3.38E-04			4.73E-09			1.93E-04		
[redacted]																		
CAH2SIO4	2.81E-10			4.95E-06						4.86E-07						1.58E-07		
[redacted]																		
CACO3	4.03E-05	0.999906		5.08E-06	0.285735		1.09E-04			5.03E-06	0.511926		1.08E-04			5.03E-06	0.511528	
[redacted]																		
ALCL3																		
CAOH2				9.49E-04														
H2CO3																		
MGOH2					0.172573					4.31E-04						2.47E-04		
[redacted]																		
NA6SO42CO3	4.49E-04			2.16E-05			4.49E-04			1.00E-04			4.49E-04			1.76E-04		
AL2SO43.16H2O																		
AL2SO43.6H2O																		
AL2SO43																		
ALCL3.6H2O																		
ALNO33.6H2O																		
ALNO33.8H2O																		
ALNO33.9H2O																		
ALOOH																		
CA2CL2O.2H2O	6.11E-04						7.17E-04						7.19E-04					
CACL2.1H2O																		
CACL2.2H2O																		
CACL2.4H2O																		
CACL2.6H2O																		
[redacted]																		
CANO32.3H2O																		
CANO32.4H2O																		
CANO32	8.07E-05						8.07E-05						8.07E-05					
CASO4.2H2O					0.264676						0.169276						0.167137	
K1ALSO4.12H2O																		
K1ALSO4																		
K2CO3.1.5H2O																		
K2CO3																		
K2SO4.1H2O																		
K2SO4																		
K3NASO42				0.001528														
KHCO3																		
KMGCL3.2H2O																		
KNO3																		
KOH.1H2O																		
KOH.2H2O																		
KOH																		
MGCL2.2H2O																		
MGCL2.4H2O																		
MGCL2.6H2O																		
[redacted]																		
MGCLOH																		
MGCO3.3H2O																		
MGNO32.2H2O																		
MGNO32.6H2O																		
MGNO32																		
MGSO4.1H2O																		
MGSO4.6H2O																		
MGSO4.7H2O																		
MGSO4OH.0.5H2O																		
MGSO4OH	2.15E-04						2.08E-04						2.08E-04					
NA2CO3.10H2O																		
NA2CO3.1H2O																		
NA2CO3.7H2O																		
NA2CO3																		
NA2SIO3.5H2O																		
NA2SIO3.6H2O																		
NA2SIO3.9H2O																		
NA2SIO3				0.0024						0.001053						6.01E-04		
NA2SO4.10H2O																		
[redacted]																		
NAALCO3OH2																		
NAALO22.2.5H2O	7.91E-09						2.55E-09						6.79E-09					
NAALO2				1.83E-06						1.82E-06						1.81E-06		
[redacted]																		
NAHSO4																		
NAOH.1H2O																		
NAOH																		
Total g/hr	1000.79	0.019644		20.2124	0.330699	980.27	1001.33	2.28E-06		20.2662	0.295456	980.771	1001.05	1.61E-08	1.45177	20.2656	0.295776	981.938
Volume, m3/hr	0.001003	7.25E-09		2.07E-05	1.31E-07	2.34562	0.001004	9.33E-13		2.07E-05	1.15E-07	2.34512	0.001003	6.61E-13	8.18E-04	2.07E-05	1.16E-07	2.34315
Enthalpy, cal/hr	-3.79E+06	-56.5226		-74822.8	-1005.24	-3.12E+06	-3.79E+06	-0.009024		-74986.9	-880.473	-3.12E+06	-3.79E+06	-0.006396	-3123.44	-74986.9	-881.916	-3.12E+06
Density, g/m3	9.97E+05	2.71E+06		9.76E+05	2.52E+06	417.914	9.98E+05	2.44E+06		9.78E+05	2.56E+06	418.217	9.98E+05	2.44E+06	1774.39	9.78E+05	2.56E+06	419.068
Vapor fraction						1						1			1			1
Solid fraction		1			1			1			1			1			1	
Organic fraction																		
Osmotic Pres, atm	0.305687			9.26932			0.800989			9.50789			1.10381			9.49207		
Redox Pot, volts	0.378475			0.260321			0.491068			0.286856			0.50541			0.304412		
E-Con, 1/ohm-cm	8.95E-04			0.047604			9.27E-04			0.051065			9.27E-04			0.051072		
E-Con, cm2/ohm-mol	83.5369			154.91			30.2655			40.1411			12.2899			14.8477		
Abs Visc, cP	0.893711			0.325484			0.893923			0.329012			0.893923			0.329026		
Rel Visc	1.00336			1.03586			1.0036			1.04709			1.0036			1.04713		
Ionic Strength	0.012273			0.26022			0.012827			0.313946			0.01283			0.313758		

04/23/01

File: Lb_Waters.xls
Infiltration: Reconciled 04/21/01, Note Book Page 84
Additional: SiO2 70.5 mg, AlCl3 9.78E-9 molal, 2.64e-6 mg/L for Al

	Case 1	Input CO2 =		0 (molal) =		0 (mg)	Case 2	Input CO2 =		0.02 (molal) =		880 (mg)	Case 3	Input CO2 =		0.065 (molal) =		2860 (mg)
					logPCo2=	-4.53383					logPCo2=	-3.56129					logPCo2=	-3.07431
Stream	LB_Infil	LB_Infil		LB_Infil_Ou	LB_Infil_Ou	LB_Infil_Out	LB_Infil	LB_Infil		LB_Infil_Ou	LB_Infil_Ou	LB_Infil_Out	LB_Infil	LB_Infil	LB_Infil	LB_Infil_Ou	LB_Infil_Ou	LB_Infil_Out
Phase	Aqueous	Solid		Aqueous	Solid	Vapor	Aqueous	Solid		Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	25	25		90	90	90	25	25		90	90	90	25	25	25	90	90	90
Pressure, atm	1	1		0.687132	0.687132	0.687132	1	1		0.687271	0.687271	0.687271	1	1	1	0.68785	0.68785	0.68785
pH	7.31516			7.93385			5.51681			7.57673			5.30746			7.33443		
Total mol/hr	55.5207	2.50E-04		1.10928	0.003336	54.4106	55.5207	9.71E-07		1.11034	0.003014	54.4103	55.4871	9.64E-07	0.033822	1.11036	0.003025	54.4103
Flow Units	molality	molality		molality	molality	molality	molality	molality		molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087			55.5087		0.999957	55.5087			55.5087		0.9996	55.5087		0.031772	55.5087		0.998775
CO2	0.002503			3.29E-07		4.26E-05	0.022641			3.06E-06		4.00E-04	0.035049		0.968228	9.40E-06		0.001225
H2SO4						2.97E-29						2.78E-28			1.65E-28			8.53E-28
H2						3.26E-22						3.26E-22			2.51E-28			3.26E-22
HCL						3.39E-13				6.95E-14		7.66E-13			9.39E-15	1.21E-13		1.34E-12
HNO3	2.24E-13			8.79E-12		2.05E-14	1.40E-11			1.99E-11		4.68E-14	2.27E-11		1.11E-15	3.48E-11		8.17E-14
O2						1.63E-22						1.63E-22			1.24E-28			1.63E-22
SICL4	5.53E-06						8.87E-08						5.48E-08					
SO3																		
[redacted]																		
ALOH3	2.40E-09	3.84E-03		8.26E-08	0.000173		2.40E-09	1		8.19E-08	0.000264		2.40E-09	1		8.19E-08	0.000288	
KCL	4.49E-09			2.48E-05			4.46E-09			2.31E-05			4.45E-09			2.30E-05		
KHSO4				8.07E-12			6.65E-13			3.12E-11			1.08E-12			5.47E-11		
MGCO3	1.97E-04			5.22E-07			2.10E-04			3.77E-06			2.10E-04			3.79E-06		
MGH2SIO4	6.21E-10			1.31E-05			1.55E-13			1.01E-05			5.9E-14			3.30E-06		
[redacted]																		
NAHCO3	2.52E-06			1.91E-06			2.96E-06			7.54E-06			2.96E-06			1.32E-05		
NAHSIO3	5.01E-07			8.18E-04			8.00E-09			3.44E-04			4.94E-09			1.97E-04		
[redacted]																		
CAH2SIO4	2.11E-10			4.57E-06			5.9E-14			4.83E-07						1.57E-07		
[redacted]																		
CACO3	6.78E-05	0.99816		5.08E-06	0.343875		1.64E-04			5.04E-06	0.568507		1.63E-04			5.04E-06	0.567874	
[redacted]																		
ALCL3																		
CAOH2				9.66E-04														
H2CO3																		
MGOH2					0.164707					4.48E-04						2.56E-04		
[redacted]																		
NA6SO42CO3	4.44E-04			2.32E-05			4.44E-04			1.03E-04			4.44E-04			1.80E-04		
AL2SO43.16H2O																		
AL2SO43.6H2O																		
AL2SO43																		
ALCL3.6H2O																		
ALNO33.6H2O																		
ALNO33.8H2O																		
ALNO33.9H2O																		
ALOOH																		
CA2CL2O.2H2O	6.88E-04						8.22E-04						8.23E-04					
CACL2.1H2O																		
CACL2.2H2O																		
CACL2.4H2O																		
CACL2.6H2O																		
[redacted]																		
CANO32.3H2O																		
CANO32.4H2O																		
CANO32	5.24E-05						5.24E-05						5.24E-05					
CASO4.2H2O					0.24161						0.142503						0.140427	
K1ALSO4.12H2O																		
K1ALSO4																		
K2CO3.1.5H2O																		
K2CO3																		
K2SO4.1H2O																		
K2SO4																		
K3NASO42				0.001122														
KHCO3																		
KMGCL3.2H2O																		
KNO3																		
KOH.1H2O																		
KOH.2H2O																		
KOH																		
MGCL2.2H2O																		
MGCL2.4H2O																		
MGCL2.6H2O																		
[redacted]																		
MGCLOH																		
MGCO3.3H2O																		
MGNO32.2H2O																		
MGNO32.6H2O																		
MGNO32																		
MGSO4.1H2O																		
MGSO4.6H2O																		
MGSO4.7H2O																		
MGSO4OH.0.5H2O																		
MGSO4OH	1.87E-04						1.78E-04						1.78E-04					
NA2CO3.10H2O																		
NA2CO3.1H2O																		
NA2CO3.7H2O																		
NA2CO3																		
NA2SIO3.5H2O																		
NA2SIO3.6H2O																		
NA2SIO3.9H2O																		
NA2SIO3				0.002395						0.001079						6.17E-04		
NA2SO4.10H2O																		
[redacted]																		
NAALCO3OH2																		
NAALO22.2.5H2O	7.00E-09						2.07E-09						5.25E-09					
NAALO2				2.01E-05						9.11E-06						5.21E-06		
[redacted]																		
NAHSO4																		
NAOH.1H2O																		
NAOH																		
Total g/hr	1000.8	0.025039		20.2064	0.33576	980.283	1001.34	7.58E-05		20.2634	0.297805	980.783	1001.06	7.52E-05	1.45195	20.2629	0.298116	981.951
Volume, m3/hr	0.001003	9.24E-09		2.07E-05	1.32E-07	2.34512	0.001004	3.10E-11		2.07E-05	1.16E-07	2.34464	0.001003	3.08E-11	8.18E-04	2.07E-05	1.16E-07	2.34266
Enthalpy, cal/hr	-3.79E+06	-72.1258		-74824.6	-1016.45	-3.12E+06	-3.79E+06	-0.30022		-75000.3	-884.884	-3.12E+06	-3.79E+06	-0.29801	-3123.83	-74998.3	-886.319	-3.12E+06
Density, g/m3	9.97E+05	2.71E+06		9.76E+05	2.54E+06	418.009	9.98E+05	2.44E+06		9.78E+05	2.58E+06	418.309	9.98E+05	2.44E+06	1774.39	9.78E+05	2.58E+06	419.16
Vapor fraction						1						1			1			1
Solid fraction		1			1			1			1			1			1	
Organic fraction																		
Osmotic Pres, atm	0.306069			8.92167			0.803335			9.17326			1.10605			9.15776		
Redox Pot, volts	0.381641			0.260318			0.488032			0.286052			0.502375			0.303512		
E-Con, 1/ohm-cm	8.88E-04			0.045894			9.28E-04			0.049533			9.28E-04			0.049545		
E-Con, cm2/ohm-mol	81.003			144.714			30.0512			38.6464			12.2611			14.3649		
Abs Visc, cP	0.89381			0.325192			0.894077			0.32882			0.894077			0.328834		
Rel Visc	1.00347			1.03493			1.00377			1.04647			1.00377			1.04652		
Ionic Strength	0.012262			0.250806			0.012961			0.306395			0.012964			0.306238		

04/23/01

Main species in aqueous

File: Lb_Waters_Main_Species.xls

	Case 1			Case 2			Case 3		
Phase	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	90	90	90	90	90	90	90	90	90
Pressure, atm *	0.68715	0.68715	0.68715	0.687288	0.687288	0.687288	0.687867	0.687867	0.687867
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality
Pore Water		logPCo2=	-4.53114		logPCo2=	-3.561029		logPCo2=	-3.074218
H2O	55.5087		0.999957	55.5087		0.9996	55.5087		0.998775
CO2	3.31E-07		4.28E-05	3.06E-06		4.00E-04	9.40E-06		0.001225
CASO4 ✓	0.004021			0.003989			0.003989		
MGSO4 ✓	6.55E-04			0.004769			0.004792		
NANO3 ✓	0.005269			0.00526			0.005256		
H2SIO3	0.00343			0.003401			0.003402		
SIO2	0.010514	0.248823		0.010429	0.288313		0.010429	0.29103	
KMGCL3	0.006803			0.010244			0.010236		
NA3HSO42	0.00424			0.001998			0.001267		
CACL2	0.023106			0.01473			0.014648		
MGCL2 ✓				0.019626			0.019778		
NA2SIO3	0.002407			0.001087			6.22E-04		
NA2SO4	0.004931			0.026629			0.0281		
NACL	0.099242			0.066133			0.065883		
Perm_2		logPCo2=	-4.53114		logPCo2=	-3.561029		logPCo2=	-3.074218
H2O	55.5087		0.999957	55.5087		0.9996	55.5087		0.998775
CO2	3.31E-07		4.28E-05	3.06E-06		4.00E-04	9.40E-06		0.001225
CASO4	0.004021			0.003989			0.003989		
MGSO4	6.55E-04			0.004769			0.004792		
NANO3	0.005269			0.00526			0.005256		
H2SIO3	0.00343			0.003401			0.003402		
SIO2	0.010514	0.248823		0.010429	0.288313		0.010429	0.29103	
KMGCL3	0.006803			0.010244			0.010236		
NA3HSO42	0.00424			0.001998			0.001267		
CACL2	0.023106			0.01473			0.014648		
MGCL2				0.019626			0.019778		
NA2SIO3	0.002407			0.001087			6.22E-04		
NA2SO4	0.004931			0.026629			0.0281		
NACL	0.099242			0.066133			0.065883		
Perm_3		logPCo2=	-4.569164		logPCo2=	-3.565243		logPCo2=	-3.075581
H2O	55.5087		0.999961	55.5087		0.999604	55.5087		0.998778
CO2	3.03E-07		3.92E-05	3.03E-06		3.96E-04	9.36E-06		0.001222
CASO4	0.004016			0.003986			0.003986		
MGSO4	6.00E-04			0.004552			0.004574		
NANO3	0.008103			0.008093			0.008086		
H2SIO3	0.003424			0.003396			0.003396		
SIO2	0.010497	0.277016		0.010414	0.318799		0.010414	0.321335	
KMGCL3	0.006952			0.011524			0.011514		
NA3HSO42	0.004223			0.001934			0.001224		
CACL2	0.026033			0.01603			0.01594		
MGCL2				0.019404			0.019552		
NA2SIO3	0.0024			0.001053			6.01E-04		
NA2SO4	0.003036			0.024872			0.026294		
NACL	0.101354			0.068628			0.068398		
Infiltration		logPCo2=	-4.533814		logPCo2=	-3.561279		logPCo2=	-3.074296
H2O	55.5087		0.999957	55.5087		0.9996	55.5087		0.998775
CO2	3.29E-07		4.26E-05	3.06E-06		4.00E-04	9.40E-06		0.001225
CASO4	0.00402			0.003989			0.003989		
MGSO4	6.51E-04			0.004704			0.004727		
NANO3	0.005266			0.005259			0.005255		
H2SIO3	0.003429			0.003401			0.003401		
SIO2	0.010511	0.249636		0.010427	0.288726		0.010427	0.291412	
KMGCL3	0.006886			0.010242			0.010233		
NA3HSO42	0.004254			0.001997			0.001264		
CACL2	0.02354			0.014961			0.014876		
MGCL2				0.01968			0.019835		
NA2SIO3	0.002395			0.001079			6.17E-04		
NA2SO4	0.004723			0.026145			0.02762		
NACL	0.099566			0.067085			0.066832		

* Pressure slightly different for different water

[illegible signature] 7/11/02

Note:

In the calculations in Pages 87 – 90 I have used mMolal as molal for $AlCl_3$; the concentration should be 1000 lower than what was used for $AlCl_3$.

As the species in page 90 does not include Al. the calculation is not changing the main species. (it was low).

Recommendations for OLI to change (modify) the model Database. see page 92.

L.Y. 04/24/01

Lietai Yang

From: Lietai Yang [ltyang@gargol.cnwra.swri.edu]
Sent: Tuesday, April 24, 2001 10:59 AM
To: 'Support@olisystems.com'
Cc: Roberto Pabalan (rpabalan); Lauren Browning (lbrowning)
Subject: Water Composition

Attention: M. Rafel

Dear Marshall,

The water containing the following species (measured or calculated at about 90oC and 1 atm) is what we want to evaporate. In our preliminary calculations using OLI, temperatures need to be as high as 130oC at 1 atm or 85oC at 40% relative humidity to completely dry this water. Very often, we are outside of the OLI limits (the ionic strength > 30 molal and the water faction < 0.65). Therefore, we would like OLI to conduct Data Servicing work for the pertinent components so that we can have a reasonable confidence in using the OLI outputs in our analysis.

In our telephone conversation more than a month ago, you have given me a verbal estimate on the cost to do a three salt data servicing. Can you expand the work and cover more salts so that we can better simulate our system? What kind of options are there for our system? Would you please provide a quote for each of the option so that we can make a decision as which option to take?

Also, we have a deadline of late July for this work.

Thanks

Lietai

Concentration for aqueous solution	
Major components	
Component	Molal
NO3-	0.15
Cl-	0.2 to 1.5
SO4--	0 to 0.2
F-	0 to 0.12
Na+	1 to 2.0
K+	0.01 to 0.15
Ca ++	0 to 0.15
SiO2 (aq)	0 to 0.15
Mg++	0 to 0.04
CO2, atm	10^-2.8 to 10^-5
Li+	0 to 7e-3
Ref: Presentation by E. Hardin, DC	
In-Drift Geochemistry Environment	
And NoteBook #430 page 90	

DOE/NRC Tech Exchange, Jan. 9 to 12, 2001
L.Y. 04/24/01

— Continued from page 67.

Calculation for Lead speciation

~~objective see page 58.~~ 04/30/01 L.Y.

File: Darrell-Pb-chem-2.XLS

Results from ESP V6.2e, April 30, 2001
Pb MW= 207.2 mg (appr. ppn 1 100 1600 2100
mM 0.004826255 0.48262548 7.722007722 10.1351351

Inputs		55.50815	55.50815	55.50815	55.50815	55.509	55.509	55.509	55.509	55.5105	55.5105	55.5105	55.5105
log(free Cl-)		-3.844664	-3.8485995	-3.848814082	-3.847987	-3.0206064	-3.024485477	-3.02469229	-3.02388856	-2.6224133	-2.62621293	-2.62641683	-2.62564581
H2O (mol)		55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)		1.50E-04	**1.50E-04**	**1.50E-04**	**1.50E-04**	1.00E-03	**1.00E-03**	**1.00E-03**	**1.00E-03**	2.50E-03	**2.50E-03**	**2.50E-03**	**2.50E-03**
LiCl (mol)													
HCl (mol)													
PbCl2 (mol)													
Pb(CH3CO2)2 (mol)		0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**0.008**	**0.008**
PbSO4 (mol)													
Total Pb (ppm)		**1653.5323**	**1653.532311**	**1653.532311**	**1653.532311**	**1653.44984**	**1653.449841**	**1653.44984**	**1653.449841**	**1653.301416**	**1653.301416**	**1653.301416**	**1653.301416**
Stream		T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase		Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C		25	80	100	120	25	80	100	120	25	80	100	120
Pressure, atm		1	1	1	2	1	1	1	2	1	1	1	2
pH		6.51158	5.79003	5.61608	5.48511	6.5137	5.79293	5.61932	5.4886	6.5173	5.79784	5.62481	5.49452
Total mol/hr		55.5183	55.5166	55.5155	55.5145	55.5199	55.5183	55.5172	55.5162	55.5229	55.5213	55.5202	55.5192
Flow Units		molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O		55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
ACETACID		1.66E-04	9.40E-04	0.00140563	0.00192277	1.66E-04	9.36E-04	0.00139933	0.00191427	1.65E-04	9.29E-04	0.00138864	0.00189985
ACET2		4.32E-16	6.32E-14	2.08E-13	5.36E-13	4.28E-16	6.27E-14	2.06E-13	5.32E-13	4.22E-16	6.17E-14	2.03E-13	5.24E-13
H2SO4													
HCL		2.32E-17	2.96E-15	1.14E-14	3.48E-14	1.54E-16	1.95E-14	7.49E-14	2.29E-13	3.79E-16	4.79E-14	1.84E-13	5.60E-13
SO3													
LIOH													
NAACET		9.22E-07	1.07E-06	1.17E-06	1.28E-06	6.13E-06	7.14E-06	7.81E-06	8.54E-06	1.53E-05	1.78E-05	1.95E-05	2.13E-05
PBACET2	PbAce2	3.49E-04	8.33E-04	0.00111146	0.00139568	3.45E-04	8.24E-04	0.00109986	0.00138116	3.39E-04	8.09E-04	0.00108061	0.00135724
PBCL2	PbCl20	2.87E-09	4.97E-09	6.06E-09	7.23E-09	1.25E-07	2.16E-07	2.63E-07	3.12E-07	7.60E-07	1.30E-06	1.57E-06	1.86E-06
PBO		1.91E-07	1.66E-06	2.78E-06	4.32E-06	1.90E-07	1.66E-06	2.78E-06	4.31E-06	1.89E-07	1.65E-06	2.77E-06	4.30E-06
LIACET													
OHION		3.74E-08	1.73E-07	2.57E-07	3.69E-07	3.77E-08	1.75E-07	2.61E-07	3.74E-07	3.82E-08	1.78E-07	2.66E-07	3.82E-07
CLION	Cl-	1.43E-04	1.42E-04	1.42E-04	1.42E-04	9.54E-04	9.45E-04	9.45E-04	9.46E-04	0.00238554	0.00236476	0.00236365	0.00236785
HION		3.46E-07	1.83E-06	2.72E-06	3.68E-06	3.46E-07	1.82E-06	2.72E-06	3.67E-06	3.44E-07	1.81E-06	2.70E-06	3.65E-06
HPBO2ION		7.76E-12	1.29E-10	2.48E-10	4.33E-10	7.81E-12	1.30E-10	2.50E-10	4.38E-10	7.88E-12	1.32E-10	2.55E-10	4.46E-10
HSO4ION													
LIION													
LISO4ION													
NAION		1.49E-04	1.49E-04	1.49E-04	1.49E-04	9.94E-04	9.93E-04	9.92E-04	9.92E-04	0.00248513	0.00248263	0.00248099	0.00247919
NASO4ION													
ACETATEION		0.0099323	0.0082469	0.00721832	0.00616983	0.00997328	0.00830005	0.0072746	0.00622659	0.0100423	0.00838921	0.00736876	0.00632124
PBACET3ION	PbAce3-	2.72E-04	4.15E-04	5.50E-04	7.15E-04	2.71E-04	4.13E-04	5.49E-04	7.14E-04	2.68E-04	4.11E-04	5.47E-04	7.13E-04
PBACETION	PbAce+	0.0043886	0.00390429	0.00350446	0.00297384	0.00435497	0.00387139	0.00347473	0.00294903	0.00429805	0.0038159	0.00342464	0.00290716
PBCL3ION	PbCl3-	2.00E-13	3.32E-13	4.23E-13	5.38E-13	5.83E-11	9.62E-11	1.22E-10	1.55E-10	8.84E-10	1.45E-09	1.83E-09	2.32E-09
PBCL4ION	PbCl4--	2.28E-17	2.18E-17	2.58E-17	3.20E-17	4.47E-14	4.24E-14	5.02E-14	6.22E-14	1.72E-12	1.62E-12	1.92E-12	2.37E-12
PBCLION	PbCl+	7.02E-06	8.31E-06	8.37E-06	8.10E-06	4.62E-05	5.46E-05	5.49E-05	5.31E-05	1.13E-04	1.33E-04	1.34E-04	1.29E-04
PBION	Pb++	0.0028181	0.00190104	0.00142172	9.87E-04	0.00281825	0.00190197	0.00142376	9.91E-04	0.00281729	0.00190227	0.00142594	9.95E-04
PBOHION	PbOH+	1.66E-04	9.38E-04	0.00140252	0.00191744	1.66E-04	9.34E-04	0.00139622	0.00190895	1.64E-04	9.27E-04	0.00138553	0.00189452
SO4ION													
PBSO4													
NACL													
LICL													
LI2SO4.1H2O													
LI2SO4													
LIACET.2H2O													
LICL.1H2O													
LICL.2H2O													
LIOH.1H2O													
NA2SO4.10H2O													
NA2SO4													
NA3HSO42													
NAACET.3H2O													
NAHSO4													
NAOH.1H2O													
NAOH													
PBHSO42													
PBOH2													
Total g/hr		1002.46	1002.46	1002.46	1002.46	1002.51	1002.51	1002.51	1002.51	1002.6	1002.6	1002.6	1002.6
Volume, m3/hr		0.0010036	0.00102915	0.00104368	0.00106094	0.00100359	0.00102916	0.00104369	0.00106095	0.00100362	0.00102919	0.00104372	0.00106097
Enthalpy, cal/hr		-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06
Density, g/m3		9.99E+05	9.74E+05	9.61E+05	9.45E+05	9.99E+05	9.74E+05	9.61E+05	9.45E+05	9.99E+05	9.74E+05	9.61E+05	9.45E+05
Vapor fraction													
Solid fraction													
Organic fraction													
Osmotic Pres, atm		0.402713	0.445424	0.452882	0.459635	0.42535	0.470514	0.47853	0.486035	0.470307	0.521914	0.532154	0.542277
Redox Pot, volts													
E-Con, 1/ohm-cm		8.59E-04	0.00138735	0.00124972	0.00127016	9.57E-04	0.00160505	0.00151392	0.00158075	0.00112722	0.00198562	0.00197524	0.00212226
E-Con, cm2/ohm-mol		105.798	171.685	143.491	141.027	106.671	180.222	159.031	161.273	107.742	191.624	180.39	189.399
Abs Visc, cP		0.896588	0.356452	0.283406	0.233459	0.896639	0.356479	0.283421	0.233472	0.896737	0.356534	0.283457	0.233502
Rel Visc		1.00659	1.00641	1.00649	1.00632	1.00665	1.00649	1.00655	1.00637	1.00676	1.00664	1.00667	1.0065
Ionic Strength		0.0131657	0.0107048	0.00933206	0.00801426	0.0140159	0.0115608	0.0101923	0.00887812	0.0155132	0.0130672	0.0117053	0.010397

[signature] 8/14/01

55.514	55.514	55.514	55.514	55.518	55.518	55.518	55.518	55.533	55.533	55.533	55.533	55.568	55.568
-2.24167791	-2.24531613	-2.24552094	-2.2448221	-2.01931139	-2.02279969	-2.0230112	-2.02238247	-1.61990097	-1.62299808	-1.62323696	-1.62279395	-1.23758404	-1.2401479
55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
6.00E-03	**6.00E-03**	**6.00E-03**	**6.00E-03**	1.00E-02	**1.00E-02**	**1.00E-02**	**1.00E-02**	2.50E-02	**2.50E-02**	**2.50E-02**	**2.50E-02**	6.00E-02	**6.00E-02**
0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**
1652.971679	**1652.971679**	**1652.971679**	**1652.971679**	**1652.576168**	**1652.576168**	**1652.576168**	**1652.576168**	**1651.144027**	**1651.144027**	**1651.144027**	**1651.144027**	**1647.779236**	**1647.779236**
T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC
Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
25	80	100	120	25	80	100	120	25	80	100	120	25	80
1	1	1	2	1	1	1	2	1	1	1	2	1	1
6.52519	5.80853	5.63669	5.50736	6.53348	5.81964	5.64902	5.52069	6.55996	5.85451	5.68747	5.56221	6.60647	5.91401
55.5299	55.5283	55.5272	55.5262	55.5379	55.5363	55.5353	55.5343	55.5677	55.5662	55.5651	55.5642	55.6373	55.6357
molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
1.62E-04	9.13E-04	0.00136542	0.00186848	1.59E-04	8.97E-04	0.00134121	0.00183568	1.51E-04	8.46E-04	0.00126472	0.00173189	1.36E-04	7.58E-04
4.10E-16	5.97E-14	1.97E-13	5.07E-13	3.97E-16	5.77E-14	1.90E-13	4.90E-13	3.57E-16	5.14E-14	1.69E-13	4.37E-13	2.93E-16	4.15E-14
8.84E-16	1.11E-13	4.22E-13	1.28E-12	1.43E-15	1.78E-13	6.75E-13	2.04E-12	3.26E-15	3.95E-13	1.48E-12	4.43E-12	6.70E-15	7.82E-13
3.63E-05	4.25E-05	4.65E-05	5.09E-05	6.01E-05	7.04E-05	7.71E-05	8.44E-05	1.47E-04	1.73E-04	1.91E-04	2.09E-04	3.37E-04	4.04E-04
3.26E-04	7.79E-04	0.00104034	0.00130765	3.13E-04	7.48E-04	0.00100015	0.00125851	2.75E-04	6.56E-04	8.82E-04	0.00111425	2.17E-04	5.15E-04
4.11E-06	6.92E-06	8.31E-06	9.75E-06	1.07E-05	1.77E-05	2.11E-05	2.46E-05	5.43E-05	8.65E-05	1.01E-04	1.15E-04	2.21E-04	3.32E-04
1.88E-07	1.64E-06	2.75E-06	4.27E-06	1.86E-07	1.63E-06	2.74E-06	4.25E-06	1.81E-07	1.60E-06	2.70E-06	4.21E-06	1.72E-07	1.54E-06
3.93E-08	1.85E-07	2.77E-07	4.01E-07	4.05E-08	1.92E-07	2.90E-07	4.20E-07	4.43E-08	2.16E-07	3.30E-07	4.84E-07	5.13E-08	2.61E-07
0.00573221	0.00568439	0.00568171	0.00569086	0.00956508	0.00948856	0.00948394	0.00949768	0.0239938	0.0238233	0.0238102	0.0238345	0.057865	0.0575244
3.42E-07	1.79E-06	2.67E-06	3.60E-06	3.38E-07	1.77E-06	2.63E-06	3.54E-06	3.27E-07	1.69E-06	2.50E-06	3.36E-06	3.05E-07	1.54E-06
8.05E-12	1.36E-10	2.64E-10	4.66E-10	8.23E-12	1.41E-10	2.75E-10	4.86E-10	8.80E-12	1.56E-10	3.09E-10	5.55E-10	9.84E-12	1.84E-10
0.00596461	0.00595857	0.00595461	0.00595029	0.00994151	0.00993134	0.00992467	0.00991744	0.0248575	0.0248311	0.024814	0.0247953	0.059672	0.0596065
0.0101893	0.00857838	0.00756793	0.00652081	0.0103385	0.00876975	0.00776914	0.00672219	0.0107813	0.00933947	0.00836998	0.00732612	0.0114483	0.0102112
2.62E-04	4.05E-04	5.42E-04	7.10E-04	2.56E-04	3.98E-04	5.36E-04	7.06E-04	2.36E-04	3.75E-04	5.13E-04	6.87E-04	2.01E-04	3.28E-04
0.0041755	0.00369698	0.00331745	0.00281738	0.00404944	0.00357527	0.00320787	0.00272538	0.00366398	0.00320575	0.0028757	0.00244587	0.00304314	0.00261732
1.15E-08	1.85E-08	2.33E-08	2.92E-08	4.98E-08	7.93E-08	9.88E-08	1.23E-07	6.38E-07	9.75E-07	1.19E-06	1.45E-06	6.32E-06	9.08E-06
5.49E-11	5.14E-11	6.04E-11	7.42E-11	4.08E-10	3.78E-10	4.42E-10	5.41E-10	1.41E-08	1.27E-08	1.47E-08	1.77E-08	3.90E-07	3.26E-07
2.61E-04	3.03E-04	3.03E-04	2.91E-04	4.15E-04	4.77E-04	4.75E-04	4.55E-04	9.00E-04	0.00100495	9.88E-04	9.35E-04	0.00168117	0.00179408
0.00281045	0.0018981	0.00142593	9.99E-04	0.00279706	0.00188783	0.00142032	9.98E-04	0.00272003	0.00182573	0.0013763	9.72E-04	0.00249431	0.00164909
1.62E-04	9.12E-04	0.0013623	0.00186313	1.59E-04	8.95E-04	0.00133806	0.0018303	1.51E-04	8.44E-04	0.00126149	0.00172636	1.36E-04	7.56E-04
1002.8	1002.8	1002.8	1002.8	1003.04	1003.04	1003.04	1003.04	1003.91	1003.91	1003.91	1003.91	1005.96	1005.96
0.00100367	0.00102925	0.00104378	0.00106102	0.00100374	0.00102932	0.00104385	0.00106108	0.00100399	0.0010296	0.00104411	0.00106132	0.00100459	0.00103026
-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.70E+06	-3.80E+06	-3.74E+06
9.99E+05	9.74E+05	9.61E+05	9.45E+05	9.99E+05	9.74E+05	9.61E+05	9.45E+05	1.00E+06	9.75E+05	9.62E+05	9.46E+05	1.00E+06	9.76E+05
0.591689	0.663697	0.681658	0.699989	0.746739	0.845622	0.873428	0.901401	1.3861	1.58986	1.65239	1.71151	2.95386	3.39164
0.00151937	0.00285785	0.00303123	0.00336031	0.00195976	0.00383421	0.00421174	0.00474246	0.00356306	0.00736989	0.00847795	0.00972613	0.00713674	0.0151858
108.925	207.7	212.159	232.042	109.283	217.334	232.652	260.181	108.403	228.893	261.535	301.261	105.434	229.617
0.896983	0.356674	0.283563	0.233593	0.897279	0.356846	0.2837	0.233711	0.898428	0.357513	0.284245	0.234174	0.901114	0.359066
1.00703	1.00704	1.00705	1.0069	1.00736	1.00752	1.00754	1.0074	1.00865	1.0094	1.00947	1.0094	1.01167	1.01379
0.0189942	0.0165659	0.0152175	0.0139207	0.0229568	0.0205447	0.0192095	0.0179241	0.0377322	0.035365	0.0340709	0.0328215	0.0720162	0.0697226

04/30/01

55.568	55.568	55.608	55.608	55.608	55.608	55.758	55.758	55.758	55.758	56.108	56.108	56.108	56.108	56.108
-1.24043187	-1.24021208	-1.01425342	-1.01642242	-1.01672427	-1.0166322	-0.61351174	-0.61476205	-0.61505729	-0.61516291	-0.2318527		-0.23140111	-0.23160612	-0.23181567
55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
6.00E-02	**6.00E-02**	1.00E-01	**1.00E-01**	**1.00E-01**	**1.00E-01**	2.50E-01	**2.50E-01**	**2.50E-01**	**2.50E-01**	6.00E-01	**6.00E-01**	**6.00E-01**	**6.00E-01**	**6.00E-01**
0.008	**0.008**	0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**0.008**	**0.008**	0.008	**0.008**	**8.00E-03**	**8.00E-03**	**8.00E-03**
1647.779236	**1647.779236**	**1643.955172**	**1643.955172**	**1643.955172**	**1643.955172**	**1629.795686**	**1629.795686**	**1629.795686**	**1629.795686**	**1598.42626**		**1.60E+03**	**1.60E+03**	**1.60E+03**
T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC	T25oC	T25oC	T80oC	T100oC	T120oC
Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Solid	Aqueous	Aqueous	Aqueous
100	120	25	80	100	120	25	80	100	120	25	25	80	100	120
1	2	1	1	1	2	1	1	1	2	1	1	1	1	2
5.75241	5.63199	6.64697	5.96425	5.80664	5.68982	6.75453	6.09086	5.94094	5.83106	6.9928		6.27985	6.13613	6.03258
55.6348	55.6337	55.7167	55.7151	55.7142	55.7132	56.0141	56.0126	56.0118	56.0109	56.7054	0.00177432	56.7069	56.7061	56.7051
molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087		55.5087	55.5087	55.5087
0.00113233	0.00155223	1.24E-04	6.82E-04	0.00101984	0.00139969	9.28E-05	5.00E-04	7.46E-04	0.00102774	4.77E-05		2.85E-04	4.22E-04	5.80E-04
1.37E-13	3.53E-13	2.43E-16	3.39E-14	1.12E-13	2.90E-13	1.41E-16	1.87E-14	6.16E-14	1.61E-13	3.98E-17		6.50E-15	2.11E-14	5.47E-14
2.89E-12	8.48E-12	9.79E-15	1.11E-12	4.05E-12	1.18E-11	1.74E-14	1.88E-12	6.68E-12	1.90E-11	2.14E-14		2.55E-12	8.88E-12	2.47E-11
4.48E-04	4.96E-04	5.42E-04	6.54E-04	7.30E-04	8.13E-04	0.00121591	0.0014784	0.00166875	0.00188166	0.00244844		0.00290199	0.00328114	0.00372185
6.97E-04	8.89E-04	1.74E-04	4.09E-04	5.57E-04	7.17E-04	9.06E-05	2.05E-04	2.82E-04	3.69E-04	2.17E-05		5.86E-05	7.94E-05	1.04E-04
3.78E-04	4.20E-04	4.59E-04	6.56E-04	7.34E-04	8.02E-04	0.00135117	0.00174409	0.00188109	0.00198776	0.00182986	1	0.0028301	0.00293603	0.00298835
2.62E-06	4.12E-06	1.65E-07	1.49E-06	2.54E-06	4.02E-06	1.44E-07	1.30E-06	2.26E-06	3.61E-06	1.12E-07		9.92E-07	1.72E-06	2.76E-06
4.06E-07	6.07E-07	5.79E-08	3.04E-07	4.80E-07	7.27E-07	7.76E-08	4.38E-07	7.11E-07	1.11E-06	1.36E-07		7.16E-07	1.20E-06	1.92E-06
0.0574868	0.0575159	0.0967713	0.0962892	0.0962223	0.0962427	0.243494	0.242794	0.242629	0.24257	0.586337		0.586947	0.58667	0.586387
2.26E-06	3.02E-06	2.85E-07	1.42E-06	2.06E-06	2.74E-06	2.30E-07	1.11E-06	1.60E-06	2.11E-06	1.32E-07		7.25E-07	1.04E-06	1.35E-06
3.73E-10	6.85E-10	1.08E-11	2.08E-10	4.31E-10	8.05E-10	1.32E-11	2.72E-10	5.82E-10	1.13E-09	2.00E-11		3.64E-10	7.96E-10	1.58E-09
0.0595626	0.0595154	0.0994738	0.0993631	0.0992875	0.0992056	0.248823	0.248563	0.248374	0.248162	0.597645		0.597195	0.596817	0.596379
0.00930329	0.00828086	0.011917	0.0108379	0.00999034	0.00900275	0.0126725	0.0118794	0.0111854	0.0103284	0.0129151		0.0120763	0.0114945	0.0107849
4.59E-04	6.31E-04	1.71E-04	2.82E-04	4.02E-04	5.65E-04	1.00E-04	1.65E-04	2.42E-04	3.57E-04	2.76E-05		5.41E-05	7.98E-05	1.20E-04
0.00234764	0.00200115	0.00255975	0.00216546	0.00194239	0.00165984	0.00153875	0.00124161	0.00111184	9.57E-04	4.65E-04		4.60E-04	4.07E-04	3.48E-04
1.08E-05	1.28E-05	2.21E-05	3.03E-05	3.54E-05	4.13E-05	1.68E-04	2.09E-04	2.36E-04	2.65E-04	5.86E-04		8.77E-04	9.51E-04	0.00103115
3.69E-07	4.36E-07	2.45E-06	2.02E-06	2.25E-06	2.62E-06	5.89E-05	4.41E-05	4.75E-05	5.38E-05	6.71E-04		6.00E-04	6.18E-04	6.69E-04
0.00173455	0.00161501	0.00224971	0.0023163	0.00221224	0.00203767	0.00310356	0.00295548	0.00275416	0.00248699	0.0021038		0.00246028	0.00223072	0.00196569
0.00124259	8.81E-04	0.00223941	0.00145833	0.00109712	7.79E-04	0.00149695	9.38E-04	7.02E-04	5.00E-04	4.73E-04		3.78E-04	2.79E-04	1.98E-04
0.00112893	0.00154641	1.24E-04	6.80E-04	0.00101633	0.00139367	9.27E-05	4.98E-04	7.43E-04	0.00102152	4.75E-05		2.83E-04	4.19E-04	5.74E-04
1005.96	1005.96	1008.3	1008.3	1008.3	1008.3	1017.06	1017.06	1017.06	1017.06	1037.02	0.493448	1037.52	1037.52	1037.52
0.00104473	0.00106189	0.00100529	0.00103103	0.00104547	0.00106257	0.00100797	0.00103404	0.00104837	0.00106525	0.00101444	8.44E-08	0.00104149	0.00105563	0.00107205
-3.72E+06	-3.70E+06	-3.80E+06	-3.75E+06	-3.73E+06	-3.71E+06	-3.82E+06	-3.76E+06	-3.74E+06	-3.72E+06	-3.85E+06	-152.412	-3.80E+06	-3.78E+06	-3.76E+06
9.63E+05	9.47E+05	1.00E+06	9.78E+05	9.64E+05	9.49E+05	1.01E+06	9.84E+05	9.70E+05	9.55E+05	1.02E+06	5.85E+06	9.96E+05	9.83E+05	9.68E+05
3.52404	3.6422	4.75906	5.45216	5.65822	5.83802	11.5272	13.1433	13.6152	14.0196	27.5054	1	31.3035	32.4057	33.3544
0.01788	0.020672	0.0110574	0.0236996	0.0280953	0.0325305	0.0248832	0.0535019	0.0637591	0.0738929	0.05392		0.115853	0.138556	0.160396
271.679	317.528	102.925	225.991	270.264	317.061	97.2154	214.353	258.582	304.215	89.9645		198.437	240.454	282.621
0.285525	0.235253	0.904161	0.360818	0.286969	0.236464	0.915683	0.367315	0.292311	0.240932	0.944055		0.382654	0.304848	0.251379
1.01402	1.01405	1.01509	1.01874	1.01915	1.01927	1.02803	1.03708	1.03812	1.03853	1.05988		1.08039	1.08264	1.08356
0.0685041	0.0673237	0.111128	0.108904	0.107754	0.106639	0.258109	0.256118	0.255138	0.254183	0.602353		0.602131	0.601331	0.60053

56.508	56.508	56.508	56.508	56.508	58.008	58.008	58.008	58.008	58.008	61.508	61.508	61.508	61.508	61.508
-0.00859005		-0.00825928	-0.0083456	-0.00849792	0.392670578		0.392848139	0.392867473	0.39286923	0.775903034		0.775911765	0.775913948	0.775916858
55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	2.50E+00	2.50E+00	2.50E+00	2.50E+00	2.50E+00	6.00E+00	6.00E+00	6.00E+00	6.00E+00	6.00E+00
0.008	0.008	8.00E-03	8.00E-03	8.00E-03	0.008	0.008	8.00E-03	8.00E-03	8.00E-03	0.008	0.008	8.00E-03	8.00E-03	8.00E-03
1562.947877		1.56E+03	1.56E+03	1.56E+03	1443.19844		1.44E+03	1.44E+03	1.44E+03	1225.029746		1.23E+03	1.23E+03	1.23E+03
T25oC Aqueous	T25oC Solid	T80oC Aqueous	T100oC Aqueous	T120oC Aqueous	T25oC Aqueous		T80oC Aqueous	T100oC Aqueous	T120oC Aqueous	T25oC Aqueous		T80oC Aqueous	T100oC Aqueous	T120oC Aqueous
25	25	80	100	120	25		80	100	120	25		80	100	120
1	1	1	1	2	1		1	1	2	1		1	1	2
7.17282		6.46074	6.31845	6.21809	7.81606		7.05745	6.89799	6.78298	8.17871		7.40103	7.19559	7.02378
57.4994	0.00121104	57.5005	57.4998	57.4988	60.4876		60.4878	60.4873	60.4865	67.4831		67.4827	67.4821	67.4816
molality	molality	molality	molality	molality	molality		molality	molality	molality	molality		molality	molality	molality
55.5087		55.5087	55.5087	55.5087	55.5087		55.5087	55.5087	55.5087	55.5087		55.5087	55.5087	55.5087
2.71E-05		1.61E-04	2.37E-04	3.23E-04	3.94E-06		2.55E-05	3.84E-05	5.28E-05	7.83E-07		5.17E-06	8.42E-06	1.29E-05
1.39E-17		2.25E-15	7.20E-15	1.83E-14	3.91E-19		7.54E-17	2.51E-16	6.56E-16	3.05E-20		6.10E-18	2.39E-17	7.66E-17
2.14E-14		2.53E-12	8.77E-12	2.41E-11	9.82E-15		1.26E-12	4.53E-12	1.28E-11	7.25E-15		9.40E-13	3.72E-12	1.19E-11
0.00344706		0.00404432	0.00454146	0.00512287	0.00587929		0.00663367	0.00726968	0.00799066	0.00898856		0.00953945	0.0101107	0.0107429
6.42E-06		1.71E-05	2.26E-05	2.89E-05	1.07E-07		3.33E-07	4.39E-07	5.38E-07	2.13E-10		9.08E-10	1.27E-09	1.63E-09
0.00169426	1	0.00253423	0.00257467	0.0025458	2.80E-04		4.94E-04	5.12E-04	5.02E-04	7.70E-06		1.82E-05	2.07E-05	2.22E-05
8.71E-08		7.62E-07	1.31E-06	2.09E-06	3.63E-08		3.14E-07	5.15E-07	7.68E-07	3.94E-10		4.52E-09	6.71E-09	8.55E-09
2.01E-07		1.09E-06	1.86E-06	3.04E-06	6.96E-07		3.80E-06	6.44E-06	1.06E-05	7.63E-07		4.97E-06	8.14E-06	1.25E-05
0.980415		0.981162	0.980967	0.980623	2.46985		2.47086	2.47097	2.47098	5.96902		5.96914	5.96917	5.96921
8.25E-08		4.60E-07	6.58E-07	8.57E-07	1.33E-08		8.85E-08	1.34E-07	1.84E-07	2.16E-09		1.93E-08	3.54E-08	6.00E-08
2.55E-11		4.64E-10	1.01E-09	2.02E-09	5.52E-11		9.11E-10	1.83E-09	3.33E-09	1.64E-12		3.58E-11	5.93E-11	8.13E-11
0.996709		0.996115	0.995618	0.995039	2.49451		2.49376	2.49312	2.4924	5.99195		5.9914	5.99083	5.9902
0.012316		0.0115419	0.0109566	0.0102663	0.0101134		0.00933521	0.00868629	0.00795088	0.00701314		0.00645783	0.00588335	0.00524668
8.84E-06		1.71E-05	2.47E-05	3.62E-05	1.92E-07		4.34E-07	6.14E-07	8.52E-07	7.64E-10		2.34E-09	3.45E-09	4.92E-09
1.73E-04		1.70E-04	1.48E-04	1.24E-04	5.15E-06		6.15E-06	5.45E-06	4.53E-06	2.51E-08		4.26E-08	4.15E-08	3.74E-08
9.80E-04		0.00141799	0.00150543	0.00158652	5.46E-04		9.30E-04	0.00100767	0.00105417	7.16E-05		1.63E-04	1.94E-04	2.22E-04
0.00242141		0.00204359	0.0020465	0.00213297	0.00706205		0.00640462	0.00631084	0.00628304	0.00792077		0.00781742	0.00778347	0.00775397
0.00130339		0.00150123	0.00134147	0.00115614	1.00E-04		1.41E-04	1.30E-04	1.12E-04	1.16E-06		2.35E-06	2.43E-06	2.32E-06
1.75E-04		1.41E-04	1.03E-04	7.20E-05	3.85E-06		3.88E-06	2.95E-06	2.06E-06	4.71E-09		7.02E-09	5.93E-09	4.53E-09
2.68E-05		1.59E-04	2.34E-04	3.17E-04	3.18E-06		2.12E-05	3.10E-05	4.09E-05	2.13E-08		2.03E-07	3.02E-07	3.90E-07
1060.56	0.336799	1060.89	1060.89	1060.89	1148.56		1148.56	1148.56	1148.56	1353.11		1353.11	1353.11	1353.11
0.00102217	5.76E-08	0.00105047	0.00106444	0.00108038	0.00105258		0.0010865	0.00110006	0.00111444	0.00112848		0.00117854	0.00119192	0.00120341
-3.89E+06	-104.027	-3.84E+06	-3.82E+06	-3.80E+06	-4.04E+06		-3.98E+06	-3.96E+06	-3.94E+06	-4.37E+06		-4.32E+06	-4.30E+06	-4.28E+06
1.04E+06	5.85E+06	1.01E+06	9.97E+05	9.82E+05	1.09E+06		1.06E+06	1.04E+06	1.03E+06	1.20E+06		1.15E+06	1.14E+06	1.12E+06
	1													
46.6479		52.9366	54.8188	56.4671	129.745		146.166	151.625	156.768	393.861		434.857	451.082	467.958
0.0833898		0.17903	0.21409	0.248112	0.166607		0.358833	0.431966	0.50465	0.252076		0.55646	0.681664	0.813759
84.5618		186.568	226.04	265.865	69.9227		155.452	189.467	224.239	47.3475		109.156	135.235	162.996
0.980913		0.400904	0.319671	0.263706	1.15754		0.478935	0.382884	0.31672	1.7811		0.733712	0.596457	0.505834
1.10126		1.13192	1.13529	1.1367	1.29955		1.35223	1.35978	1.36521	1.99962		2.07157	2.11827	2.18038
1.00116		1.00041	0.999699	0.998986	2.50169		2.50034	2.49961	2.49885	5.99987		5.99922	5.99861	5.99795

2/19/02

04/20/01

65.508		65.508		65.508		65.508	
0.788251827		0.812764335		0.824778413		0.837991615	
55.5		55.5		55.5		55.5	
1.00E+01	1.00E+01	1.00E+01		1.00E+01		1.00E+01	
0.008	0.008	8.00E-03		8.00E-03		8.00E-03	
1215.989202		1.22E+03	1.22E+03	1.22E+03			
T25oC Aqueous	T25oC Solid	T80oC Aqueous	T80oC Solid	T100oC Aqueous	T100oC Solid	T120oC Aqueous	T120oC Solid
25	25	80	80	100	100	120	120
1	1	1	1	1	1	2	2
8.18065		7.40073		7.19105		7.01279	
67.8273	3.82786	68.5395	3.47141	68.9034	3.28918	69.3154	3.08288
molality	molality	molality	molality	molality	molality	molality	molality
55.5087		55.5087		55.5087		55.5087	
7.54E-07		4.65E-06		7.37E-06		1.09E-05	
2.92E-20		5.48E-18		2.10E-17		6.62E-17	
7.31E-15		9.70E-13		3.90E-12		1.28E-11	
0.00909345		0.00979866		0.0104224		0.0110943	
1.68E-10		4.64E-10		5.28E-10		5.42E-10	
6.67E-06		1.22E-05		1.23E-05		1.17E-05	
3.11E-10		2.25E-09		2.65E-09		2.61E-09	
7.38E-07		4.56E-06		7.27E-06		1.08E-05	
6.14118		6.49777		6.68003		6.88639	
2.05E-09		1.73E-08		3.17E-08		5.41E-08	
1.31E-12		1.83E-11		2.40E-11		2.54E-11	
6.16401		6.51981		6.70145		6.90711	
0.00690827		0.00619916		0.0055727		0.00489726	
6.26E-10		1.33E-09		1.66E-09		1.97E-09	
2.06E-08		2.44E-08		2.02E-08		1.53E-08	
6.60E-05		1.32E-04		1.48E-04		1.61E-04	
0.00792758		0.00785593		0.00783915		0.00782752	
9.77E-07		1.46E-06		1.31E-06		1.08E-06	
3.58E-09		3.20E-09		2.12E-09		1.24E-09	
1.70E-08		1.07E-07		1.30E-07		1.35E-07	
	1		1		1		1
1363.17	223.712	1384	202.88	1394.65	192.23	1406.71	180.173
0.00113236	1.03E-04	0.00119318	9.38E-05	0.00121171	8.88E-05	0.00122833	8.33E-05
-4.39E+06	-3.76E+05	-4.37E+06	-3.39E+05	-4.37E+06	-3.20E+05	-4.37E+06	-2.99E+05
1.20E+06	2.16E+06	1.16E+06	2.16E+06	1.15E+06	2.16E+06	1.15E+06	2.16E+06
	1		1		1		1
409.175		485.783		522.232		563.726	
0.25476		0.571139		0.70737		0.656677	
28.825		68.0926		85.6438		105.144	
1.81938		0.782387		0.653406		0.574165	
2.04259		2.209		2.32051		2.47492	
6.17194		6.52767		6.70929		6.91494	

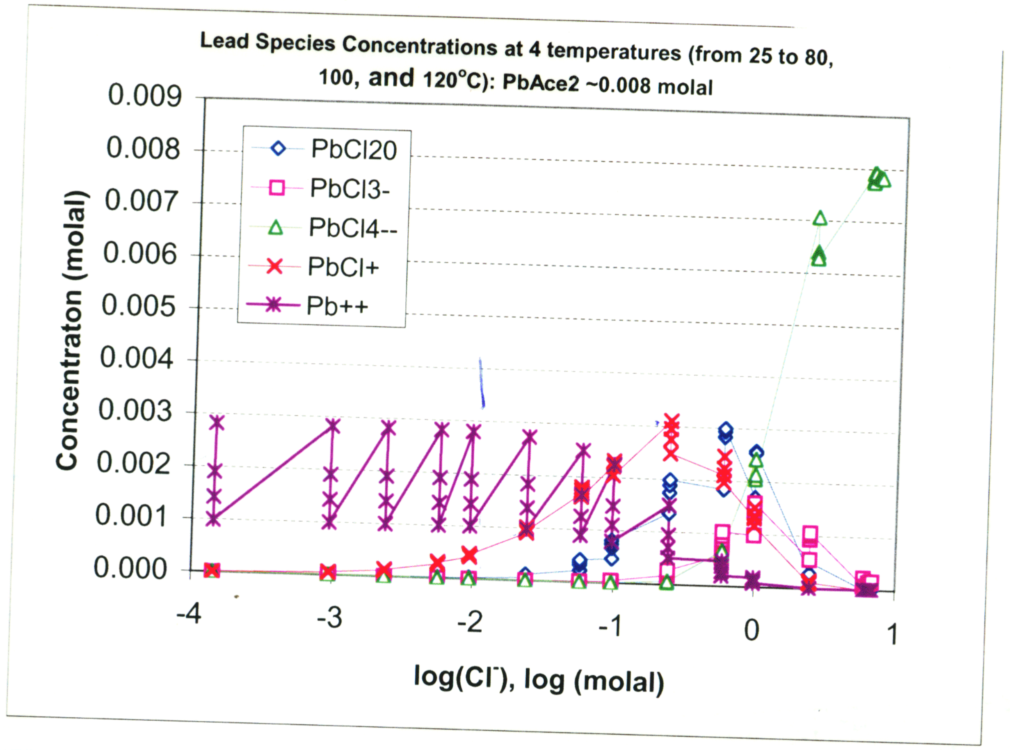
Use PbCl2

55.50015	55.50015	55.50015	55.50015
-1.8369669	-1.85995415	-1.87435286	-1.89209504
55.5	55.5	55.5	55.5
1.50E-04	1.50E-04	1.50E-04	1.50E-04
8.00E-03	0.008	0.008	0.008
0	0	0	0
1654.159349	1654.159349	1654.159349	1654.159349
T25oC Aqueous	T80oC Aqueous	T100oC Aqueous	T120oC Aqueous
25	80	100	120
1	1	1	2
5.01255	4.22608	4.01149	3.82742
55.5225	55.5218	55.5213	55.5208
molality	molality	molality	molality
55.5087	55.5087	55.5087	55.5087
7.30E-14	1.02E-11	4.15E-11	1.37E-10
5.88E-05	1.16E-04	1.57E-04	2.14E-04
3.94E-10	3.21E-09	5.37E-09	8.23E-09
1.23E-09	4.93E-09	6.71E-09	8.54E-09
0.0145557	0.0138053	0.0133551	0.0128205
1.12E-05	6.91E-05	1.14E-04	1.75E-04
5.21E-16	7.04E-15	1.24E-14	1.90E-14
1.50E-04	1.50E-04	1.50E-04	1.50E-04
4.18E-07	7.53E-07	1.03E-06	1.44E-06
5.16E-09	5.18E-09	6.47E-09	8.51E-09
0.00147783	0.00211366	0.00248063	0.00290016
0.00645301	0.00570207	0.00524893	0.00471121
1.12E-05	6.91E-05	1.14E-04	1.75E-04
1002.08	1002.08	1002.08	1002.08
0.00100317	0.00102874	0.00104325	0.00106048
-3.79E+06	-3.74E+06	-3.72E+06	-3.70E+06
9.99E+05	9.74E+05	9.61E+05	9.45E+05
0.50182	0.555016	0.564604	0.569371
0.00197114	0.00416898	0.00484612	0.00538884
242.627	526.233	620.335	701.198
0.893319	0.355571	0.282715	0.232941
1.00292	1.00392	1.00404	1.00409
0.0210092	0.0195082	0.0186051	0.0175332

2/19/02

Pb J.Y. 04/30/01

File: Darrel_~~Pd~~_Chem_2. XLS



J. Yang

3/14/02

05/07/01

Using HCl as Cl⁻ source

J.Y. 05/07/01

File: ~~Darrel~~ Darrel_Chem-3.XLS

Results from ESP V6.2e, May 07, 2001

Pb MW= 207.2 mg (appr. ppm) mM

	1	100	1600	2100
mM	0.004826255	0.482625483	7.722007722	10.1351351

Not Right, Organic shown a

Fix Pd, varying H

Inputs		55.50815			55.509			55.5105			55.518		
log(free Cl-)		-3.84496777	-3.84912081	-3.849427752	-3.02213927	-3.027649027	-3.028626724	-2.62589349	-2.63339216	-2.63574364	-2.03412879	-2.0498616	-2.05881615
H2O (mol)		55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)													
LiCl (mol)													
HCl (mol)		1.50E-04	1.50E-04	1.50E-04	1.00E-03	1.00E-03	1.00E-03	2.50E-03	2.50E-03	2.50E-03	1.00E-02	1.00E-02	1.00E-02
PbCl2 (mol)													
Pb(CH3CO2)2 (mol)		0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008
PbSO4 (mol)													
Total Pb (ppm)		1653.53231	1653.532311	1653.532311	1653.482828	1653.482828	1653.482828	1653.40036	1653.400363	1653.400363	1652.938713	1652.938713	1652.938713
Stream		T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC
Phase		Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C		25	80	100	25	80	100	25	80	100	25	80	100
Pressure, atm		1	1	1	1	1	1	1	1	1	1	1	1
pH		6.31747	5.7487	5.585	5.69171	5.53244	5.421	5.25263	5.22865	5.17119	4.26961	4.29633	4.28398
Total mol/hr		55.5181	55.5165	55.5155	55.5192	55.5176	55.5166	55.5211	55.5197	55.5187	55.5307	55.5297	55.5292
Flow Units		molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O		55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
ACETACID		2.58E-04	0.00102201	0.00149034	0.00102468	0.00157784	0.00202571	0.00250455	0.00281922	0.00317107	0.00994188	0.0100031	0.0100932
ACET2		1.03E-15	7.47E-14	2.34E-13	1.64E-14	1.78E-13	4.33E-13	9.78E-14	5.69E-13	1.06E-12	1.54E-12	7.16E-12	1.07E-11
H2SO4													
HCL		3.63E-17	3.25E-15	1.22E-14	1.02E-15	3.54E-14	1.17E-13	6.96E-15	1.76E-13	5.14E-13	2.59E-13	5.68E-12	1.47E-11
SO3													
LIOH													
NAACET													
PBACET2	PbAce2	3.47E-04	8.31E-04	0.00111009	3.22E-04	8.00E-04	0.0010764	2.73E-04	7.09E-04	9.74E-04	6.49E-05	1.88E-04	2.81E-04
PBCL2	PbCl20	2.91E-09	5.07E-09	6.20E-09	1.35E-07	2.42E-07	3.02E-07	8.89E-07	1.66E-06	2.13E-06	1.85E-05	3.66E-05	4.96E-05
PBO		7.92E-08	1.40E-06	2.47E-06	4.65E-09	5.65E-07	1.30E-06	6.58E-10	1.57E-07	4.79E-07	9.91E-12	3.30E-09	1.36E-08
LIACET													
OHION		2.39E-08	1.57E-07	2.40E-07	5.67E-09	9.57E-08	1.65E-07	2.07E-09	4.78E-08	9.31E-08	2.19E-10	5.70E-09	1.23E-08
CLION	Cl-	1.43E-04	1.42E-04	1.41E-04	9.50E-04	9.38E-04	9.36E-04	0.0023665	0.00232599	0.00231343	0.00924424	0.00891535	0.00873341
HION		5.41E-07	2.01E-06	2.92E-06	2.29E-06	3.31E-06	4.28E-06	6.30E-06	6.69E-06	7.63E-06	6.12E-05	5.81E-05	6.00E-05
HPBO2ION		2.06E-12	9.89E-11	2.05E-10	2.87E-14	2.43E-11	7.38E-11	1.48E-15	3.36E-12	1.54E-11	2.34E-18	8.40E-15	5.78E-14
HSO4ION													
LIION													
LISO4ION													
NAION													
NASO4ION													
ACETATEION		0.00983352	0.0081498	0.00712146	0.009271	0.00766362	0.00665158	0.00826233	0.00682668	0.00588239	0.00344836	0.00287521	0.00247394
PBACET3ION	PbAce3-	2.68E-04	4.09E-04	5.42E-04	2.35E-04	3.70E-04	4.91E-04	1.77E-04	2.92E-04	3.93E-04	1.76E-05	3.27E-05	4.77E-05
PBACETION	PbAce+	0.00441159	0.00394066	0.00354478	0.00435718	0.00405099	0.00369977	0.00415818	0.00406188	0.00382143	0.00242975	0.00265005	0.00273069
PBCL3ION	PbCl3-	2.03E-13	3.38E-13	4.32E-13	6.23E-11	1.07E-10	1.39E-10	1.03E-09	1.82E-09	2.43E-09	8.36E-08	1.54E-07	2.13E-07
PBCL4ION	PbCl4--	2.31E-17	2.21E-17	2.63E-17	4.74E-14	4.67E-14	5.64E-14	1.95E-12	1.98E-12	2.45E-12	6.39E-10	6.65E-10	8.49E-10
PBCLION	PbCl+	7.12E-06	8.47E-06	8.57E-06	4.96E-05	6.14E-05	6.34E-05	1.32E-04	1.71E-04	1.83E-04	7.20E-04	0.00101253	0.00116833
PBION	Pb++	0.00285882	0.00193931	0.00145543	0.00301021	0.00213846	0.00164224	0.00324952	0.00244018	0.00195	0.0047489	0.00402158	0.00357237
PBOHION	PbOH+	1.08E-04	8.71E-04	0.00133805	2.68E-05	5.80E-04	0.00102706	1.05E-05	3.25E-04	6.77E-04	1.53E-06	5.96E-05	1.52E-04
SO4ION													
PBSO4													
NACL													
LICL													
LI2SO4.1H2O													
LI2SO4													
LIACET.2H2O													
LICL.1H2O													
LICL.2H2O													
LIOH.1H2O													
NA2SO4.10H2O													
NA2SO4													
NA3HSO42													
NAACET.3H2O													
NAHSO4													
NAOH.1H2O													
NAOH													
PBHSO42													
PBOH2													
Total g/hr		1002.46	1002.46	1002.46	1002.49	1002.49	1002.49	1002.54	1002.54	1002.54	1002.82	1002.82	1002.82
Volume, m3/hr		0.00100358	0.00102915	0.00104368	0.00100357	0.00102915	0.00104369	0.00100356	0.00102916	0.0010437	0.00100352	0.00102915	0.00104373
Enthalpy, cal/hr		-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06
Density, g/m3		9.99E+05	9.74E+05	9.61E+05	9.99E+05	9.74E+05	9.61E+05	9.99E+05	9.74E+05	9.61E+05	9.99E+05	9.74E+05	9.61E+05
Vapor fraction													
Solid fraction													
Organic fraction													
Osmotic Pres, atm		0.399634	0.441542	0.448931	0.409212	0.445792	0.45213	0.432242	0.464567	0.46809	0.626246	0.684864	0.692779
Redox Pot, volts													
E-Con, 1/ohm-cm		8.53E-04	0.00137392	0.00123363	9.07E-04	0.00151537	0.00140992	0.00100107	0.0017619	0.00172624	0.00151449	0.00304401	0.00339023
E-Con, cm2/ohm-mol		105.01	171.232	142.711	101.152	172.812	153.642	95.6798	172.625	166.533	84.4347	174.331	196.566
Abs Visc, cP		0.896553	0.356439	0.283396	0.896378	0.35639	0.283352	0.89606	0.356302	0.283277	0.894534	0.355887	0.282953
Rel Visc		1.00655	1.00637	1.00646	1.00635	1.00624	1.0063	1.006	1.00599	1.00603	1.00428	1.00482	1.00488
Ionic Strength		0.0131037	0.0106401	0.00926062	0.0134665	0.0111108	0.00972117	0.0140556	0.0118853	0.010539	0.0174592	0.015845	0.0148276

J. Yang 3/14/02

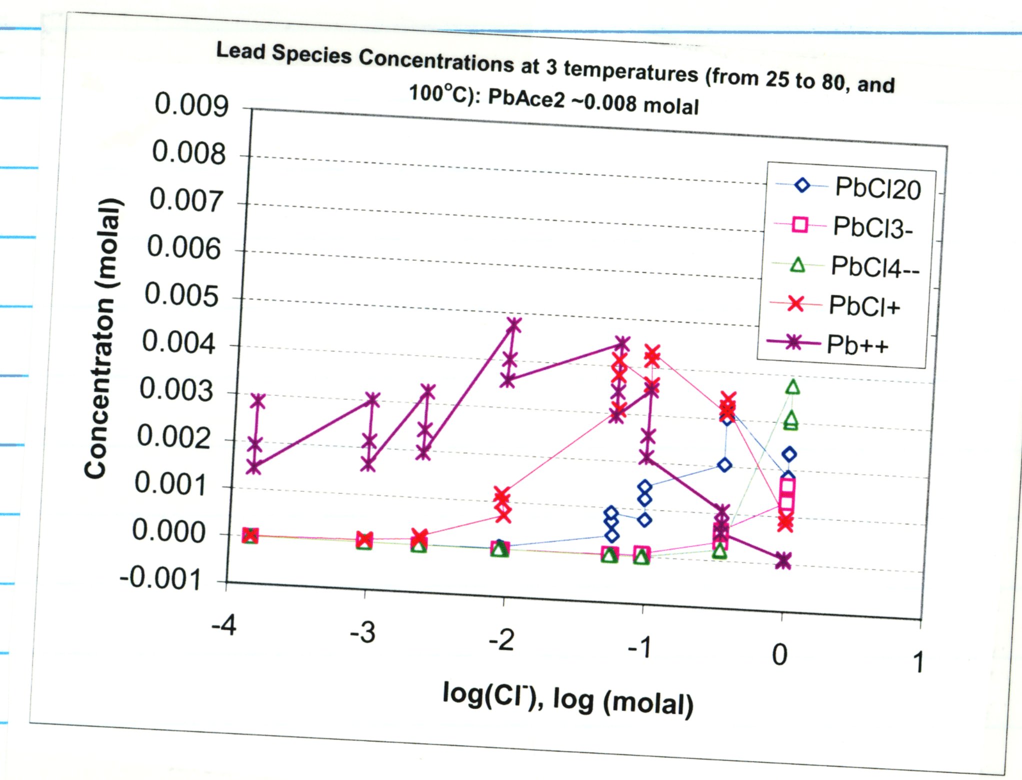
is liquid here

Cl

55.568			55.608			55.858			56.508		
-1.2514035	-1.2618484	-1.2675411	-1.0237413	-1.0304616	-1.033932	-0.4705748	-0.4710319	-0.4719064	-0.010338	-0.0098188	-0.0100157
55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
6.00E-02	6.00E-02	6.00E-02	1.00E-01	1.00E-01	1.00E-01	3.50E-01	3.50E-01	3.50E-01	1.00E+00	1.00E+00	1.00E+00
0.008	0.008	0.008	0.008	0.008	0.008	0.008	0.008	#REF!	0.008	0.008	0.008
1649.94426	1649.94426	1649.94426	1647.54995	1647.54995	1647.54995	1633.28045	1633.28045	#REF!	1595.51838	1595.51838	1595.51838
T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC
Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
25	80	100	25	80	100	25	80	100	25	80	100
1	1	1	1	1	1	1	1	1	1	1	1
1.44218	1.45217	1.45657	1.17321	1.18612	1.19189	0.593389	0.615492	0.624962	0.0966449	0.130527	0.143912
55.6241	55.6227	55.622	55.7027	55.7012	55.7005	56.1952	56.196	56.1953	57.4843	57.4855	57.485
molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
0.0159891	0.0159911	0.0159919	0.0159957	0.0159969	0.0159974	0.0160009	0.0160011	0.0160013	0.016002	0.016002	0.0160021
3.99E-12	1.83E-11	2.70E-11	4.00E-12	1.83E-11	2.70E-11	4.02E-12	1.84E-11	2.72E-11	4.07E-12	1.87E-11	2.75E-11
9.84E-10	2.24E-08	5.58E-08	3.00E-09	6.81E-08	1.69E-07	3.88E-08	8.55E-07	2.10E-06	3.70E-07	7.75E-06	1.88E-05
2.60E-10	5.97E-10	8.82E-10	5.23E-11	1.12E-10	1.59E-10	8.22E-13	1.75E-12	2.28E-12	8.11E-15	1.66E-14	2.03E-14
4.16E-04	7.10E-04	8.97E-04	7.78E-04	0.00122121	0.0014816	0.00203736	0.00301655	0.00328434	0.00183637	0.00234924	0.0023296
1.53E-17	4.09E-15	1.70E-14	3.07E-18	7.62E-16	3.04E-15	4.74E-20	1.17E-17	4.29E-17	4.45E-22	1.06E-19	3.64E-19
3.57E-13	9.06E-12	2.06E-11	2.01E-13	5.18E-12	1.18E-11	6.07E-14	1.64E-12	3.82E-12	2.20E-14	6.20E-13	1.47E-12
0.0560527	0.0547207	0.0540081	0.0946801	0.0932263	0.0924843	0.338396	0.33804	0.33736	0.976477	0.977645	0.977202
0.0440203	0.0440183	0.0440175	0.0840199	0.0840187	0.0840181	0.334054	0.334053	0.334051	0.984154	0.984147	0.984136
5.84E-27	1.64E-23	1.19E-22	6.55E-28	1.73E-24	1.22E-23	2.94E-30	8.04E-27	5.27E-26		2.53E-29	1.59E-28
8.97E-06	7.25E-06	6.47E-06	5.02E-06	4.11E-06	3.69E-06	1.47E-06	1.25E-06	1.15E-06	5.02E-07	4.48E-07	4.16E-07
1.84E-13	2.62E-13	3.92E-13	2.07E-14	2.78E-14	4.03E-14	9.57E-17	1.33E-16	1.80E-16	3.27E-19	4.57E-19	5.91E-19
4.48E-06	4.10E-06	4.09E-06	1.76E-06	1.49E-06	1.43E-06	1.22E-07	1.04E-07	9.11E-08	4.41E-09	3.55E-09	2.94E-09
1.17E-05	1.88E-05	2.46E-05	3.78E-05	5.65E-05	7.11E-05	3.98E-04	5.67E-04	6.45E-04	0.00130757	0.00159759	0.00165685
6.71E-07	6.34E-07	7.78E-07	4.12E-06	3.70E-06	4.43E-06	2.35E-04	2.12E-04	2.36E-04	0.00377816	0.00301113	0.00311512
0.00308755	0.00381001	0.00413013	0.00365048	0.00416271	0.0043371	0.00310832	0.00343018	0.00324283	9.71E-04	9.68E-04	8.45E-04
0.00448115	0.00345778	0.00294443	0.00352951	0.00255565	0.00210556	0.00105131	7.75E-04	5.92E-04	1.08E-04	7.55E-05	5.43E-05
1.73E-09	5.67E-08	1.41E-07	6.68E-10	2.04E-08	4.87E-08	4.35E-11	1.32E-09	2.89E-09	1.38E-12	3.97E-11	8.18E-11
1004.64	1004.64	1004.64	1006.1	1006.1	1006.1	1014.89	1015.21	1015.21	1038.91	1038.91	1038.91
0.00100428	0.00102995	0.00104453	0.001005	0.00103069	0.00104523	0.00100956	0.00103541	0.0010498	0.00102188	0.00104827	0.00106245
-3.80E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.81E+06	-3.75E+06	-3.73E+06	-3.83E+06	-3.78E+06	-3.76E+06
1.00E+06	9.75E+05	9.62E+05	1.00E+06	9.76E+05	9.63E+05	1.01E+06	9.81E+05	9.67E+05	1.02E+06	9.91E+05	9.78E+05
2.79267	3.18697	3.3024	4.61178	5.26491	5.45671	16.3361	18.6238	19.2792	50.5164	57.1693	59.1302
0.0187763	0.0318795	0.0353741	0.0337778	0.0566981	0.0627863	0.122812	0.203574	0.224789	0.32364	0.532328	0.586645
277.305	482.908	543.415	314.323	541.111	607.667	346.33	588.777	659.174	328.098	553.596	618.333
0.895419	0.357043	0.283954	0.897696	0.358523	0.28519	0.911567	0.367656	0.292802	0.946289	0.390301	0.311688
1.00528	1.00808	1.00844	1.00783	1.01226	1.01283	1.02341	1.03804	1.03986	1.06239	1.10198	1.10693
0.0605565	0.0582064	0.056986	0.0982648	0.0958536	0.0946778	0.340551	0.34002	0.339308	0.989227	0.988352	0.988259

05/07/01

File: Darrel_chem_3.XLS



05/07/01

L.g.

Changing Pb Concentration

05/7/01

HCl or NaCl 0.01 molal, varying Pb

Inputs	55.518			55.526			55.534	
log(free Cl-)	-2.0341288	-2.0498616	-2.0588162	-2.0371767	-2.050764708	-2.0576253	-2.039691	-2.0531662
H2O (mol)	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)								
LiCl (mol)								
HCl (mol)	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02	1.00E-02
PbCl2 (mol)								
Pb(CH3CO2)	0.008	0.008	0.008	0.016	0.016	0.016	0.024	0.024
PbSO4 (mol)								
Total Pb (p	1652.93871	1652.93871	1652.93871	3297.32848	3297.32848	3297.32848	4933.23545	4933.23545
Stream	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature	25	80	100	25	80	100	25	80
Pressure, atr	1	1	1	1	1	1	1	1
pH	4.26961	4.29633	4.28398	4.75128	4.74589	4.71099	4.91736	4.89176
Total mol/hr	55.5307	55.5297	55.5292	55.5459	55.5433	55.5417	55.5591	55.5548
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
ACETACID	0.00994188	0.0100031	0.0100932	0.00998609	0.0101558	0.0103848	0.00999553	0.0102484
ACET2	1.54E-12	7.16E-12	1.07E-11	1.56E-12	7.38E-12	1.14E-11	1.56E-12	7.52E-12
H2SO4								
HCL	2.59E-13	5.68E-12	1.47E-11	8.26E-14	1.97E-12	5.39E-12	5.51E-14	1.37E-12
SO3								
LIOH								
NAACET								
PBACET2	6.49E-05	1.88E-04	2.81E-04	6.58E-04	0.00156992	0.0020841	0.00151745	0.0032918
PBCL2	1.85E-05	3.66E-05	4.96E-05	1.90E-05	3.55E-05	4.68E-05	1.95E-05	3.58E-05
PBO	9.91E-12	3.30E-09	1.36E-08	9.96E-11	2.67E-08	9.54E-08	2.29E-10	5.50E-08
LIACET								
OHION	2.19E-10	5.70E-09	1.23E-08	6.82E-10	1.64E-08	3.37E-08	1.02E-09	2.33E-08
CLION	0.00924424	0.00891535	0.00873341	0.00917959	0.00889683	0.00875739	0.0091266	0.00884777
HION	6.12E-05	5.81E-05	6.00E-05	2.07E-05	2.11E-05	2.29E-05	1.43E-05	1.53E-05
HPBO2ION	2.34E-18	8.40E-15	5.78E-14	7.31E-17	1.96E-13	1.11E-12	2.50E-16	5.72E-13
HSO4ION								
LIION								
LISO4ION								
NAION								
NASO4ION								
ACETATEIO	0.00344836	0.00287521	0.00247394	0.0107427	0.00840083	0.00694609	0.0160026	0.0120416
PBACET3IO	1.76E-05	3.27E-05	4.77E-05	5.56E-04	7.98E-04	9.94E-04	0.00191169	0.00239818
PBACETION	0.00242975	0.00265005	0.00273069	0.00829069	0.00791502	0.00752473	0.0132394	0.0119396
PBCL3ION	8.36E-08	1.54E-07	2.13E-07	8.53E-08	1.49E-07	2.02E-07	8.68E-08	1.49E-07
PBCL4ION	6.39E-10	6.65E-10	8.49E-10	6.83E-10	6.75E-10	8.43E-10	7.17E-10	6.96E-10
PBCLION	7.20E-04	0.00101253	0.00116833	7.84E-04	0.00103327	0.00115004	8.36E-04	0.00108189
PBION	0.0047489	0.00402158	0.00357237	0.00568929	0.00447551	0.00379699	0.00647163	0.00499451
PBOHION	1.53E-06	5.96E-05	1.52E-04	5.21E-06	1.75E-04	4.06E-04	8.31E-06	2.62E-04
SO4ION								
PBSO4								
NACL								
LICL								
LI2SO4.1H2								
LI2SO4								
LIACET.2H2								
LICL.1H2O								
LICL.2H2O								
LIOH.1H2O								
NA2SO4.10								
NA2SO4								
NA3HSO42								
NAACET.3H								
NAHSO4								
NAOH.1H2C								
NAOH								
PBHSO42								
PBOH2								
Total g/hr	1002.82	1002.82	1002.82	1005.42	1005.42	1005.42	1008.02	1008.02
Volume, m3/	0.00100352	0.00102915	0.00104373	0.00100411	0.00102979	0.00104438	0.00100474	0.00103046
Enthalpy, cal	-3.79E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06
Density, g/m	9.99E+05	9.74E+05	9.61E+05	1.00E+06	9.76E+05	9.63E+05	1.00E+06	9.78E+05
Vapor fractio								
Solid fraction								
Organic fract								
Osmotic Pre	0.626246	0.684864	0.692779	0.864097	0.92287	0.923326	1.11098	1.17732
Redox Pot, v								
E-Con, 1/ohr	0.00151449	0.00304401	0.00339023	0.00199547	0.00369618	0.0038595	0.00238711	0.00423884
E-Con, cm2/	84.4347	174.331	196.566	77.0645	146.439	154.115	70.5421	128.481
Abs Visc, cP	0.894534	0.355887	0.282953	0.899649	0.357825	0.284485	0.904682	0.359727
Rel Visc	1.00428	1.00482	1.00488	1.01003	1.01029	1.01032	1.01568	1.01566
Ionic Strengt	0.0174592	0.015845	0.0148276	0.0261681	0.0225712	0.0204945	0.0335127	0.0282823

Inputs	55.508			55.516			55.524		
log(free Cl-)	-2.0193114	-2.0227997	-2.0230112	-2.025621	-2.0301598	-2.0308074	-2.0298126	-2.0353935	-2.0366916
H2O (mol)	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)	1.00E-02			1.00E-02			1.00E-02		
HCl (mol)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pb(CH3CO2)	0.008	0.008	0.008	0.016	0.016	0.016	0.024	0.024	0.024
Total Pb (p	1652.57617	1652.57617	1652.57617	3296.60714	3296.60714	3296.60714	4932.15901	4932.15901	4932.15901
Stream	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature	25	80	100	25	80	100	25	80	100
Pressure, atr	1	1	1	1	1	1	1	1	1
pH	6.53348	5.81964	5.64902	6.56595	5.84016	5.65837	6.57775	5.84234	5.65215
Total mol/hr	55.5379	55.5363	55.5353	55.5521	55.5487	55.5467	55.5645	55.5597	55.5568
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
ACETACID	1.59E-04	8.97E-04	0.00134121	2.34E-04	0.00128168	0.00189087	2.85E-04	0.00154341	0.00226913
ACET2	3.97E-16	5.77E-14	1.90E-13	8.57E-16	1.18E-13	3.78E-13	1.27E-15	1.71E-13	5.44E-13
HCL	1.43E-15	1.78E-13	6.75E-13	1.28E-15	1.63E-13	6.36E-13	1.22E-15	1.58E-13	6.28E-13
NAACET	6.01E-05	7.04E-05	7.71E-05	9.29E-05	1.03E-04	1.09E-04	1.14E-04	1.23E-04	1.26E-04
PBACET2	3.13E-04	7.48E-04	0.00100015	0.00105031	0.0022413	0.00281032	0.00192337	0.00388007	0.00472394
PBCL2	1.07E-05	1.77E-05	2.11E-05	1.33E-05	2.20E-05	2.66E-05	1.48E-05	2.47E-05	3.02E-05
PBO	1.86E-07	1.63E-06	2.74E-06	2.88E-07	2.39E-06	3.87E-06	3.56E-07	2.85E-06	4.52E-06
OHION	4.05E-08	1.92E-07	2.90E-07	4.47E-08	2.06E-07	3.02E-07	4.67E-08	2.10E-07	3.02E-07
CLION	0.00956508	0.00948856	0.00948394	0.00942712	0.00932911	0.00931521	0.00933657	0.00921736	0.00918985
HION	3.38E-07	1.77E-06	2.63E-06	3.20E-07	1.72E-06	2.62E-06	3.16E-07	1.73E-06	2.69E-06
HPBO2ION	8.23E-12	1.41E-10	2.75E-10	1.40E-11	2.21E-10	4.04E-10	1.80E-11	2.68E-10	4.71E-10
NAION	0.00994151	0.00993134	0.00992467	0.00990871	0.00989878	0.00989325	0.00988729	0.0098792	0.00987549
ACETATEIO	0.0103385	0.00876975	0.00776914	0.0166827	0.0133791	0.011391	0.0211498	0.0164042	0.0136493
PBACET3IO	2.56E-04	3.98E-04	5.36E-04	0.00138469	0.00182168	0.00220723	0.00321496	0.00386689	0.00444595
PBACETION	0.00404944	0.00357527	0.00320787	0.0087406	0.00729434	0.00637332	0.0129668	0.0105777	0.00917881
PBCL3ION	4.98E-08	7.93E-08	9.88E-08	6.12E-08	9.68E-08	1.22E-07	6.75E-08	1.07E-07	1.37E-07
PBCL4ION	4.08E-10	3.78E-10	4.42E-10	5.17E-10	4.74E-10	5.59E-10	5.84E-10	5.35E-10	6.38E-10
PBCLION	4.15E-04	4.77E-04	4.75E-04	5.48E-04	6.28E-04	6.33E-04	6.35E-04	7.35E-04	7.51E-04
PBION	0.00279706	0.00188783	0.00142032	0.00403169	0.00271427	0.00206298	0.0049635	0.00337802	0.0026074
PBOHION	1.59E-04	8.95E-04	0.00133806	2.34E-04	0.00127841	0.00188544	2.85E-04	0.00153923	0.00226249
Total g/hr	1003.04	1003.04	1003.04	1005.64	1005.64	1005.64	1008.24	1008.24	1008.24
Volume, m3/	0.00100374	0.00102932	0.00104385	0.00100435	0.00102997	0.00104451	0.00100499	0.00103065	0.0010452
Enthalpy, cal	-3.79E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06
Density, g/m	9.99E+05	9.74E+05	9.61E+05	1.00E+06	9.76E+05	9.63E+05	1.00E+06	9.78E+05	9.65E+05
Osmotic Pre	0.746739	0.845622	0.873428	0.98958	1.09018	1.10503	1.21115	1.31384	1.31833
E-Con, 1/ohr	0.00195976	0.00383421	0.00421174	0.00243097	0.004507	0.00475458	0.00279862	0.00503295	0.00518353
E-Con, cm2/	109.283	217.334	232.652	93.9058	176.948	182.035	82.7234	151.296	152.429
Abs Visc, cP	0.897279	0.356846	0.2837	0.902355	0.358763	0.285211	0.90736	0.360651	0.286698
Rel Visc	1.00736	1.00752	1.00754	1.01306	1.01293	1.0129	1.01868	1.01826	1.01818
Ionic Strengt	0.0229568	0.0205447	0.0192095	0.0315263	0.0272444	0.0249768	0.0386649	0.0328668	0.0298929

[signature]

8/14/02

05/07/01

HCl or NaCl 0.001 molal, Varying Pb

	55.509			55.517			55.525	
	-3.0221393	-3.027649	-3.0286267	-3.027862	-3.0339757	-3.0353068	-3.0349207	-3.0428335
	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
	0.008	0.008	0.008	0.016	0.016	0.016	0.024	0.024
	1653.48283	1653.48283	1653.48283	3298.41109	3298.41109	3298.41109	4923.56436	4923.56436
	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC
	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
	25	80	100	25	80	100	25	80
	1	1	1	1	1	1	1	1
	5.69171	5.53244	5.421	5.89266	5.63433	5.49473	6.03894	5.68594
	55.5192	55.5176	55.5166	55.5334	55.5301	55.5281	55.5413	55.5353
	molality	molality	molality	molality	molality	molality	molality	molality
	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
	0.00102468	0.00157784	0.00202571	0.00105398	0.00193043	0.00255285	0.00109963	0.00237612
	1.64E-14	1.78E-13	4.33E-13	1.73E-14	2.67E-13	6.87E-13	1.89E-14	4.04E-13
	1.02E-15	3.54E-14	1.17E-13	6.16E-16	2.68E-14	9.50E-14	4.19E-16	2.26E-14
	3.22E-04	8.00E-04	0.0010764	0.00108763	0.00236521	0.00298046	0.00292528	0.00577626
	1.35E-07	2.42E-07	3.02E-07	1.57E-07	2.75E-07	3.44E-07	1.79E-07	3.15E-07
	4.65E-09	5.65E-07	1.30E-06	1.48E-08	1.12E-06	2.26E-06	3.65E-08	1.80E-06
	5.67E-09	9.57E-08	1.65E-07	9.29E-09	1.25E-07	2.01E-07	1.35E-08	1.45E-07
	9.50E-04	9.38E-04	9.36E-04	9.38E-04	9.25E-04	9.22E-04	9.23E-04	9.06E-04
	2.29E-06	3.31E-06	4.28E-06	1.48E-06	2.69E-06	3.71E-06	1.09E-06	2.47E-06
	2.87E-14	2.43E-11	7.38E-11	1.49E-13	6.23E-11	1.56E-10	5.30E-13	1.16E-10
	0.009271	0.00766362	0.00665158	0.0155426	0.0121686	0.0101948	0.0233749	0.0173905
	2.35E-04	3.70E-04	4.91E-04	0.00132926	0.00173938	0.00208384	0.00537827	0.00607192
	0.00435718	0.00405099	0.00369977	0.00924549	0.00795787	0.00704582	0.0175502	0.0144767
	6.23E-11	1.07E-10	1.39E-10	7.16E-11	1.20E-10	1.56E-10	8.07E-11	1.34E-10
	4.74E-14	4.67E-14	5.64E-14	5.72E-14	5.47E-14	6.60E-14	6.81E-14	6.44E-14
	4.96E-05	6.14E-05	6.34E-05	6.20E-05	7.49E-05	7.76E-05	7.71E-05	9.35E-05
	0.00301021	0.00213846	0.00164224	0.00422272	0.00293344	0.00226101	0.00597352	0.00421064
	2.68E-05	5.80E-04	0.00102706	5.53E-05	9.31E-04	0.00155165	1.00E-04	0.00137467
	1002.49	1002.49	1002.49	1005.09	1005.09	1005.09	1010	1010
	0.00100357	0.00102915	0.00104369	0.00100418	0.0010298	0.00104435	0.00100519	0.00103088
	-3.79E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06
	9.99E+05	9.74E+05	9.61E+05	1.00E+06	9.76E+05	9.62E+05	1.00E+06	9.80E+05
	0.409212	0.445792	0.45213	0.713559	0.767197	0.770127	1.22475	1.31061
	9.07E-04	0.00151537	0.00140992	0.00140127	0.00223354	0.00200821	0.00211463	0.00328625
	101.152	172.812	153.642	82.7724	134.873	116.969	64.4307	102.379
	0.896378	0.35639	0.283352	0.901509	0.358333	0.284892	0.911528	0.362116
	1.00635	1.00624	1.0063	1.01211	1.01172	1.01177	1.02336	1.0224
	0.0134665	0.0111108	0.00972117	0.0220324	0.0177664	0.0154618	0.0356494	0.0285792

	55.508			55.516			55.524		
	-3.0206064	-3.0244855	-3.0246923	-3.0265535	-3.031428	-3.032148	-3.030547	-3.036453	-3.037882
	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
	1.00E-03			1.00E-03			1.00E-03		
	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
	0.008	0.008	0.008	0.016	0.016	0.016	0.024	0.024	0.024
	1653.44984	1653.44984	1653.44984	3298.34545	3298.345	3298.345	4933.9207	4933.921	4933.921
	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC
	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
	25	80	100	25	80	100	25	80	100
	1	1	1	1	1	1	1	1	1
	6.5137	5.79293	5.61932	6.55103	5.81891	5.63378	6.56485	5.82342	5.62969
	55.5199	55.5183	55.5172	55.5341	55.5307	55.5287	55.5555	55.5506	55.5479
	molality	molality	molality	molality	molality	molality	molality	molality	molality
	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
	1.66E-04	9.36E-04	0.00139933	2.40E-04	0.001318	0.001948	2.91E-04	0.00158	0.002328
	4.28E-16	6.27E-14	2.06E-13	8.99E-16	1.24E-13	4.00E-13	1.32E-15	1.79E-13	5.71E-13
	1.54E-16	1.95E-14	7.49E-14	1.35E-16	1.76E-14	6.93E-14	1.28E-16	1.69E-14	6.78E-14
	6.13E-06	7.14E-06	7.81E-06	9.39E-06	1.04E-05	1.09E-05	1.15E-05	1.23E-05	1.26E-05
	3.45E-04	8.24E-04	0.00109986	0.00111358	0.002381	0.002987	0.0020104	0.004067	0.004961
	1.25E-07	2.16E-07	2.63E-07	1.50E-07	2.56E-07	3.16E-07	1.64E-07	2.81E-07	3.51E-07
	1.90E-07	1.66E-06	2.78E-06	2.92E-07	2.41E-06	3.89E-06	3.59E-07	2.87E-06	4.53E-06
	3.77E-08	1.75E-07	2.61E-07	4.23E-08	1.91E-07	2.77E-07	4.46E-08	1.96E-07	2.79E-07
	9.54E-04	9.45E-04	9.45E-04	9.41E-04	9.30E-04	9.29E-04	9.32E-04	9.19E-04	9.16E-04
	3.46E-07	1.82E-06	2.72E-06	3.26E-07	1.76E-06	2.70E-06	3.21E-07	1.78E-06	2.77E-06
	7.81E-12	1.30E-10	2.50E-10	1.34E-11	2.06E-10	3.72E-10	1.73E-11	2.52E-10	4.35E-10
	9.94E-04	9.93E-04	9.92E-04	9.91E-04	9.90E-04	9.89E-04	9.89E-04	9.88E-04	9.88E-04
	0.00997328	0.00830005	0.0072746	0.0161472	0.012735	0.010738	0.0205275	0.015682	0.012931
	2.71E-04	4.13E-04	5.49E-04	0.00141449	0.001833	0.002201	0.0032468	0.003857	0.004401
	0.00435497	0.00387139	0.00347473	0.00913788	0.00768	0.006732	0.0134169	0.01103	0.009613
	5.83E-11	9.62E-11	1.22E-10	6.86E-11	1.12E-10	1.44E-10	7.43E-11	1.22E-10	1.59E-10
	4.47E-14	4.24E-14	5.02E-14	5.51E-14	5.16E-14	6.17E-14	6.16E-14	5.76E-14	6.96E-14
	4.62E-05	5.46E-05	5.49E-05	5.92E-05	6.95E-05	7.09E-05	6.78E-05	8.01E-05	8.30E-05
	0.00281825	0.00190197	0.00142376	0.00403724	0.002721	0.002065	0.0049712	0.003392	0.002621
	1.66E-04	9.34E-04	0.00139622	2.40E-04	0.001315	0.001943	2.90E-04	0.001576	0.002321
	1002.51	1002.51	1002.51	1005.11	1005.11	1005.11	1007.88	1007.88	1007.88
	0.00100359	0.00102916	0.00104369	0.0010042	0.00103	0.001044	0.001005	0.001031	0.001045
	-3.79E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06	-3.80E+06	-3.74E+06	-3.72E+06
	9.99E+05	9.74E+05	9.61E+05	1.00E+06	9.76E+05	9.62E+05	1.00E+06	9.78E+05	9.64E+05
	0.42535	0.470514	0.47853	0.727264	0.787624	0.789959	0.991411	1.06557	1.06455
	9.57E-04	0.00160505	0.00151392	0.00144606	0.002322	0.002112	0.0018283	0.002882	0.002585
	106.671	180.222	159.031	85.4197	138.677	120.406	73.4845	117.443	101.622
	0.896639	0.356479	0.283421	0.901761	0.35842	0.284959	0.90679	0.360321	0.286461
	1.00665	1.00649	1.00655	1.0124	1.01197	1.01201	1.01804	1.01733	1.01734
	0.0140159	0.0115608	0.0101923	0.0225396	0.01822	0.015933	0.0296775	0.023851	0.020869

05/07/01

May 10/01

Lietai Yang

To: Yi-ming Pan (ypan)
Cc: Darrell Dunn (ddunn); Gustavo Cragnolino; Vijay Jain (vjain)
Subject: RE: Pb speciations

Enclosed are the results of more calculations.

It seems that Pb Acetate does not decociate easily (only ~30%). If Cl- is not abosulately required, then just add PbCl2 alone (not adding other clorides in order to maintain low Cl- conc) would allow you to achieve 3000 ppm Pb++ (with only a small percentage of Cl complex). A slight amount of HCl helps only slightly for Pb++. If too much HCl, then the Cl- is too much and complex will be formed.

It is an interesting try with the PbSO4. If nothing else is added, the Pb is dissociated into Pb++ almost completely at T> 80oC. Is SO4-- bad for the test?

Regards.

Lietai

Darrell_Pb_Chem_4.xls

7/14/02

File: Darrell_Pb_chem_4.xls 05/10/01

Results from ESP V6.2e, May 10, 2001
Pb MW= 207.2 mg (appr. ppm: 1, 100, 1600, 2100, 5000
mM: 0.00482625, 0.482625483, 7.722007722, 10.1351351, 24.13127413

		PbSO4 only, Pb++ >96% at T>80oC				PbSO4 only, Pb++ >96% at T>80oC			
Inputs		55.508			55.508	55.524			55.524
log(free Cl-)		#VALUE!		#VALUE!	#VALUE!		#VALUE!	#VALUE!	#VALUE!
free Pb++ percentage		1.831875		98.41475	96.640875	0.610625		99.02625	97.86625
H2O (mol)		55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)									
LiCl (mol)									
HCl (mol)									
PbCl2 (mol)									
Pb(CH3CO2)2 (mol)									
PbSO4 (mol)		0.008	0.008	0.008	0.008	0.024	0.024	0.024	0.024
Total Pb (ppm)		1657.77572	1657.77572	1657.775724	1653.82927	4973.327173	4973.327173	4973.32717	4937.594948
Stream		T25oC	T25oC	T80oC	T100oC	T25oC	T25oC	T80oC	T100oC
Phase		Aqueous	Solid	Aqueous	Aqueous	Aqueous	Solid	Aqueous	Aqueous
Temperature, C		25	25	80	100	25	25	80	100
Pressure, atm		1	1	1	1	1	1	1	1
pH		5.73849		4.42531	4.2933	5.73849		4.38333	4.26491
Total mol/hr		55.5003	0.00785158	55.5159	55.5158	55.5003	0.0238516	55.5479	55.5476
Flow Units		molality	molality	molality	molality	molality	molality	molality	molality
H2O		55.5087		55.5087	55.5087	55.5087		55.5087	55.5087
ACETACID									
ACET2									
H2SO4		1.64E-24		8.06E-20	2.72E-19	1.64E-24		1.77E-19	5.58E-19
HCL									
SO3		2.12E-28		2.88E-23	1.62E-22	2.12E-28		6.34E-23	3.32E-22
LIOH									
NAACET									
PBACET2	PbAce2								
PBCL2	PbCl20								
PBO		4.01E-10		9.02E-09	2.33E-08	4.01E-10		1.35E-08	3.69E-08
LIACET									
OHION		5.71E-09		8.12E-09	1.34E-08	5.71E-09		8.40E-09	1.43E-08
CLION	Cl-								
HION		1.88E-06		4.56E-05	6.22E-05	1.88E-06		5.57E-05	7.37E-05
HPBO2ION		2.52E-15		3.23E-14	1.06E-13	2.52E-15		4.80E-14	1.73E-13
HSO4ION		2.37E-08		8.25E-05	2.08E-04	2.37E-08		1.82E-04	4.42E-04
LIION									
LISO4ION									
NAION									
NASO4ION									
ACETATEION									
PBACET3ION	PbAce3-								
PBACETION	PbAce+								
PBCL3ION	PbCl3-								
PBCL4ION	PbCl4--								
PBCLION	PbCl+								
PBION	Pb++	1.47E-04		0.00787318	0.00773127	1.47E-04		0.0237663	0.0234879
PBOHION	PbOH+	1.90E-06		1.28E-04	2.70E-04	1.90E-06		2.38E-04	5.16E-04
SO4ION		1.48E-04		0.00791873	0.00779339	1.48E-04		0.0238219	0.0235615
PBSO4			1				1		
NACL									
LICL									
LI2SO4.1H2O									
LI2SO4									
LIACET.2H2O									
LICL.1H2O									
LICL.2H2O									
LIOH.1H2O									
NA2SO4.10H2O									
NA2SO4									
NA3HSO42									
NAACET.3H2O									
NAHSO4									
NAOH.1H2O									
NAOH									
PBHSO42									
PBOH2									
Total g/hr		999.894	2.3811	1002.28	1002.28	999.894	7.23332	1007.13	1007.13
Volume, m3/hr		0.00100301	3.76E-07	0.00102858	0.00104309	0.00100301	1.14E-06	0.00102863	0.00104311
Enthalpy, cal/hr		-3.79E+06	-1726.33	-3.74E+06	-3.72E+06	-3.79E+06	-5244.25	-3.74E+06	-3.72E+06
Density, g/m3		9.97E+05	6.32E+06	9.74E+05	9.61E+05	9.97E+05	6.32E+06	9.79E+05	9.66E+05
Vapor fraction									
Solid fraction			1				1		
Organic fraction									
Osmotic Pres, atm		0.00694981		0.332325	0.338766	0.00694981		0.807405	0.822341
Redox Pot, volts									
E-Con, 1/ohm-cm		4.35E-05		0.00458415	0.00552881	4.35E-05		0.0124207	0.014987
E-Con, cm2/ohm-mol		5.45124		589.394	720.881	1.81708		532.349	651.382
Abs Visc, cP		0.890996		0.356378	0.283348	0.890996		0.359893	0.286181
Rel Visc		1.00031		1.0062	1.00629	1.00031		1.01612	1.01635
Ionic Strength		5.92E-04		0.0317119	0.0313193	5.92E-04		0.095414	0.0946149

		PbSO4 only, Pb++ 99.9% T>80oC			
Inputs		55.58			55.58
log(free Cl-)		#VALUE!	#VALUE!	#VALUE!	#VALUE!
free Pb++ percentage		0.1831875		99.537125	98.957125
H2O (mol)		55.5	55.5	55.5	55.5
NaCl (mol)					
LiCl (mol)					
HCl (mol)					
PbCl2 (mol)					
Pb(CH3CO2)2 (mol)					
PbSO4 (mol)		0.08	0.08	0.08	0.08
Total Pb (ppm)		16577.75724	16577.75724	16577.75724	16185.7613
Stream		T25oC	T25oC	T80oC	T100oC
Phase		Aqueous	Solid	Aqueous	Aqueous
Temperature, C		25	25	80	100
Pressure, atm		1	1	1	1
pH		5.73849		4.35769	4.24442
Total mol/hr		55.5003	0.0798516	55.6597	55.6593
Flow Units		molality	molality	molality	molality
H2O		55.5087		55.5087	55.5087
ACETACID					
ACET2					
H2SO4		1.64E-24		2.85E-19	8.73E-19
HCL					
SO3		2.12E-28		1.02E-22	5.19E-22
LIOH					
NAACET					
PBACET2	PbAce2				
PBCL2	PbCl20				
PBO		4.01E-10		1.72E-08	4.79E-08
LIACET					
OHION		5.71E-09		9.92E-09	1.68E-08
CLION	Cl-				
HION		1.88E-06		6.83E-05	8.90E-05
HPBO2ION		2.52E-15		6.32E-14	2.37E-13
HSO4ION		2.37E-08		3.15E-04	7.59E-04
LIION					
LISO4ION					
NAION					
NASO4ION					
ACETATEION					
PBACET3ION	PbAce3-				
PBACETION	PbAce+				
PBCL3ION	PbCl3-				
PBCL4ION	PbCl4--				
PBCLION	PbCl+				
PBION	Pb++	1.47E-04		0.0796297	0.0791657
PBOHION	PbOH+	1.90E-06		3.83E-04	8.48E-04
SO4ION		1.48E-04		0.079698	0.0792546
PBSO4			1		
NACL					
LICL					
LI2SO4.1H2O					
LI2SO4					
LIACET.2H2O					
LICL.1H2O					
LICL.2H2O					
LIOH.1H2O					
NA2SO4.10H2O					
NA2SO4					
NA3HSO42					
NAACET.3H2O					
NAHSO4					
NAOH.1H2O					
NAOH					
PBHSO42					
PBOH2					
Total g/hr		999.894	24.2161	1024.11	1024.11
Volume, m3/hr		0.00100301	3.83E-06	0.00102911	0.00104348
Enthalpy, cal/hr		-3.79E+06	-17557	-3.75E+06	-3.73E+06
Density, g/m3		9.97E+05	6.32E+06	9.95E+05	9.81E+05
Vapor fraction					
Solid fraction			1		
Organic fraction					
Osmotic Pres, atm		0.00694981		1.69549	1.73876
Redox Pot, volts					
E-Con, 1/ohm-cm		4.35E-05		0.0351338	0.0424026
E-Con, cm2/ohm-mol		0.545124		451.956	553.078
Abs Visc, cP		0.890996		0.3714	0.295452
Rel Visc		1.00031		1.04862	1.04927
Ionic Strength		5.92E-04		0.319039	0.317689

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PbSO4 +HCl, still not soluble at 25oC				PbSO4 only, 50, 65 oC				PbSO4 only, 30, 35, 40 oC						soluble above 40oC ----> PbSO4 only, 50, 65 oC		
55.525			55.525	55.525			55.525	55.525						55.525		
	#VALUE!	-3.12351658	-3.15215599		#VALUE!	#VALUE!	#VALUE!		#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!		#VALUE!	#VALUE!
0.67675		98.76583333	97.8875	0.610625		99.72833333	99.47666667	0.658166667						99.80291667		99.7575
55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03	1.00E-03
0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024
4973.11828	4973.11828	4973.11828	4937.447873	4973.327173	4973.327173	4973.327173	4937.594948	4973.307277	4973.307277	4973.307277	4973.307277	4973.307277	4973.307277	4937.594948	4937.594948	4937.594948
T25oC	T25oC	T80oC	T100oC	ec	T25oC	T50oC	T65oC	T30oC	T30oC	T35oC	T35oC	T40oC	T40oC	T43oC	T45oC	T47.5oC
Aqueous	Solid	Aqueous	Aqueous	Aqueous	Solid	Aqueous	Aqueous	Aqueous	Solid	Aqueous	Solid	Aqueous	Solid	Aqueous	Aqueous	Aqueous
25	25	80	100	25	25	50	65	30	30	35	35	40	40	43	45	47.5
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
3.02476		3.72865	3.88385	5.73849		4.6521	4.50222	5.63615		5.53815		5.44433		4.73382	4.70967	4.68039
55.5023	0.0238339	55.5489	55.5487	55.5003	0.0238516	55.5479	55.5479	55.5003	0.0238397	55.5003	0.0238277	55.5004	0.0238157	55.5479	55.5479	55.5479
molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
55.5087		55.5087	55.5087	55.5087		55.5087	55.5087	55.5087		55.5087		55.5087		55.5087	55.5087	55.5087
4.23E-19		3.53E-18	3.15E-18	1.64E-24		2.26E-20	6.70E-20	3.14E-24		5.92E-24		1.10E-23		1.31E-20	1.53E-20	1.86E-20
5.33E-13		1.55E-12	2.58E-12													
5.47E-23		1.26E-21	1.87E-21	2.12E-28		4.29E-24	1.71E-23	4.34E-28		8.77E-28		1.75E-27		2.19E-24	2.66E-24	3.38E-24
1.23E-08		5.60E-07	7.34E-07													
1.55E-15		6.67E-10	6.43E-09	4.01E-10		2.75E-09	6.18E-09	5.14E-10		6.51E-10		8.14E-10		1.87E-09	2.09E-09	2.40E-09
1.12E-11		1.86E-09	5.94E-09	5.71E-09		3.37E-09	5.43E-09	6.52E-09		7.39E-09		8.31E-09		2.66E-09	2.85E-09	3.10E-09
9.96E-04		7.52E-04	7.04E-04													
9.88E-04		2.51E-04	1.77E-04	1.88E-06		2.97E-05	4.21E-05	2.38E-06		2.99E-06		3.71E-06		2.46E-05	2.60E-05	2.78E-05
1.92E-23		5.23E-16	1.25E-14	2.52E-15		6.05E-15	1.74E-14	3.36E-15		4.40E-15		5.67E-15		3.62E-15	4.20E-15	5.04E-15
1.20E-05		8.02E-04	0.00103902	2.37E-08		3.93E-05	8.73E-05	3.72E-08		5.78E-08		8.87E-08		2.65E-05	2.97E-05	3.42E-05
5.96E-12		1.99E-10	2.56E-10													
4.06E-15		1.02E-13	1.17E-13													
3.72E-06		2.47E-04	2.94E-04													
1.62E-04		0.0237038	0.023493	1.47E-04		0.0239348	0.0238744	1.58E-04		1.69E-04		1.81E-04		0.0239527	0.0239481	0.0239418
3.86E-09		5.28E-05	2.16E-04	1.90E-06		6.90E-05	1.29E-04	2.41E-06		3.04E-06		3.79E-06		5.11E-05	5.57E-05	6.20E-05
1.54E-04		0.0232019	0.0229649	1.48E-04		0.0239645	0.0239165	1.60E-04		1.72E-04		1.84E-04		0.0239773	0.0239741	0.0239696
	1				1				1		1		1			
999.936	7.22796	1007.16	1007.16	999.894	7.23332	1007.13	1007.13	999.898	7.22971	999.901	7.22608	999.905	7.22245	1007.13	1007.13	1007.13
0.00100303	1.14E-06	0.00102867	0.00104315	0.00100301	1.14E-06	0.00101209	0.00101959	0.00100446	1.14E-06	0.00100609	1.14E-06	0.00100789	1.14E-06	0.00100912	0.00100993	0.00101099
-3.79E+06	-5240.35	-3.74E+06	-3.72E+06	-3.79E+06	-5244.25	-3.77E+06	-3.76E+06	-3.79E+06	-5238.65	-3.78E+06	-5233.05	-3.78E+06	-5227.45	-3.78E+06	-3.78E+06	-3.77E+06
9.97E+05	6.32E+06	9.79E+05	9.66E+05	9.97E+05	6.32E+06	9.95E+05	9.88E+05	9.95E+05	6.32E+06	9.94E+05	6.32E+06	9.92E+05	6.32E+06	9.98E+05	9.97E+05	9.96E+05
	1				1				1		1		1			
0.0505751		0.827987	0.842271	0.00694981		0.769715	0.790557	0.00760471		0.00827393		0.0089532		0.758797	0.761988	0.765897
4.57E-04		0.0125842	0.0151223	4.35E-05		0.00849462	0.0104305	5.21E-05		6.16E-05		7.21E-05		0.00761246	0.00786243	0.00817726
18.3239		521.263	657.28	1.81708		358.221	443.115	2.18038		2.58423		3.02944		320.078	330.855	344.463
0.89098		0.359815	0.286131	0.890996		0.55557	0.440112	0.798339		0.720282		0.653849		0.627616	0.605544	0.57968
1.00029		1.0159	1.01617	1.00031		1.01526	1.01579	1.00033		1.00035		1.00037		1.01494	1.01504	1.01515
0.00163319		0.0948638	0.0941309	5.92E-04		0.0958675	0.0957112	6.39E-04		6.86E-04		7.33E-04		0.095911	0.0959	0.0958847

J. Yang 8/14/02

05/10/01

	Pb Acetate only, ~20% dissociation			Low PbCl2 only, ~70% dissociation			High PbCl2, ~50% dissociation			High PbCl2 + HCl, ~40% dissociation			High PbCl2 + HCl, ~50% dissociation		
Inputs	55.508			55.508			55.524			55.548			55.525		
log(free Cl-)	#VALUE!	#VALUE!	#VALUE!	-1.8411161	-1.8641965	-1.8786667	-1.4092551	-1.4456332	-1.46690316	-1.221682	-1.249497005	-1.265039439	-1.399787513	-1.43607891	-1.457362518
free Pb++ pe	35.2255	23.760125	17.766	80.795	71.45	65.805	65.38375	54.1108333	48.0741667	55.804583	43.835	37.80508333	64.96625	53.80791667	47.84333333
H2O (mol)	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
NaCl (mol)															
LiCl (mol)															
HCl (mol)										0.0240	0.0240	0.0240	0.0010	0.0010	0.0010
PbCl2 (mol)				0.008	0.008	0.008	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024	0.024
Pb(CH3CO2	0.008	0.008	0.008												
PbSO4 (mol)															
Total Pb (p	1653.54881	1653.54881	1653.54881	1654.17586	1654.17586	1654.17586	4940.58737	4940.58737	4940.58737	4936.2716	4936.27159	4936.27159	4938.330453	4938.330453	4938.330453
Stream	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC	T25oC	T80oC	T100oC
Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature	25	80	100	25	80	100	25	80	100	25	80	100	25	80	100
Pressure, atr	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
pH	6.51121	5.78951	5.6155	5.01191	4.22524	4.01052	4.87276	4.10336	3.8972	1.7128	1.72158	1.72502	3.08643	3.08946	3.0856
Total mol/hr	55.5179	55.5163	55.5152	55.5224	55.5216	55.5212	55.563	55.5598	55.5581	55.608	55.6043	55.6023	55.5879	55.5847	55.5829
Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
H2O	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
ACETACID	1.67E-04	9.41E-04	0.00140676												
ACET2	4.32E-16	6.33E-14	2.09E-13												
H2SO4															
HCL				7.24E-14	1.02E-11	4.12E-11	2.54E-13	3.31E-11	1.29E-10	5.56E-10	1.22E-08	2.99E-08	1.59E-11	3.49E-10	8.56E-10
SO3															
LIOH															
NAACET															
PBACET2	3.49E-04	8.34E-04	0.00111357												
PBCL2				5.79E-05	1.14E-04	1.55E-04	7.12E-04	0.00120603	0.00151997	0.0012932	0.00210902	0.00261222	7.35E-04	0.00124544	0.00156987
PBO	1.91E-07	1.66E-06	2.78E-06	3.94E-10	3.21E-09	5.37E-09	3.90E-10	3.18E-09	5.33E-09	1.48E-16	4.06E-14	1.72E-13	1.03E-13	2.96E-11	1.26E-10
LIACET															
OHION	3.73E-08	1.73E-07	2.57E-07	1.23E-09	4.92E-09	6.69E-09	9.82E-10	4.03E-09	5.58E-09	6.93E-13	1.72E-11	3.87E-11	1.61E-11	3.91E-10	8.62E-10
CLION				0.0144173	0.0136711	0.0132231	0.0389713	0.0358399	0.0341269	0.060023	0.0562993	0.0543201	0.0398302	0.0366371	0.0348849
HION	3.46E-07	1.83E-06	2.73E-06	1.12E-05	6.92E-05	1.14E-04	1.64E-05	9.77E-05	1.58E-04	0.0240038	0.0240041	0.0240045	0.00100042	0.00100953	0.00102432
HPBO2ION	7.76E-12	1.29E-10	2.47E-10	5.21E-16	7.02E-15	1.23E-14	3.97E-16	5.61E-15	1.01E-14	1.07E-25	3.06E-22	2.25E-21	1.72E-21	5.05E-18	3.67E-17
HSO4ION															
LIION															
LISO4ION															
NAION															
NASO4ION															
ACETATEIO	0.00992488	0.00823729	0.00720813												
PBACET3IO	2.73E-04	4.15E-04	5.50E-04												
PBACETION	0.00439465	0.00391021	0.00350981												
PBCL3ION				4.08E-07	7.35E-07	1.01E-06	1.36E-05	2.04E-05	2.56E-05	3.86E-05	5.70E-05	7.12E-05	1.44E-05	2.16E-05	2.71E-05
PBCL4ION				4.98E-09	5.00E-09	6.25E-09	5.24E-07	4.24E-07	4.75E-07	2.44E-06	2.00E-06	2.27E-06	5.67E-07	4.59E-07	5.15E-07
PBCLION				0.00146812	0.00210134	0.00246722	0.00756908	0.00969268	0.0107621	0.0092764	0.0113151	0.0122441	0.00766133	0.009813	0.0108997
PBION	0.00281804	0.00190081	0.00142128	0.0064636	0.005716	0.0052644	0.0156921	0.0129866	0.0115378	0.0133931	0.0105204	0.00907322	0.0155919	0.0129139	0.0114824
PBOHION	1.66E-04	9.39E-04	0.00140365	1.12E-05	6.92E-05	1.14E-04	1.63E-05	9.77E-05	1.58E-04	9.15E-09	3.08E-07	7.78E-07	2.65E-07	9.38E-06	2.42E-05
SO4ION															
PBSO4															
NACL															
LICL															
LI2SO4.1H2(															
LI2SO4															
LIACET.2H2(															
LICL.1H2O															
LICL.2H2O															
LIOH.1H2O															
NA2SO4.10I															
NA2SO4															
NA3HSO42															
NAACET.3H															
NAHSO4															
NAOH.1H2O															
NAOH															
PBHSO42															
PBOH2															
Total g/hr	1002.45	1002.45	1002.45	1002.07	1002.07	1002.07	1006.52	1006.52	1006.52	1007.4	1007.4	1007.4	1006.98	1006.98	1006.98
Volume, m3/l	0.00100357	0.00102914	0.00104368	0.00100317	0.00102874	0.00104325	0.00100352	0.0010291	0.00104359	0.001004	0.00102955	0.00104402	0.00100396	0.00102954	0.00104404
Enthalpy, cal	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06	-3.79E+06	-3.74E+06	-3.72E+06
Density, g/m:	9.99E+05	9.74E+05	9.61E+05	9.99E+05	9.74E+05	9.61E+05	1.00E+06	9.78E+05	9.64E+05	1.00E+06	9.78E+05	9.65E+05	1.00E+06	9.78E+05	9.65E+05
Vapor fractio															
Solid fraction															
Organic fract															
Osmotic Pre:	0.398979	0.441381	0.44882	0.496001	0.548371	0.557701	1.34727	1.4627	1.47646	2.30507	2.56226	2.62153	1.38485	1.50333	1.51697
Redox Pot, v															
E-Con, 1/ohr	8.42E-04	0.00134847	0.00120263	0.00195608	0.00413712	0.00480857	0.00507711	0.0102679	0.0116704	0.0139325	0.0246203	0.0274052	0.00544585	0.0108291	0.0122636
E-Con, cm2/	105.598	169.936	140.389	245.286	532.001	627.068	212.291	440.277	507.461	291.411	528.078	596.075	218.605	445.776	511.934
Abs Visc, cP	0.896579	0.356447	0.283403	0.893308	0.355564	0.28271	0.897024	0.357695	0.284459	0.897929	0.358398	0.285051	0.897047	0.357715	0.284474
Rel Visc	1.00658	1.0064	1.00648	1.00291	1.0039	1.00402	1.00708	1.00992	1.01023	1.00809	1.0119	1.01234	1.0071	1.00998	1.01028
Ionic Strengt	0.0130155	0.0105535	0.00918003	0.0208813	0.0193878	0.0184885	0.0546785	0.0488481	0.0456917	0.073462	0.0668827	0.0634713	0.0554381	0.0495741	0.046396

J. Yang 8/29/02

Below 40℃, solid $PbSO_4$ forms, but above 40℃, No solid forms.

Called OLI, found out that they only have data to 40℃. above 40℃, the software assumed a infinity solubility for $PbSO_4$.

I should not rely on the results for T > 40℃

L.Y.

05/11/01.

L. Yang
8/19/02

May 11/01

OLI Contacted. There is no data for $PbSO_4$ above 40℃. The solubility was assumed infinity at T > 40℃.

Lietai Yang

From: Jim Berthold [Support@olisystems.com]
Sent: Friday, May 11, 2001 10:47 AM
To: Yang Lietai
Subject: PbSO4

pbso4.zip   Databook Tour.PDF   OLI Tips 2 Load DataBase.doc

Lietai,

Attached are several files. The first is the revised lead sulfate database. I extended the applicable temperature range to 100 C. Be advised, we make no guarantee above 40 C. The data is from Seidell. The compressed file is PBSO4.ZIP and contains the OLI/ESP database PBSO4. This is an ESP type database.

The second file is a tour of the OLI/Databook. You should review this since it will help you determine the contents of the database I just provided.

The final file is instructions for importing the database into the OLI/Analyzers. You can not use the ESP format database directly.

To use this database decompress the zip file into the following folder:

c:\oli65\esp

This assumes you have OLI65 installed. If you are still using oli62, then install in \oli62\esp

When decompressed, there will be approximately 39 files.

Take the tour to see how to generate a model with a private database. When you do this for real, substitute PBSO4 for GEOCHEM as explained in the tour.

Give me a call if you have questions.

Jim Berthold
OLI Systems, Inc.
Customer Relations
support@olisystems.com
www.olisystems.com
(973) 539-4996 extension 24
(973) 539-5922 FAX

L. Yang
8/19/02

SOLUBILITIES

INORGANIC AND METAL-ORGANIC COMPOUNDS

K - Z

A Compilation of Solubility Data
from the Periodical Literature

VOLUME II

FOURTH EDITION

by
William F. Linke, Ph.D.
American Cyanamid Co., Stamford, Conn.

A Revision and Continuation of the Compilation
Originated by
Atherton Seidell, Ph.D.
U. S. National Institutes of Health

J. Yang 3/14/02

1965

American Chemical Society
Washington, D.C.

LEAD

LEAD SULFATE $PbSO_4$

SOLUBILITY IN WATER

(Average curve from gravimetric results of Dibbits (1874), Beck and Stegmüller (1910) and Pleissner (1907) and conductivity results of Böttger (1903) and Kohlrausch (1904-05).

t°	Gms. $PbSO_4$ per Liter	t°	Gms. $PbSO_4$ per Liter
0	0.028	20	0.041
5	0.031	25	0.045
10	0.035	30	0.049
15	0.038	35	0.052
18	0.040	40	0.056

Later determinations of the solubility of lead sulfate in water by Crockford and Brawleys, 1934; Purdum and Rutherford, 1933; Kolthoff and Rosenblum, 1933; and Huybrechts and de Langeron, 1930, gave an average curve from which the following values were taken.

t°	Gms. $PbSO_4$ per Liter	t°	Gms. $PbSO_4$ per liter
0	0.0330	25	0.0452
5	0.0354	30	0.0476
10	0.0380	35	0.0500
15	0.0403	40	0.0526
20	0.0427	50	0.0574

Used this J.Y. 05/14/01

Koizumi, 1950 reports that the effect of dissolved CO_2 on the solubility of $PbSO_4$ is negligible.

SOLUBILITY OF LEAD SULFATE IN SULFURIC ACID SOLUTIONS

Results of Crockford and Brawley, 1936; Crockford and Addlestone, 1936

In agreement with Donk, 1916, analyses of the solid phases showed that $PbSO_4$ is the only one at these temperatures. The eutectic temperature for $PbSO_4 + H_2SO_4$ was found to be 5.4°. The acid concentration of 104 percent H_2SO_4 corresponds to 80.5 percent SO_3.

Gms. H_2SO_4 per 1000 gms. aq. solvent	Gms. $PbSO_4$ per 1000 gms. sat. solution at: 0°	25°	35°	50°
0.0	0.033	0.0445	0.0497	0.0577
0.05	0.008	0.0100	0.0110	0.0240
0.1	0.007	0.0080	0.0100	0.0210
0.2	0.0064	0.0070	0.0080	0.0180
0.5	0.0052	0.0060	0.0066	0.0150
1.0	0.0046	0.0052	0.0051	0.0130
2.0	0.0034	0.0038	0.0045	0.0120
5.0	0.0020	0.0025	0.0043	0.0115
10.0	0.0018	0.0022	0.0042	0.0113
50.0	0.0016	0.0020	0.0040	0.0103

(Cont.)

Lietai Yang

From: Lietai Yang [ltyang@gargol.cnwra.swri.edu]
Sent: Monday, May 14, 2001 12:01 PM
To: 'ypan@gargol.cnwra.swri.edu'; 'Darrell Dunn (ddunn)'; 'Gustavo Cragnolino'; 'Vijay Jain (vjain)'
Cc: 'Narasi Sridhar (nsridhar)'
Subject: RE: Initial tests for the effect of trace elements

J.Y. 05/14/01

PbSO4_Solubility.xls

Yi-Ming

Regarding the solubility of PbSO4 in water, I contacted OLI and realized that they only have the data up to 40oC for PbSO4(from Seidell). For temperatures greater than 40oC, they assigned a solubility of infinity. This is why we saw no solids at these temperatures. The OLI results at temperatures above 40oC are wrong.

As suggested by Gustavo, I looked at the book, a revision of Seidell's book, and got the solubility data from 0oC to 50oC. The extrapolation to 100oC shows only about 55ppm of Pb solubility (see enclosed file).

I guess you cannot use PbSO4 in the tests.

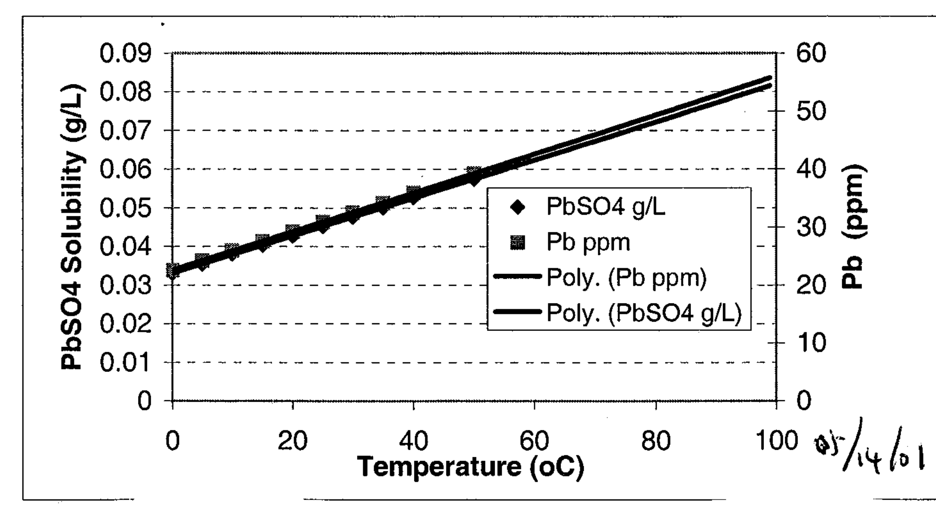
Thanks

Lietai

File: PbSO4_Solubility

Solubility of PbSO4 in Water
MW(PbSO4)= 303.25
AW(Pb)= 207.2

Temp, oC	PbSO4 (g/l	Pb (ppm)
0	0.033	22.54773
5	0.0354	24.18757
10	0.038	25.96406
15	0.0403	27.53556
20	0.0427	29.1754
25	0.0452	30.88356
30	0.0476	32.5234
35	0.05	34.16323
40	0.0526	35.93972
50	0.0574	39.21939
99		



05/14/01

Page 1320, Linke, Solubilities of Inorganic and Metal Organic Compounds -Seidell, Fouth Edition, Volume 2. (1965) American Chemical Society, Washington, D.C.

J. Yang 3/14/02

Lietai Yang

From: Lietai Yang [ltyang@gargol.cnwra.swri.edu]
Sent: Tuesday, May 15, 2001 11:16 AM
To: 'gcragnolino@gargol.cnwra.swri.edu'; 'ypan@gargol.cnwra.swri.edu'; 'Darrell Dunn (ddunn)'; 'Vijay Jain (vjain)'
Cc: 'Narasi Sridhar (nsridhar)'
Subject: RE: Initial tests for the effect of trace elements

Darrell_Pb_Chem_5.xls

Enclosed file shows the amount of NaCl and HCl needed to achieve the same pH and free Cl- concentrations as with the PbCl2 (5000 ppm total Pb) solution. There are two sets of data, one set is to match the pH and Cl- concentration at 25oC and the other set is to match the pH and Cl- at 95oC. The set for 95oC is probably what you want to use.

Yi-Ming, I will do a run to see what is the maximum achievable Pb++ later.

Thanks

Lietai

-----Original Message-----
From: Gustavo Cragnolino [mailto:gcragnolino@gargol.cnwra.swri.edu]
Sent: Monday, May 14, 2001 3:57 PM
To: ltyang@gargol.cnwra.swri.edu; ypan@gargol.cnwra.swri.edu; 'Darrell Dunn (ddunn)'; 'Gustavo Cragnolino'; 'Vijay Jain (vjain)'
Cc: 'Narasi Sridhar (nsridhar)'
Subject: RE: Initial tests for the effect of trace elements

It is obvious from Lietai's findings that we should go ahead with PbCl2.
Lietai, could you do the calculation to see how much HCl should be added to NaCl to have the same pH that that for PbCl2 as a guide for solution preparation.

3/19/02

From: Yi-Ming Pan [mailto:ypan@gargol.cnwra.swri.edu]
Sent: Friday, May 11, 2001 12:06 PM
To: 'Darrell Dunn (ddunn)'; ltyang@gargol.cnwra.swri.edu; 'Gustavo Cragnolino'; 'Vijay Jain (vjain)'
Cc: Narasi Sridhar (nsridhar)
Subject: Initial tests for the effect of trace elements

FYI regarding the initial test conditions based on the conclusion of today's meeting, which will include four polarization curve measurements(i.e., two solutions and two materials).

I. Test Solutions
Solution A (from Leitai's calculation)
Total Pb as PbCl2: 5,000 ppm
Free Pb++ concentration: 2,400 ppm
Cl concentration: 0.034 molal
pH: 3.9
Temperature: 95C

Solution B
NaCl solution with the same Cl concentration and pH in Solution A

II. Test Materials
Crevice specimens for both alloys 22 and 825

Please let me know if you have any questions and/or comments on the initial test conditions.

Thanks,
Yiming

Note:
For the free Pb++ concentration, the calculation for Solution A is based on a 5,000 ppm of PbCl2 that was used by Catholic U. The Pb++ concentration depends on the amount of PbCl2 and the resultant Cl concentration. Leitai will perform additional calculations to determine the maximum. In addition, the reference cited in the database for PbSO4 will be evaluated to confirm the almost complete solubility and dissociation of PbSO4 at temperatures above 45C.

3/19/02

Calculation Results requested by Gustavo: 5/15/01

Results from ESP V6.2e, May 15, 2001

Pb MW=	207.2 mg (appr. pp	1	100	1600	2100	5000
	mM	0.004826255	0.48262548	7.72200772	10.1351351	24.13127413

		PbCl2			NaCl alone			NaCl +HCl			NaCl +HCl		
	Inputs	55.5243			55.5			55.5000164			55.500142		
	log(free Cl-)	-1.404523	-1.4169044	-1.45669574	-1.4044575	-1.4044575	-1.4044575	-1.40535888	-1.4053589	-1.40535888	-1.455343	-1.45534296	-1.455343
	free Pb++ percentage	65.18272	61.227572	49.44074074									
Added	H2O (mol)	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5
	NaCl (mol)				3.94E-02	0.039398	0.039398	3.93E-02	0.0393	0.0393	3.49E-02	0.0349	0.0349
	LiCl (mol)												
	HCl (mol)							1.64E-05	0.0000164	0.0000164	1.42E-04	0.000142	0.000142
	PbCl2 (mol)	0.0243	0.0243	0.0243	0	0	0	0	0	0	0	0	0
	Pb(CH3CO2)2 (mol)												
	PbSO4 (mol)												
	Total Pb (ppm)	5001.897	5001.89746	5001.897458	0	0	0	0	0	0	0	0	0
	Stream	T25oC	T50oC	T95oC	T25oC	T50oC	T95oC	T25oC	T50oC	T95oC	T25oC	T50oC	T95oC
	Phase	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
	Temperature, C	25	50	95	25	50	95	25	50	95	25	50	95
	Pressure, atm	1	1	1	1	1	1	1	1	1	1	1	1
	pH	4.87136	4.48004	3.94454	6.99582	6.63394	6.16706	4.85876	4.86259	4.87051	3.91848	3.92222	3.9307
	Total mol/hr	55.5637	55.5626	55.5593	55.5788	55.5788	55.5788	55.5786	55.5786	55.5786	55.5701	55.5701	55.5701
	Flow Units	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality	molality
	H2O	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087	55.5087
	ACETACID												
	ACET2												
	H2SO4												
	HCL	2.58E-13	2.89E-12	9.50E-11	1.95E-15	2.10E-14	6.42E-13	2.67E-13	1.24E-12	1.27E-11	2.09E-12	9.72E-12	9.95E-11
	SO3												
	LIOH												
	NAACET												
PbAce2	PBACET2												
PbCl20	PBCL2	7.31E-04	8.99E-04	0.00146933									
	PBO	3.90E-10	1.18E-09	4.72E-09									
	LIACET												
	OHION	9.80E-10	2.09E-09	5.17E-09	1.20E-07	2.78E-07	8.31E-07	8.73E-10	4.70E-09	4.20E-08	9.94E-11	5.35E-10	4.78E-09
Cl-	CLION	0.039398	0.0382909	0.0349385	0.0394042	0.0394042	0.0394042	0.0393225	0.0393225	0.0393225	0.0350475	0.0350475	0.0350475
	HION	1.64E-05	4.07E-05	1.42E-04	1.20E-07	2.78E-07	8.31E-07	1.64E-05	1.64E-05	1.64E-05	1.42E-04	1.42E-04	1.42E-04
	HPBO2ION	3.96E-16	1.66E-15	8.80E-15									
	HSO4ION												
	LIION												
	LISO4ION												
	NAION				0.0394042	0.0394042	0.0394042	0.0393061	0.0393061	0.0393061	0.0349055	0.0349055	0.0349055
	NASO4ION												
	ACETATEION												
PbAce3-	PBACET3ION												
PbAce+	PBACETION												
PbCl3-	PBCL3ION	1.41E-05	1.60E-05	2.50E-05									
PbCl4--	PBCL4ION	5.51E-07	4.39E-07	4.81E-07									
PbCl+	PBCLION	0.007702	0.00846979	0.0106534									
Pb++	PBION	0.015839	0.0148783	0.0120141									
PbOH+	PBOHION	1.64E-05	4.07E-05	1.41E-04									
	SO4ION												
	PBSO4												
	NACL												
	LICL												
	LI2SO4.1H2O												
	LI2SO4												
	LIACET.2H2O												
	LICL.1H2O												
	LICL.2H2O												
	LIOH.1H2O												
	NA2SO4.10H2O												
	NA2SO4												
	NA3HSO42												
	NAACET.3H2O												
	NAHSO4												
	NAOH.1H2O												
	NAOH												
	PBHSO42												
	PBOH2												
	Total g/hr	1006.61	1006.61	1006.61	1002.15	1002.15	1002.15	1002.15	1002.15	1002.15	1001.89	1001.89	1001.89
	Volume, m3/hr	0.001004	0.00101256	0.00103971	0.00100367	0.00101273	0.00103991	0.00100367	0.00101273	0.0010399	0.0010036	0.00101265	0.0010398
	Enthalpy, cal/hr	-3.79E+06	-3.77E+06	-3.72E+06	-3.80E+06	-3.77E+06	-3.73E+06	-3.80E+06	-3.77E+06	-3.73E+06	-3.79E+06	-3.77E+06	-3.72E+06
	Density, g/m3	1.00E+06	9.94E+05	9.68E+05	9.98E+05	9.90E+05	9.64E+05	9.98E+05	9.90E+05	9.64E+05	9.98E+05	9.89E+05	9.64E+05
	Vapor fraction												
	Solid fraction												
	Organic fraction												
	Osmotic Pres, atm	1.36239	1.43054	1.49046	1.82257	1.95211	2.15158	1.81885	1.94813	2.14718	1.62415	1.73982	1.91813
	Redox Pot, volts												
	E-Con, 1/ohm-cm	0.00513	0.00762454	0.011466	0.0043955	0.00673052	0.0112319	0.00438687	0.00671736	0.0112101	0.00397137	0.00607298	0.0101191
	E-Con, cm2/ohm-mol	211.851	317.709	490.589	111.976	173.008	296.465	111.988	173.028	296.504	113.739	175.498	300.273
	Abs Visc, cP	0.897091	0.552121	0.300156	0.894471	0.550071	0.298887	0.894464	0.550065	0.298883	0.894106	0.549789	0.298709
	Rel Visc	1.00715	1.00896	1.01029	1.00421	1.00522	1.00602	1.0042	1.0052	1.006	1.0038	1.0047	1.00542
	Ionic Strength	0.055253	0.0531866	0.0469792	0.0394043	0.0394044	0.039405	0.0393225	0.0393226	0.0393226	0.0350475	0.0350475	0.0350475

Continued on page 175

J. Yang 8/19/02

08/17/01

- OLI ESP V6.5/CSP V2.2

Installation test

The following results were obtained with OLI ESP6.5/CSP V2.2. The out streams ~~is~~ are (J.Y. 08/17/01) the outlets of a Mixer Unit. The input was specified such that the outlet streams have three phases at equilibrium. Therefore the deliquescence point can be calculated using

$$RH\% = \frac{P_{H_2O}}{P^0_{H_2O}} \times 100\%$$

$P^0_{H_2O}$ (pure water pressure) ; P_{H_2O} (saturated solution pressures)

Pure Water			Saturated MgCl2.6H2O			Saturated KCl			Saturated KNO3		
Stream	out	out	out	out	out	out	out	out	out	out	out
Phase	Aqueous	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor	Aqueous	Solid	Vapor
Temperature, C	50	50	50	50	50	50	50	50	50	50	50
Pressure, atm	0.122062	0.122062	0.042846	0.042846	0.042846	0.099473	0.099473	0.099473	0.108012	0.108012	0.108012
pH	6.63553		4.02062			6.53346			6.67919		
Total mol/hr	55.5494	5.56E-04	31.65322	5.6	2.91E-04	67.43978	4.01989	6.56E-04	73.64116	0.954069	6.56E-04
Flow Units	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr	mol/hr
H2O	55.5494	5.56E-04	23.6979		2.91E-04	55.5493		6.56E-04	55.5493		6.56E-04
HCL			9.19E-10		1.05E-09	1.19E-12		4.15E-14			
KCL						0.069739	4.01989				
NANO3											
OHION	2.32E-07		3.32E-10			1.17E-07					
HION	2.32E-07		4.29E-06			1.17E-07					
KION						5.91037			9.04593		
NO3ION									9.04593		
KNO3										0.954069	
MGION			2.65177								
MGOHION			4.29E-06								
CLION			5.30354			5.91037					
MGCL2.6H2O				5.6							
Total g/hr	1000.74	0.010008	679.404	1138.5	0.005242	1446.57	299.688	0.011809	1915.31	96.4595	0.011809
Volume, L/hr	1.01296	0.120502	0.520828	0.72576	0.179988	1.19307	0.150826	0.174532	1.42356	0.045738	0.160719
Enthalpy, cal/hr	-3.77E+06	-31.9963	-2.11E+06	-3.33E+06	-16.7588	-4.37E+06	-4.18E+05	-37.7559	-4.77E+06	-1.12E+05	-37.756
Density, g/L	987.94	0.083049	1304.47	1568.7	0.029123	1212.47	1986.97	0.067661	1345.44	2108.95	0.073477
Vapor fraction		1			1			1			1
Solid fraction				1			1			1	
Organic fraction											
Osmotic Pres, atm			1685.61			306.311			167.504		
Redox Pot, volts											
E-Con, 1/ohm-cm	1.69E-07		0.119412			0.626119			0.438156		
E-Con, cm2/ohm-mol			5.96409			56.0055			49.1453		
Abs Visc, cP	0.547218		8.07183			0.690691			0.889968		
Rel Visc	1		14.7507			1.26219			1.62635		
Ionic Strength	2.32E-07		18.6341			5.90604			9.03931		

Relative Humidities at 50oC

Rel. Hum%	1	35.10142387	81.49407678	88.48945618
ASTM Value	Value	35	81.2	84.8
	Error	+-0.1	+-0.3	+-2.5

J. Yang 8/17/01

J.Y. 08/17/01

~~From the table in page 115.~~

The calculated Rel. Humidity (deliquescence point) for the saturated salts are given at the bottom of the table in page 115.

The ASTM values (see page 117) are also given in table of page 115.

The calculated RH values are close to the ASTM values, although it should be noted that for $MgCl_2 \cdot 6H_2O$. The error is $\frac{35.1 - 30.5}{30.5} = 0.15 = 15\%$ which is quite significant.

J. Yang 08/17/01

E 104 — page 3 (ASTM)

12. Keywords

ANNEXES

(Mandatory Information)

A1. EQUILIBRIUM RELATIVE HUMIDITY VALUES FOR SELECTED SATURATED AQUEOUS SALT SOLUTIONS

Information potentially subject to copyright protection was redacted from this location. The redacted material was extracted from an ASTM manual.

J. Yang 8/17/01

SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE	
2. Project Title: Evolution of Near Field Environment and Container Life Source Term	Project No. 20-01402-561 and 20-01402-571
3. SRN Title: OLI Software ESP V.6.5 and CSP V2.2	
4. Originator/Requestor: L. Yang	Date: 08/17/01

5. Summary of Actions

- ■ Release of new software
- ☐ Release of modified software:
  - ☐ Enhancements made
  - ☐ Corrections made
- ☐ Change of access software
- ☐ Software Retirement

6. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
N. Sridhar	RO	A
L. Yang	RO	A
R. Pabalan	RO	A
V. Jain	RO	A

7. Element Manager Approval: Date:

8. Remarks: Installation test was performed by L. Yang on 08/17/01 and the results compares with ESP6.2 (scientific Notebook # 430, p.115).

The comparison with literature data is recorded in Scientific Notebook #430, pages 116 to 117.

CNWRA Form TOP-6 (05/98)

L.Y. 08/17/01

SOFTWARE SUMMARY FORM

01. Summary Date: 08/17/01	02. Summary prepared by (Name and phone) L. Yang (210)522 2483	03. Summary Action: Updating
04. Software Date: 03/26/2001	05. Short Title: OLI Software ESP 6.5 and CSP V2.2	
06. Software Title: ESP6.5/CSP2.2		07. Internal Software ID:

08. Software Type:
- ☐ Automated Data System
- ■ Computer Program
- ☐ Subroutine/Module

09. Processing Mode:
- ■ Interactive
- ☐ Batch
- ☐ Combination

10. Application Area

a. General:
- ■ Scientific/Engineering
- ☐ Auxiliary Analyses
- ☐ Total System PA
- ☐ Subsystem PA
- ☐ Other

b. Specific:

11. Submitting Organization and Address:

CNWRA/SwRI
6220 Culebra Road
San Antonio, TX 78228

12. Technical Contact(s) and Phone:

N. Sridhar (210) 522-5538
L. Yang (210) 522-2483

13. Software Application:
This software predicts the speciation of an aqueous solution at given some chemistry conditions. It also predicts metals stability diagrams.

14. Computer Platform PC	15. Computer Operating System: Windows NT/95/98	16. Programming Language(s): N/A	17. Number of Source Program Statements: N/A
18. Computer Memory Requirements: 40 MB	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements
16 MB RAM required, single user hardware key required

23. Software Availability: ☐ Available ■ Limited ☐ In-House ONLY

24. Documentation Availability: ■ Available ☐ Preliminary ☐ In-House ONLY

25. It is required that OLI systems be paid an annual fee to obtain a "Hardware Key" to allow access each year

Software User: N. Sridhar and L. Yang Date: 08/18/01

CNWRA Form TOP-4-1 (05/98)

L.Y. 08/17/01

Simulation of Evaporation Process for YM waters

Lietai Yang

From: Roberto Pabalan [rpabalan@gargol.cnwra.swri.edu]
Sent: Tuesday, September 04, 2001 11:34 AM
To: Lietai Yang
Subject: YM water compositions for OLI simulation

YM waters to simulate.doc

Lietai:

See attached file giving the YM water compositions for evaporative simulation using the OLI software.

Thanks.

bobby

Software version 6.7.

use total pressure of 0.85 Bar

and f_{CO_2} = 1.02E-3 Bar

— Bobby. 09/04/01

J. Yang 8/14/02

09/10/01

Yucca Mountain water compositions for OLI simulation.

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

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

Sample Name:		
	UZ-14/1542.3-1542.8	UZ_a
	UZ-14/85.2-85.6	UZ_b
	NRG-6/158.2-158.6	NRG_a
	NRG-6/244.6-245.0	NRG_b
	Average J13	AVG-J13

J. Yang 8/14/02

Chemistry model:

YM_Water

Using Water Analyzer of OLI Tool kit ~~of ESP 6.5~~

With Sample Manager. The samples of Ion inputs were reconciled:

Sample: UZ_B

Template Reconcile Units LastResult Help

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	49.9	51.2303	CL-1	60.	59.99975
MG+2	13.2	13.19999	CO3-2		
NA+1	43.5	43.5	HCO3-1	131.	130.9997
AL+3	0.3	0.299999	NO3-1	22.	21.99999
			SO4-2	66.	65.99991

Calc. pH 7.6863

<PgDn>

~~SiO_2: 143 mg/L = 0.00238 mol/kg~~ ; added ~ 1 mg/L Ca^{++} for reconciliation J.y. 09/18/01

Note: Neutral SiO_2 not included here as it is neutral, it can't be included in ESP directly.

SiO_2: 89.8 mg/L = 1.498 E-3 mol/kg.

J. Yang 8/10/02

Sample UZ-A, Calculated reconciled pH = 7.31

Template Reconcile Units LastResult Help

YM_Water Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	3.6	3.599623	CL-1	20.	19.99789
MG+2	0.5	0.4999487	CO3-2	46.	45.99516
NA+1	207.	206.9782	HCO3-1	384.	488.9661
AL+3	13.8	13.79854	NO3-1	4.	3.999582
			SO4-2	28.	27.99708

<PgDn>

not included : SiO_2 : 143 ~~84.8~~ mg/L = 0.00238 mol/kg ~~= 1.498 E-3 mol/kg~~
added HCO_3^{-1} during reconciliation. J.y. 09/18/01

Sample: NRG-A, Calculated pH = 7.93

Template Reconcile Units LastResult Help

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	122.	122.959	CL-1	185.	184.9998
MG+2	23.3	23.29997	CO3-2		
NA+1	35.6	35.59985	HCO3-1	34.	33.99998
AL+3			NO3-1	32.	31.99995
			SO4-2	159.	158.9996

1.621E-3 mol/kg

J. Yang 8/10/02

Not included: SiO_2 : 97.4 mg/L , added Ca^{+2}

Sample NRG-B

lculate pH Reconcile pH Help

YM_WATER Study
YM_WATER Model
Sample NRG_B

Sample NRG_B

Measured pH: 0.0

Calculated pH: 7.4225

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	33.	32.99988	CL-1	49.	48.99978
MG+2	4.9	4.899972	CO3-2		
NA+1	72.	75.96943	HCO3-1	61.	60.99961
AL+3	0.6	0.5999973	NO3-1	40.	39.99986
			SO4-2	115.	114.9992

~~Not included: SiO_2: 51 mg/L~~ ; 0.849 E-3 mol/kg added Na+ to reconcile.

Sample AVG_J13, Calculated pH: 8.07

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			CL-1	7.14	7.139547
CA+2	13.	12.9992	CO3-2		
K+1	45.8 (5.04)	45.79733	F-1	2.18	2.179869
MG+2	2.01	2.009874	HCO3-1	128.9	191.3923
NA+1	45.8	45.79708	NO3-1	8.78	8.779436
			SO4-2	18.4	18.39886

w/James 11/27/01 wrong page 132

1.01E-3 mol/kg ← Not included: SiO_2: 61 mg/L; ~ 60 mg HCO_3-1 was added

The above files are converted into OLI stream files using OLI Stream Manager under: OLI Toolkit.

new OLI stream files.

original files

Utility Send Help

YM_WATER Study
YM_WATER Model
Sample AVG_J13

WORKING WITH WHICH ESP STREAM?

New OLI Stream	Based On:	Sent To:
AVG_J13	AVG_J13	
NRG_B	NRG_B	
NRG_A	NRG_A	
UZ_B	UZ_B	
UZ_A	UZ_A	

Successfully created OLI Stream AVG_J13
<Esc> Quit <F1> Help <F3> End (Save) <F10> Actions <Enter> Continue

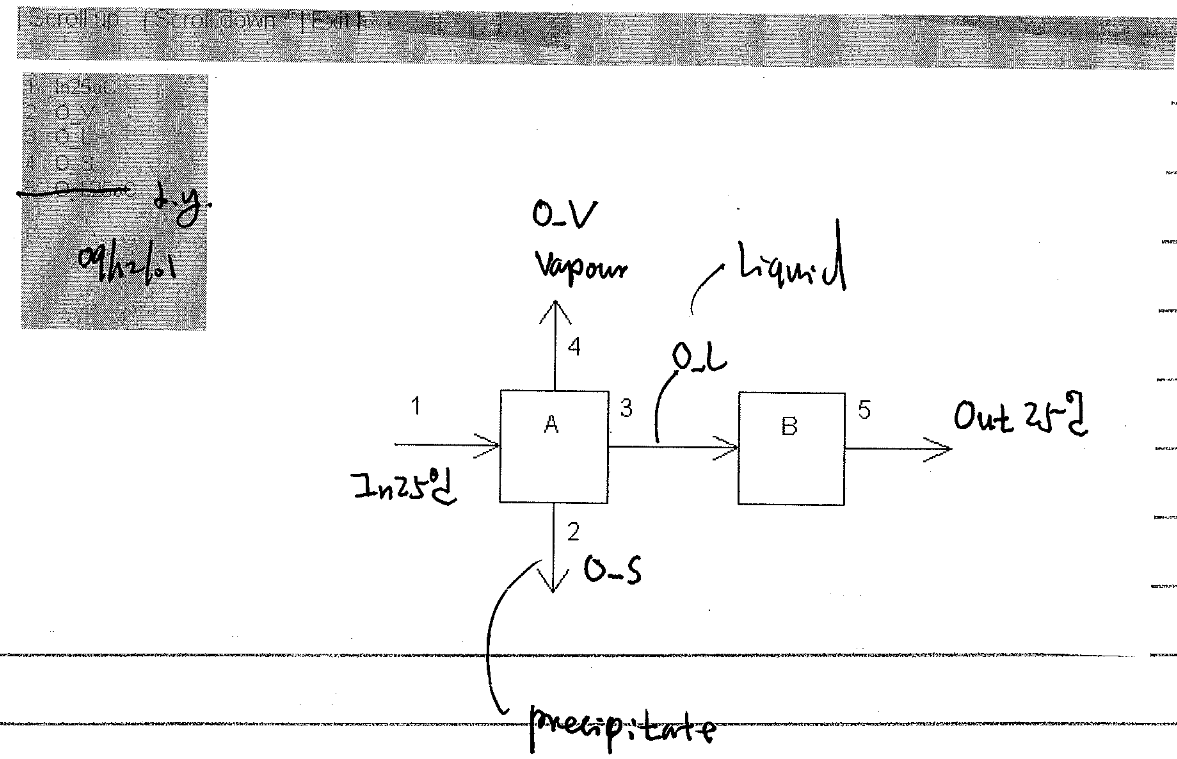
J. yar 8/14/02

Back to ESP. Created a new Process

YM_Water — process Name

~~YM_Water — process~~ J.y. 09/12/01

Process Build:



A — a Separator,

B — a Mixer.

A — set to ~~Isothermal~~ Dewpoint operation at constant P = 0.85 atm. J.y. 12/13/01

B — set to Isothermal at const. 25°C.

Stream Out 25°C is the composition for liquid sampled at the O_L stream condition (T and P). J. Yang 8/14/02

Load the OLI stream files in Page 125 for In25°C.
" *.smp "

YM_WATER Study
YM_WATER Model
OLI Stream UZ_A

OLI Stream UZ_A

ALOH3	0.511914E-03			
CAOH2	0.899044E-04			
H2CO3	0.864287E-02			
HCL	0.564627E-03			
HNO3	0.645682E-04			
MGOH2	0.205902E-04			
NA6SO42CO3	0.145866E-03			
NAOH	0.813669E-02			
SCALE ALOH3PPT	0.100000D+01	273.150	373.150	
SCALE ALOOHPPT	0.738618D+00	373.250	523.150	EXCL TR
SCALE NAALCO3OH2PPT	0.121568D+00			
SCALE CACO3PPT	0.114807D+00			

<PgUp> <PgDn>

SiO_2 to add: 2.38 E-3 mol/kg.
H_2O 55.508 mol

YM_WATER Study
YM_WATER Model
OLI Stream UZ_B

OLI Stream UZ_B

ALOH3	0.111237E-04			
CAOH2	0.127884E-02			
H2CO3	0.186058E-02			
HCL	0.169314E-02			
HNO3	0.354971E-03			
MGOH2	0.543344E-03			
NA3HSO42	0.563604E-04			
NA6SO42CO3	0.287317E-03			
SCALE ALOH3PPT	0.100000D+01	273.150	373.150	
SCALE CACO3PPT	0.100000D+01			
SCALE ALOOHPPT	0.738477D+00	373.250	523.150	EXCL TR
SCALE CASO4.2H2O	0.130814D-01	273.150	373.150	

<PgUp> <PgDn>

SiO_2: 1.495E-3 mol/kg.

J. Yang 8/14/02

```
                                          YM_WATER Study
                                          YM_WATER Model
OLI Stream NRG_A                          OLI Stream NRG_A

CAOH2            0.307026E-02
H2CO3            0.557630E-03
H2SO4            0.623280E-03
HCL              0.522202E-02
HNO3             0.516468E-03
MGOH2            0.959356E-03
NA3HSO42         0.516545E-03
SCALE CACO3PPT             0.969737D+00
SCALE CASO4.2H2O           0.565979D-01   273.150   373.150
SCALE CASO4PPT             0.405024D-01   373.150   523.150   EXCL TR
END
<PgUp>
```

1.621 E-3 mol/kg SiO_2.

```
                                          YM_WATER Study
                                          YM_WATER Model
OLI Stream NRG_B                          OLI Stream NRG_B

ALOH3            0.222466E-04
CAOH2            0.823735E-03
H2CO3            0.496991E-03
HCL              0.138268E-02
HNO3             0.645378E-03
MGOH2            0.201688E-03
NA3HSO42         0.956701E-04
NA6SO42CO3       0.503138E-03
SCALE ALOH3PPT             0.100000D+01   273.150   373.150
SCALE ALOOHPPT             0.738476D+00   373.250   523.150   EXCL TR
SCALE CACO3PPT             0.167579D+00
SCALE CASO4.2H2O           0.154617D-01   273.150   373.150
<PgUp>                                                          <PgDn>
```

0.849 E-3 mol/kg SiO_2.

8/14/02


```
                                          YM_WATER Study
                                          YM_WATER Model
OLI Stream AVG_J13                        OLI Stream AVG_J13

CAOH2            0.324475E-03
H2CO3            0.304212E-02
H6F6             0.191308E-04
HNO3             0.141648E-03
KMGCL3           0.671532E-04
KOH              0.110464E-02
MGOH2            0.155731E-04
NA6SO42CO3       0.958015E-04
NAOH             0.141802E-02
SCALE CACO3PPT             0.100000D+01
SCALE CAF2PPT              0.104042D+00
END
<PgUp>
```

SiO_2: 1.01E-3 mol/kg.

Re ajust the chemistry model to include SiO_2 and every chemical species in the above 5 waters.

→ YM-Water (still call it this name)

The reconciled file on page 124 has an error. this table is redone. see page 132

8/14/02

Verification of the reconciled stream:

File: YM_Water_Recociliation_Verification.xls

From Page 121 UZ_A

Species	FW	mg/L					mol/L				
		UZ-14/1542.3-1542.8	UZ-14/85.2-85.6	NRG-6/158.2-158.6	NRG-6/244.6-245.0	Average J13	UZ-14/1542.3-1542.8	UZ-14/85.2-85.6	NRG-6/158.2-158.6	NRG-6/244.6-245.0	Average J13
		UZ_A	UZ_B	NRG_A	NRG_B	AVG_J13	UZ_A	UZ_B	NRG_A	NRG_B	AVG_J13
Ca2+	40	3.6	49.9	122	33	13	9.00E-05	1.25E-03	3.05E-03	8.25E-04	3.25E-04
Mg2+	24.3	0.5	13.2	23.3	4.9	2.01	2.06E-05	5.43E-04	9.59E-04	2.02E-04	8.27E-05
Na+	23	207	43.5	35.6	72	45.8	9.00E-03	1.89E-03	1.55E-03	3.13E-03	1.99E-03
K+	39.1					5.04					1.29E-04
SiO2(aq)	60.09	143	89.8	97.4	51	61	2.38E-03	1.49E-03	1.62E-03	8.49E-04	1.02E-03
Al3+	27	13.8	0.3	0	0.6	0	5.11E-04	1.11E-05	0.00E+00	2.22E-05	0.00E+00
HCO3-	61	384	131	34	61	128.9	6.30E-03	2.15E-03	5.57E-04	1.00E-03	2.11E-03
CO32-	60	46					7.67E-04				
Total CO32-							7.06E-03	2.15E-03	5.57E-04	1.00E-03	2.11E-03
Cl-	35.5	20	60	185	49	7.14	5.63E-04	1.69E-03	5.21E-03	1.38E-03	2.01E-04
NO3-	62	4	22	32	40	8.78	6.45E-05	3.55E-04	5.16E-04	6.45E-04	1.42E-04
SO42-	96	28	66	159	115	18.4	2.92E-04	6.88E-04	1.66E-03	1.20E-03	1.92E-04
F-	19				na	2.18					1.15E-04
pH		8.6	6.9	6.8	7.2	7.41					
charge bal.		1.02%	-0.91%	-0.26%	-2.26%	-0.31%					
water type		Na-HCO3	Ca-Na-HCO3-Cl-SO4	Ca-Mg-Cl-SO4	Na-Ca-SO4-Cl	Na-Ca-HCO3	Na-HCO3	Ca-Na-HCO3-Cl-SO4	Ca-Mg-Cl-SO4	Na-Ca-SO4-Cl	Na-Ca-HCO3

Recociled Compounds: from page 127

Compound	UZ-A
AlOH3	5.12E-04
CaOH2	8.99E-05
H2CO3	8.64E-03
H6F6	
H2SO4	
HCl	5.65E-04
HNO3	6.46E-05
KMgCl3	
KOH	
MgOH2	2.06E-05
Na3HSO42	
Na6SO42CO3	1.46E-04
NaOH	8.14E-03

compared well.

J.Y. 9/13/01

From Reconciled ~~Compounds~~ ions from Reconciled compound above

Species	
Ca2+	**8.99E-05**
Mg2+	**2.06E-05**
Na+	**9.01E-03**
K+	**0.00E+00**
SiO2(aq)	
Al3+	**5.12E-04**
HCO3-	
CO32-	
Total CO32-	**8.79E-03**
Cl-	**5.65E-04**
NO3-	**6.46E-05**
SO42-	**2.92E-04**
F-	**0**

$(8.79-1.72)\times10^{-3} = 7.07E\text{-}3$

added	HCO3-
by mol/L	1.72E-03
by mg/L	104.97

The reconciled file included the added 104.97 mg/L of HCO_3^- (see page 123)

J. Yang A Ulmor

Concentration factor.

J.Y. 09/20/01

In DOE's Report. Page 15, and Page 13 (ANL-EBS-MD-000041 REV (April 2000))

The concentration factor is the ratio of the initial water mass divided by the water mass at the time of analysis.

— My understanding is not to include the solutes in the water, not solid either!

J. Yang 09/20/01

09/17/01 Found an error for AVG-J13 reconciled Result. (page. 124) K+ should be 5.04 mg/L

Newly reconciled results are given in page 132

J. Yang 3/19/02

Reconciliation of AVG-J13 (from pages 124 and 129.

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
AL+3			OH-1		
CA+2	13.	13.00001	CL-1	7.14	7.139998
H+1			CO3-2		
K+1	5.04	5.040011	F-1	2.18	2.179998
MG+2	2.01	2.01	H3SIO4-1		
NA+1	45.8	46.21689	HCO3-1	128.9	128.9002
			HSO4-1		
			NO3-1	8.78	8.779968
			SO4-2	18.4	18.39999

<PgDn>

PH = 8.186

SiO_2 : 61 mg/L not included. = 1.01E-3 mol/kg.
~~Na+1 ; 0.4 mg/L added for reconsilation~~

After converted into OLI Stream Files:

YM_WATER Study
YM_WATER Model
OLI Stream AVG_J13

OLI Stream AVG_J13

CAOH2	0.324456E-03
H2CO3	0.201730E-02
H6F6	0.191296E-04
HNO3	0.141640E-03
KMGCL3	0.671493E-04
KOH	0.617918E-04
MGOH2	0.155721E-04
NA6SO42CO3	0.957958E-04
NAOH	0.143607E-02
SCALE CACO3PPT	0.999470D+00
SCALE CAF2PPT	0.117995D+00
END	

<PgUp>

H_2O: 55.509 mol/hr

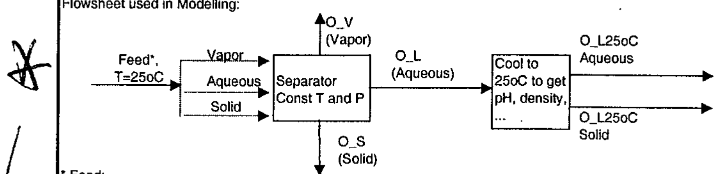
J. Y. 8/14/02

Summary of Modeling Results with OLI ESP 6.5
9/21/2001
File: YM_Water_Total_Ionic.xls

Sheet Contents
This workbook contains the fowllong worksheets:

Original_Data:	Data from OLI (Zero rows deleted, the number column shows the original row number)
Stream_O_L	Data for Syream O_L
Stream_O_L_Ignored_Zero_Rows	Data for Syream O_L after deleted the zero rows for the O_L stram)
Chart_Stream_O_L	Chart according to data on Stream_O_L_Ignored_Zero_Rows
Stream_O_L_Ions_Only	Data for Syream O_L after deleted non ionic rows)
Chart_Stream_O_L_Ions	Chart according to data on Stream_O_L_Ions_Only

Flowsheet used in Modelling:



* Feed:
UZ_A: UZ-14/1542.3-1542.8
UZ_B: UZ-14/85.2-85.6
NRG_A: NRG-6/158.2-158.6
NRG_B: NRG-6/244.6-245.0
AVG_J13: Average J13

Notations of Selected Labels:

Water	Feed Name
Variable T, oC	Temperature
Variable Con of added CO2 to Feed (molal)	CO2 added to the feed to adjust the P(CO2) in the O_L stream
[redacted] Pressure,atm	
Conc. Factor (Derived)	Concentration factor: Ratio of Water in O_V to Water in O_L **
P of Pure H2O at T	Vapour Pressure of H2O at T
R Humidity at T	Relative Humidity in the Separator or Streams D_H of O_L
P(CO2, atm)	Fugacity of CO2 in Separator
Ionic Strg.* (Software Maximum, 30)	
X(H2O) (Software Minimum, 0.65)	Mole Fraction of water in O_L stream

For Molecular Phase output Results, please see the fowlloing five Spreadsheet Files:
YM_Water_UZ_A.xls
YM_Water_UZ_B.xls
YM_Water_NRG_A.xls
YM_Water_NRG_B.xls
YM_Water_AVG_J13.xls

* Flow Sheet shown in page 126 was abandoned.
J. Y. 09/21/01

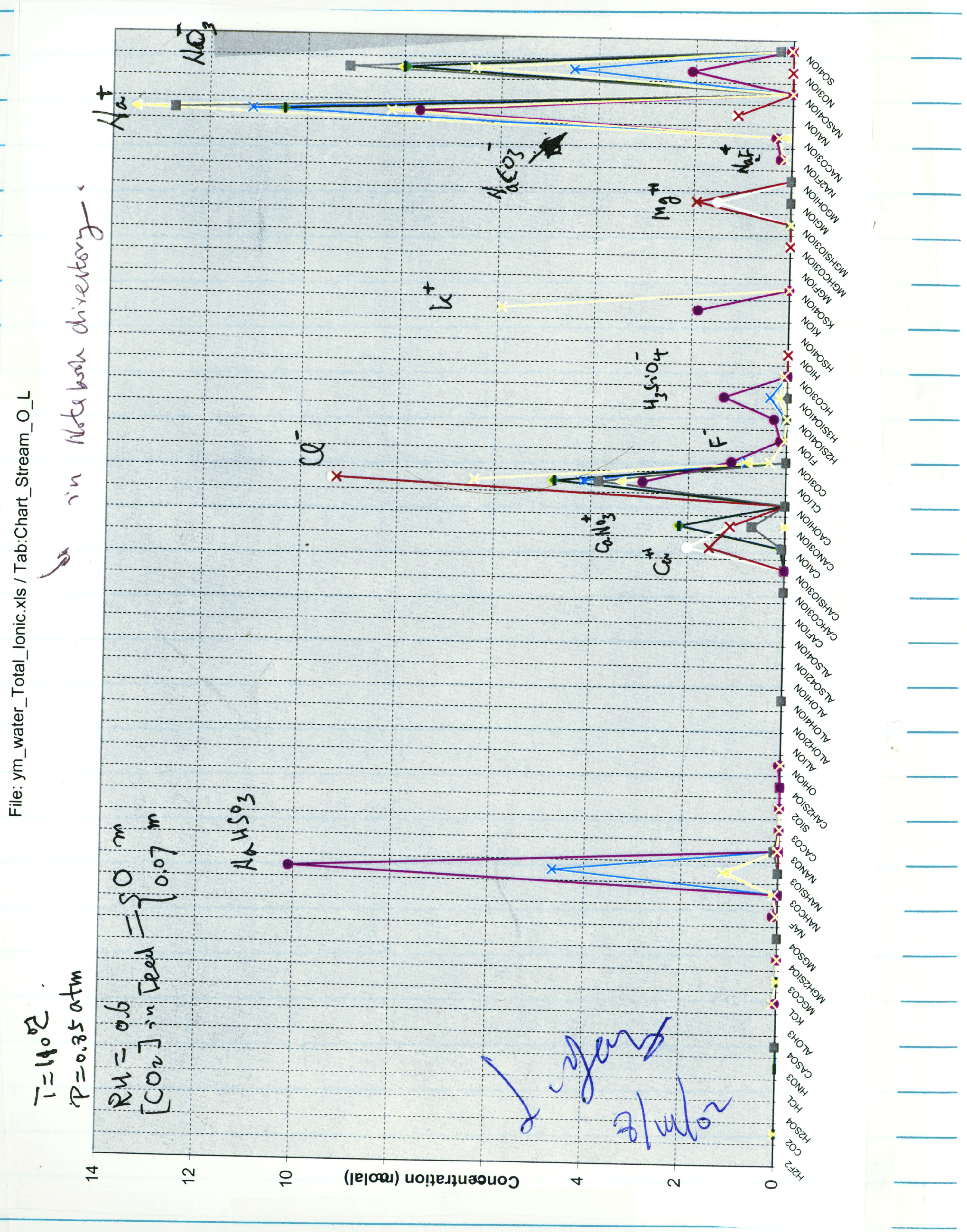
Example outputs →

** — Definition see page 131

Water	UZ_A
Variable T, oC	110
Variable Con of added CO2 to Feed (molal)	0
[redacted]	0.85
Conc. Factor (Derived)	1.0E+06
P of Pure H2O at T	1.40844
R Humidity at T	0.603504587
P(CO2, atm)	6.91E-05
Ionic Strg.* (Maximum, 30)	12.0397
X(H2O) (Minimum, 0.65)	0.68058068

	Stream	UZ_A	UZ_A	O_V	O_L
	Phase	Aqueous	Solid	Vapor	Aqueous
	Temperature,C	25	25	110	110
	Pressure,atm	1	1	0.85	0.85
	pH	7.33586			10.6325
	Totalmol/hr	55.53845	9.76E-04	55.5265	8.17E-05
	FlowUnits	mol/hr	mol/hr	mol/hr	mol/hr
1	H2O	55.5178		55.52198	5.56E-05
2	H2F2				
3	CO2	7.33E-04		0.00451583	1.12E-13
4	H2SO4	1.49E-27			
5	HCL	1.39E-17		5.25E-12	1.36E-21
6	HF				
7	HNO3	9.41E-15		4.69E-12	8.33E-18
9	SIF4				
10	SO3				
11	CASO4	1.34E-06			3.89E-17
12	ALOH3	2.40E-09	5.12E-04		2.56E-15
13	KCL				
14	KHSO4				
15	MGCO3	7.95E-08			6.25E-14
16	MGH2SIO4	6.21E-11			3.09E-13
17	MGSO4	1.42E-07			3.30E-18
18	NAF				
19	NAHCO3	2.45E-05			2.44E-08
20	NAHSIO3	5.82E-06			4.69E-06
21	NANO3	6.14E-10			4.23E-08
23	CACO3	8.56E-07			8.75E-13
24	SIO2	0.0019037	4.64E-04		1.90E-09
25	CAH2SIO4	3.12E-11			1.37E-13
26	OHION	2.43E-07			2.00E-08
31	ALION	2.40E-15			
32	ALOH2ION	2.25E-11			1.93E-21
33	ALOH4ION	1.45E-08			5.49E-09
34	ALOHION	3.09E-13			1.21E-28
35	ALSO42ION	3.02E-18			
36	ALSO4ION	2.03E-16			
37	CAFION				
38	CAHCO3ION	4.92E-06			4.09E-15
39	CAHSIO3ION	6.59E-09			1.84E-13
40	CAION	8.28E-05			2.25E-14
41	CANO3ION	6.62E-10			2.43E-13
42	CAOHION	2.28E-10			2.22E-14
43	CLION	5.65E-04			4.18E-06
44	CO3ION	1.11E-05			8.21E-07
45	FION				
46	H2SIO4ION	1.53E-11			3.92E-08
47	H3SIO4ION	6.57E-06			3.75E-07
48	HCO3ION	0.0080102			1.24E-08
49	HF2ION				
50	HION	5.10E-08			9.90E-18
51	HSO4ION	9.21E-10			1.17E-18
52	KION				
53	KSO4ION				
54	MGFION				
55	MGHCO3ION	3.43E-06			4.88E-16
56	MGHSIO3ION	2.50E-09			5.30E-14
57	MGION	1.69E-05			5.80E-16
58	MGOHION	4.50E-10			2.84E-14
59	NA2FION				
60	NACO3ION	2.33E-07			1.64E-07
61	NAION	0.0089796			1.11E-05
62	NASO4ION	1.78E-06			6.43E-10
63	NO3ION	4.57E-06			4.53E-06
65	SIF6ION				
66	SO4ION	2.88E-04			6.64E-08
74	NA6SO42CO3				
75	MGOH2				
84	ALOOH				
95	CASO4.2H2O				
108	KNO3				
117	MGF2				
129	NA2CO3				
131	NA2SO4				
133	NAALCO3OH2				
136	NACL				
181	Totalg/hr	1001.07	0.0678034	1000.45	0.00227164
182	Volume,L/hr	1.00359	2.90E-05	2040.29	1.47E-06
1.83E+02	Enthalpy,cal/hr	-3.80E+06	-2.58E+02	-3.17E+06	-6.64E+00
184	Density,g/L	997.49	2337.16	0.490345	1550.28
185	Vaporfraction			1	
186	Solidfraction		1		
187	Organicfraction				
188	OsmoticPres,atn	0.479577			877.248
189	RedoxPot,volts				
190	E-Con,1/ohm-cn	8.37E-04			0.6401
191	E-Con,cm2/ohm	40.9822			0.043295
192	AbsVisc,cP	0.894802			1.61256
193	RelVisc	1.00458			6.3342

J. Y. 8/14/02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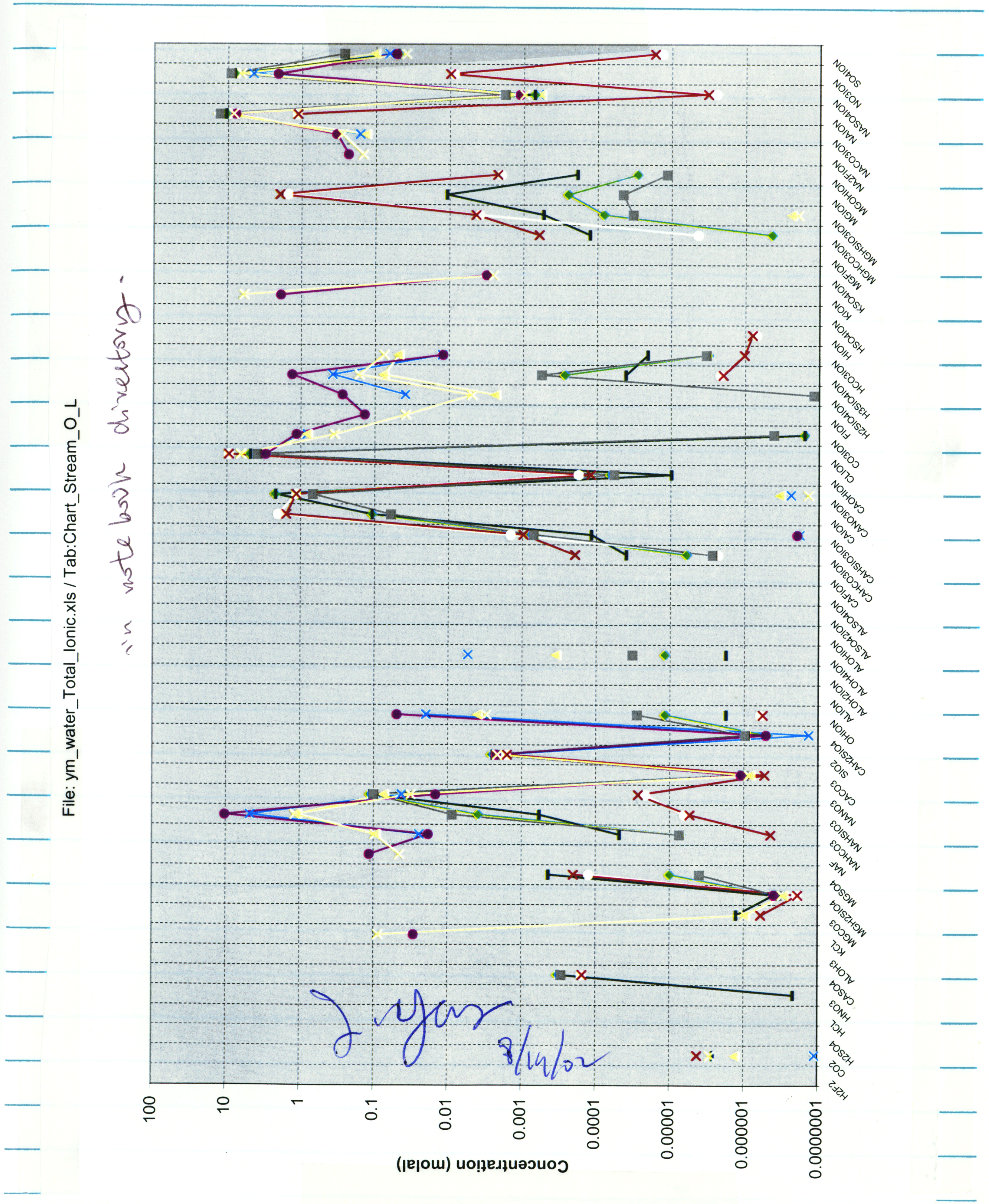
P=0.35 atm
RH = 0.6
8/14/02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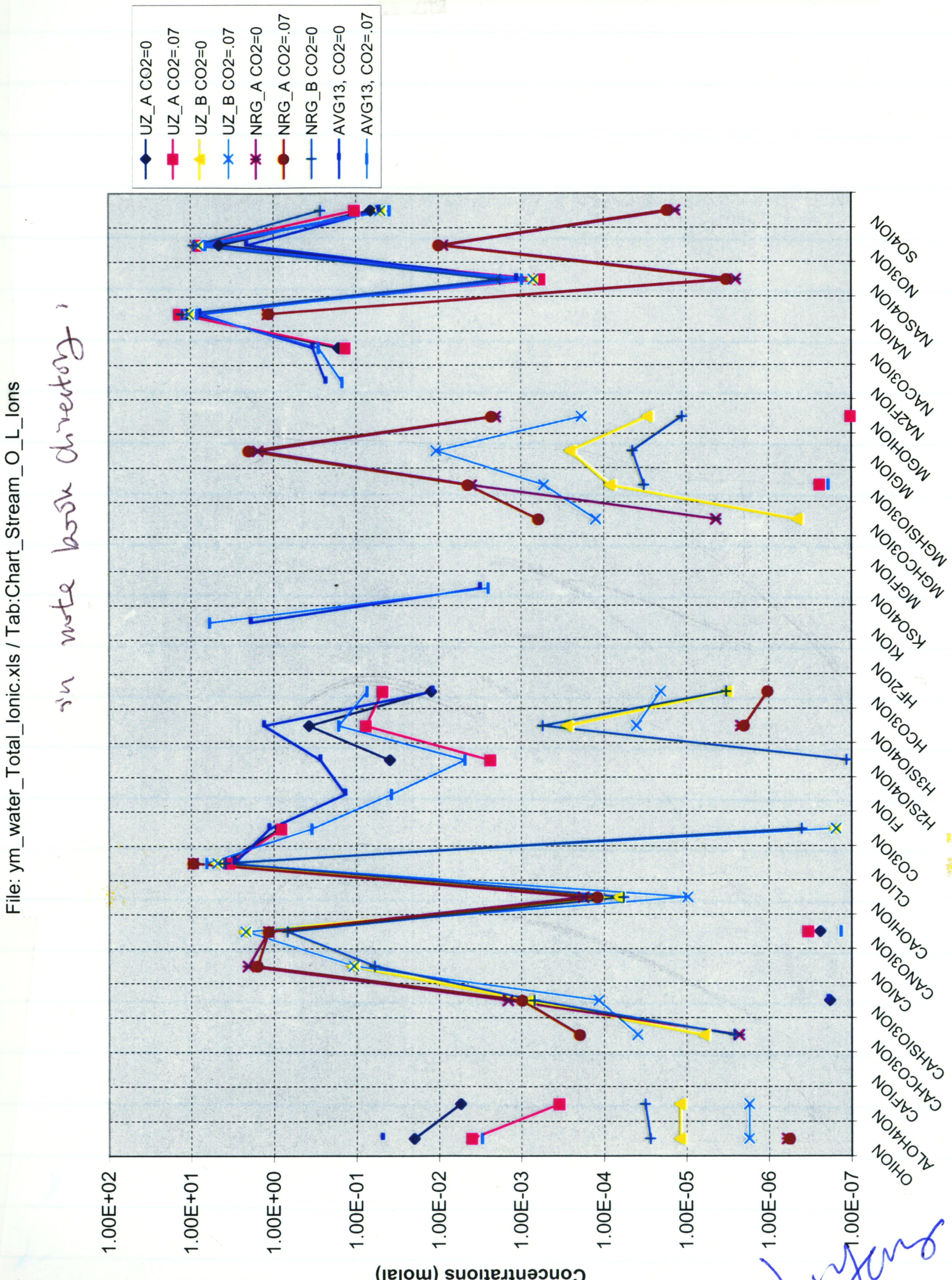
Concentration (molal)
in note book directory.
8/14/02



in note book directory

[signature]

8/14/02

T = 110 °C

P = 0.85 atm.

File: ym_water_EVap.xls / Tab: Ym_water_total_ionic

This Sheet is copied from the sheet with Zero Rows Deleted in File: ym_water_Total_Ionic.xls

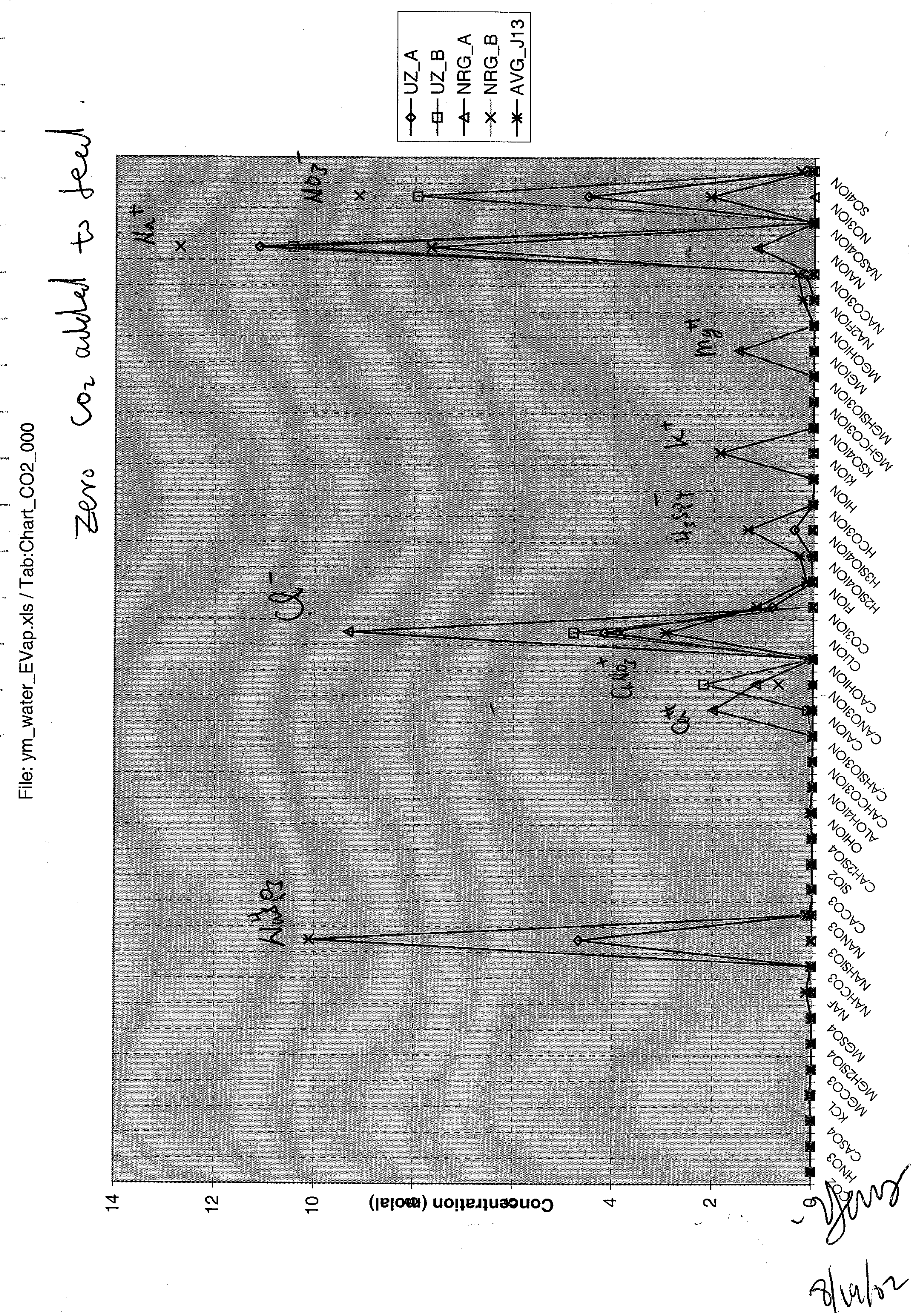
Source:

	CO2 in Feed (molal)	0	0.07	0	0.07	0	0.07	0	0	0.07
	Molals (C>1e-7)	UZ_A	UZ_A	UZ_B	UZ_B	NRG_A	NRG_A	NRG_B	AVG_J13	AVG_J13
3	CO2	1.12E-07	1.3E-06		2.6E-06		4.18E-06			2.84E-06
7	HNO3				2.17E-07					
11	CASO4			0.000325	0.000324	0.000155	0.00015	0.000289		
13	KCL								0.028511	0.086039
15	MGCO3		9.54E-07		1.28E-06		5.84E-07			9.61E-07
16	MGH2SIO4	3.09E-07	2.86E-07	4E-07	4E-07	1.91E-07	1.85E-07	3.56E-07	3.9E-07	3.02E-07
17	MGSO4			9.98E-06	0.000437	0.000124	0.000199	3.99E-06		
18	NAF								0.113455	0.044046
19	NAHCO3	0.024407	0.091638	7.23E-06	4.78E-05		4.32E-07	7.39E-06	0.018008	0.094567
20	NAHSIO3	4.682643	1.066844	0.003832	0.000579	6.27E-06	5.32E-06	0.008704	10.10267	1.153555
21	NANO3	0.042275	0.071294	0.110955	0.111682	2.12E-05	2.66E-05	0.099309	0.014468	0.031341
23	CACO3	8.74E-07	8.09E-07	1.13E-06	1.13E-06		5.25E-07	1.01E-06	1.1E-06	8.55E-07
24	SIO2	0.001901	0.00169	0.002552	0.002545	0.001621	0.001567	0.002289	0.0022	0.00214
25	CAH2SIO4	1.37E-07		4.89E-07				9.65E-07	5.04E-07	
26	OHION	0.01998	0.003928	1.17E-05	1.77E-06	5.99E-07	5.57E-07	2.8E-05	0.048496	0.003034
33	ALOH4ION	0.00549	0.000345	1.17E-05	1.78E-06			3.23E-05		
38	CAHCO3ION			6.02E-06	3.98E-05	2.28E-06	0.000194	2.7E-06		
39	CAHSIO3ION	1.84E-07		0.000781	0.000118	0.001439	0.000967	0.000704	1.94E-07	
40	CAION			0.107076	0.107546	2.008151	1.550909	0.060095		
41	CANO3ION	2.43E-07	3.32E-07	2.184817	2.180375	1.142855	1.133872	0.686056		1.37E-07
42	CAOHION			6.53E-05	9.81E-06	0.000176	0.000119	5.83E-05		
43	CLION	4.174277	3.398285	4.791008	4.768404	9.332072	9.247634	3.850956	2.951193	6.417751
44	CO3ION	0.820127	0.802104	1.55E-07	1.57E-07			4.07E-07	1.130449	0.344798
45	FION								0.135464	0.037656
46	H2SIO4ION	0.039129	0.002319					1.18E-07	0.271092	0.004832
47	H3SIO4ION	0.375021	0.075066	0.000272	4.1E-05	2.16E-06	1.96E-06	0.000559	1.30611	0.163199
48	HCO3ION	0.012392	0.046864	3.14E-06	2.08E-05		1.02E-06	3.34E-06	0.011915	0.074018
50	HION					7.07E-07	7.96E-07			
52	KION								1.875587	5.909292
53	KSO4ION								0.003127	0.002515
55	MGHCO3ION			4.38E-07	0.000127	4.33E-06	0.000609			
56	MGHSIO3ION		2.38E-07	8.13E-05	0.000537	0.003906	0.004337	3.3E-05		1.93E-07
57	MGION			0.000248	0.010787	1.512397	1.945774	4.52E-05		
58	MGOHION			2.85E-05	0.000188	0.001997	0.002232	1.14E-05		
59	NA2FION								0.230504	0.146505
60	NACO3ION	0.16341	0.133033						0.332792	0.282526
61	NAION	11.12424	13.5169	10.44812	10.45521	1.149296	1.121734	12.71917	7.672066	8.259885
62	NASO4ION	0.000643	0.00058	0.000711	0.000715	2.47E-06	3.21E-06	0.001804	0.001125	0.000979
63	NO3ION	4.52175	8.046178	7.956995	8.004133	0.008664	0.009744	9.135558	2.080597	6.557243
66	SO4ION	0.06638	0.101892	0.049773	0.049974	1.34E-05	1.66E-05	0.268687	0.052131	0.038773

P_{CO_2} (from Data File) (atm) 2.36E-5, 1.09E-3

[signature]

8/14/02


File: ym_water_EVap.xls / Tab:Chart_CO2_000
Zero Co2 added to feed.
UZ_A
UZ_B
NRG_A
NRG_B
AVG_J13
Concentration (molal)
SO4ION
NO3ION
NASO4ION
NAION
NACO3ION
NA2FION
MGOHION
MGION
MGHSIO3ION
MGHCO3ION
KSO4ION
KION
HION
HCO3ION
H3SIO4ION
H2SIO4ION
FION
CO3ION
CLION
CAOHION
CANO3ION
CAION
CAHSIO3ION
CAHCO3ION
ALOH4ION
OHION
CAH2SIO4
SIO2
CACO3
NANO3
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NAF
MGSO4
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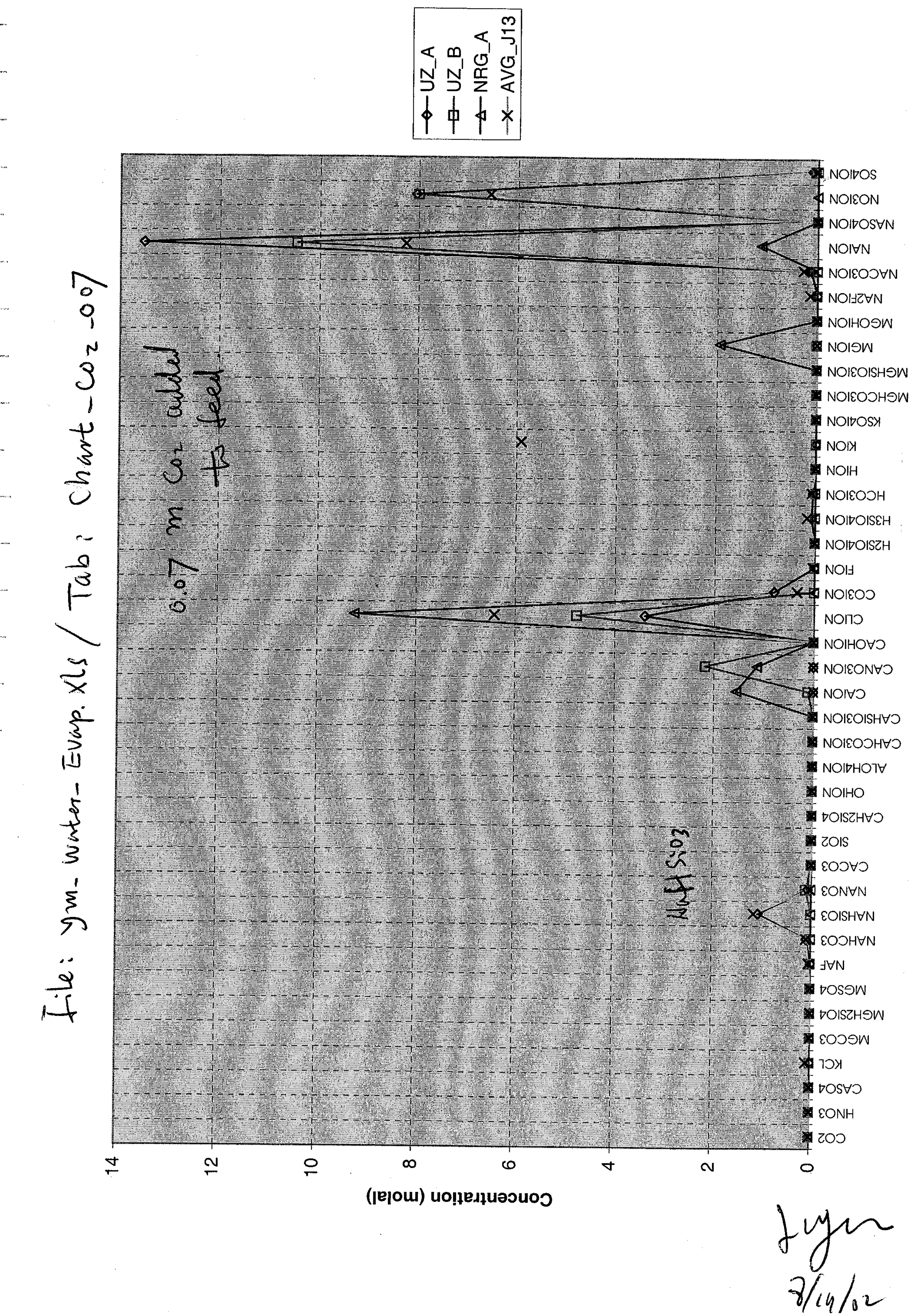
MGCO3
KCL
CASO4
HNO3
8/14/02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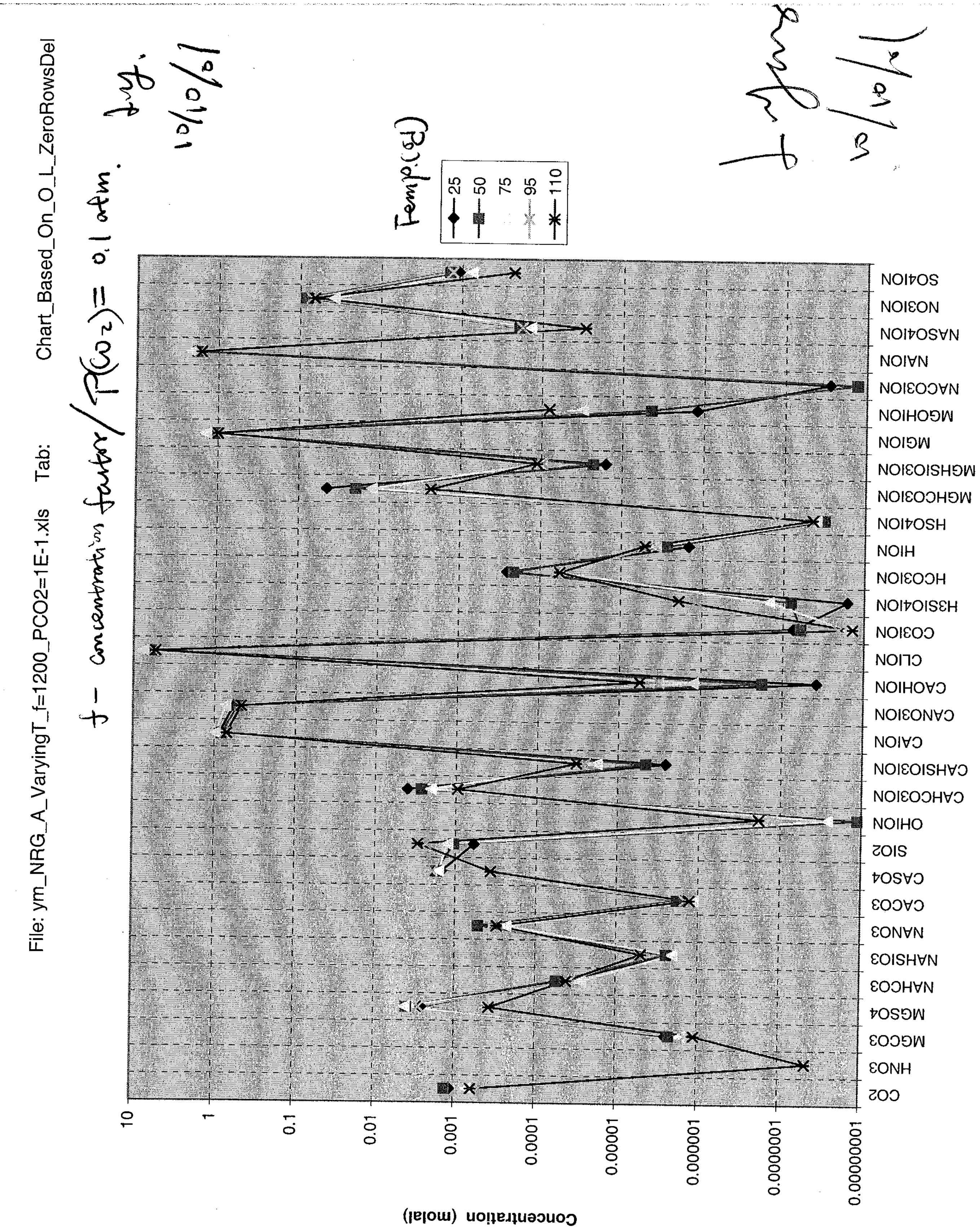
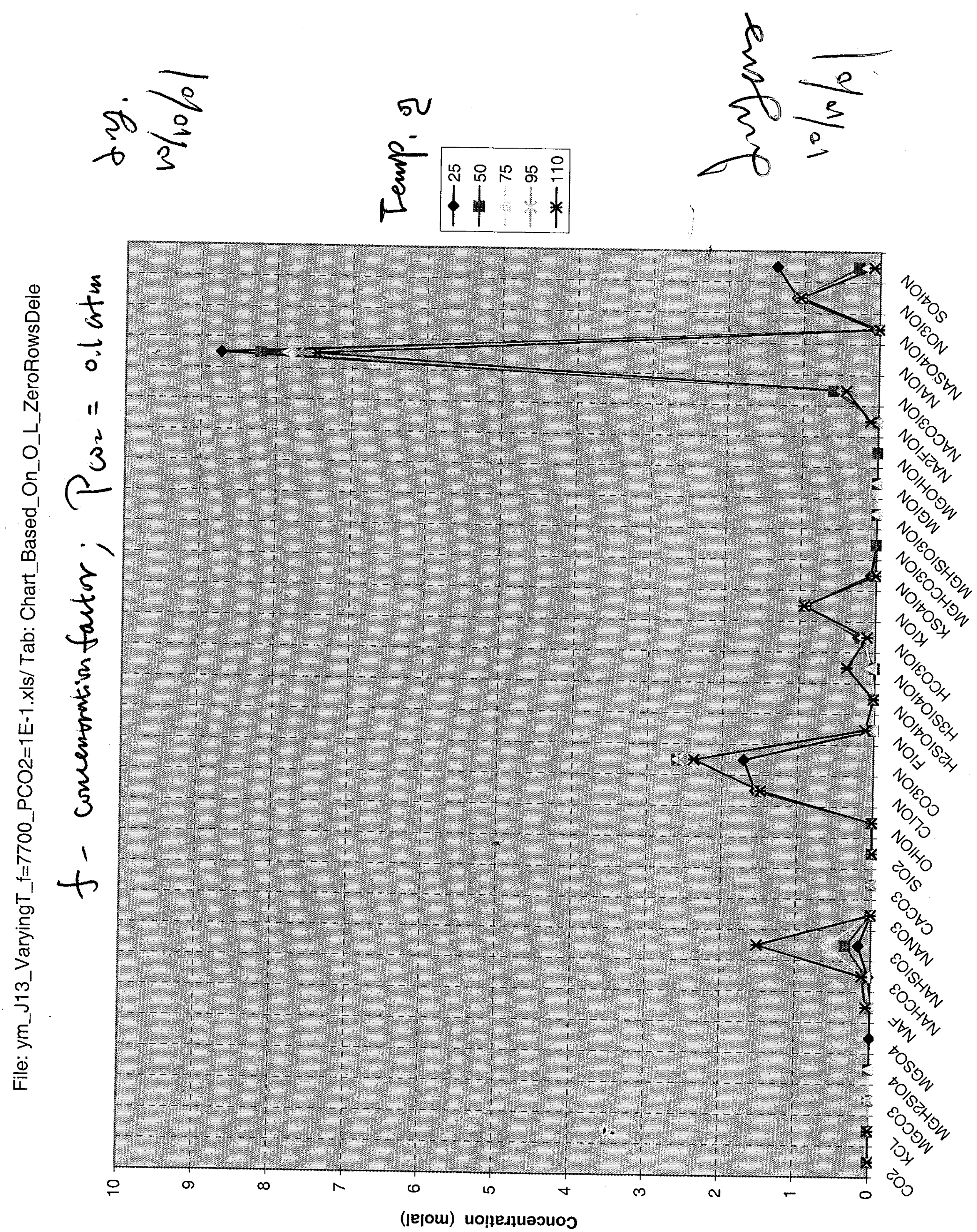
0.07 m Co2 added to feed
UZ_A
UZ_B
NRG_A
AVG_J13
Concentration (molal)
SO4ION
NO3ION
NASO4ION
NAION
NACO3ION
NA2FION
MGOHION
MGION
MGHSIO3ION
MGHCO3ION
KSO4ION
KION
HION
HCO3ION
H3SIO4ION
H2SIO4ION
FION
CO3ION
CLION
CAOHION
CANO3ION
CAION
CAHSIO3ION
CAHCO3ION
ALOH4ION
OHION
CAH2SIO4
SIO2
CACO3
NANO3
NAHSIO3
NAHCO3
NAF
MGSO4
MGH2SIO4
MGCO3
KCL
CASO4
HNO3
CO2
8/14/02

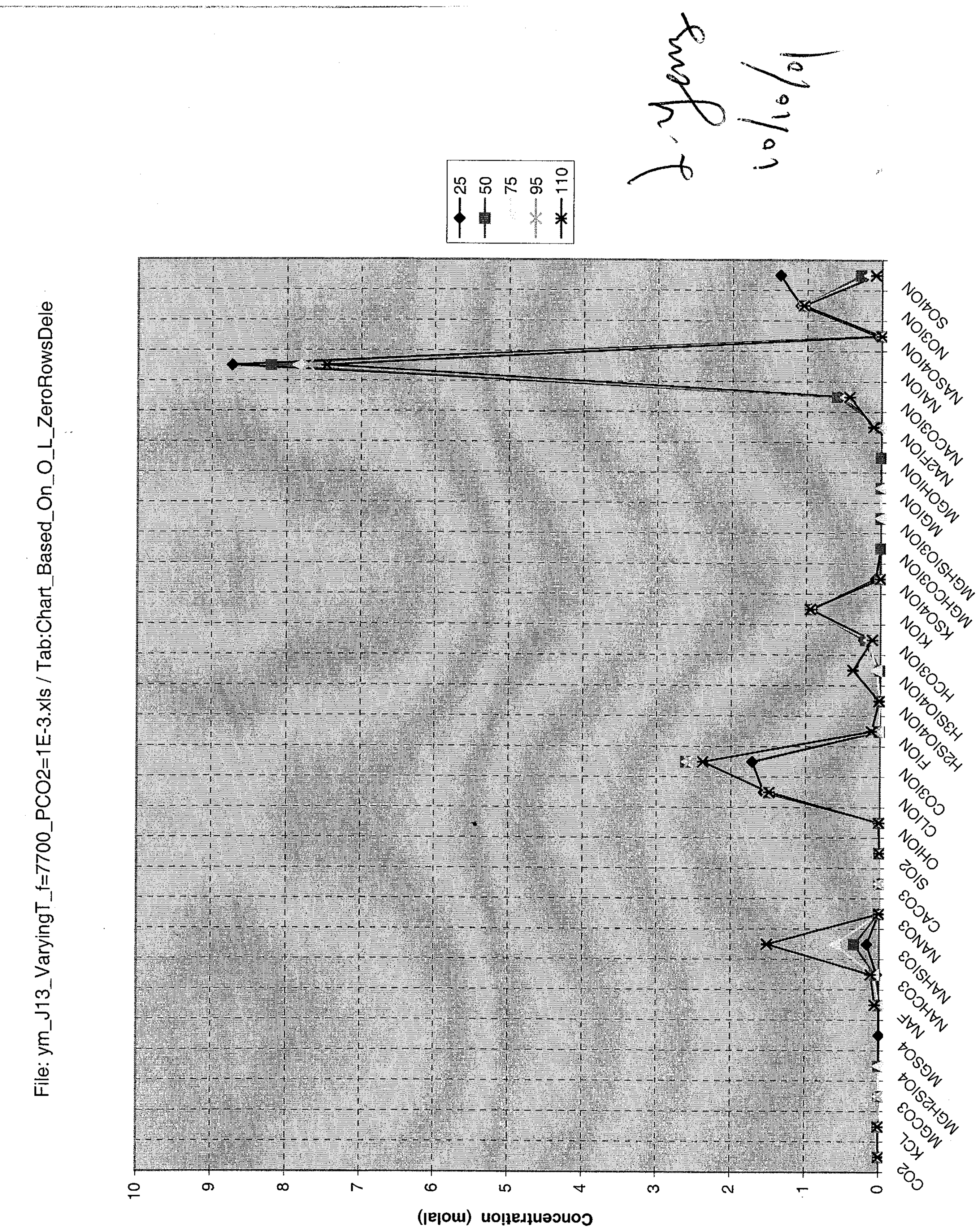
Pages 69 through 139 copied and given to QA for record

J. Yang

10/05/01




File: ym_J13_VaryingT_f=7700_PCO2=1E-1.xls/ Tab: Chart_Based_On_O_L_ZeroRowsDele
f - concentration factor; P$_{CO_2}$ = 0.1 atm
Temp. °C
25
50
75
95
110
Concentration (molal)
0
1
2
3
4
5
6
7
8
9
10
CO2
KCL
MGCO3
MGH2SIO4
MGSO4
NAF
NAHCO3
NAHSIO3
NANO3
CACO3
SIO2
OHION
CLION
CO3ION
FION
H2SIO4ION
H3SIO4ION
HCO3ION
KION
KSO4ION
MGHCO3ION
MGHSIO3ION
MGION
MGOHION
NA2FION
NACO3ION
NAION
NASO4ION
NO3ION
SO4ION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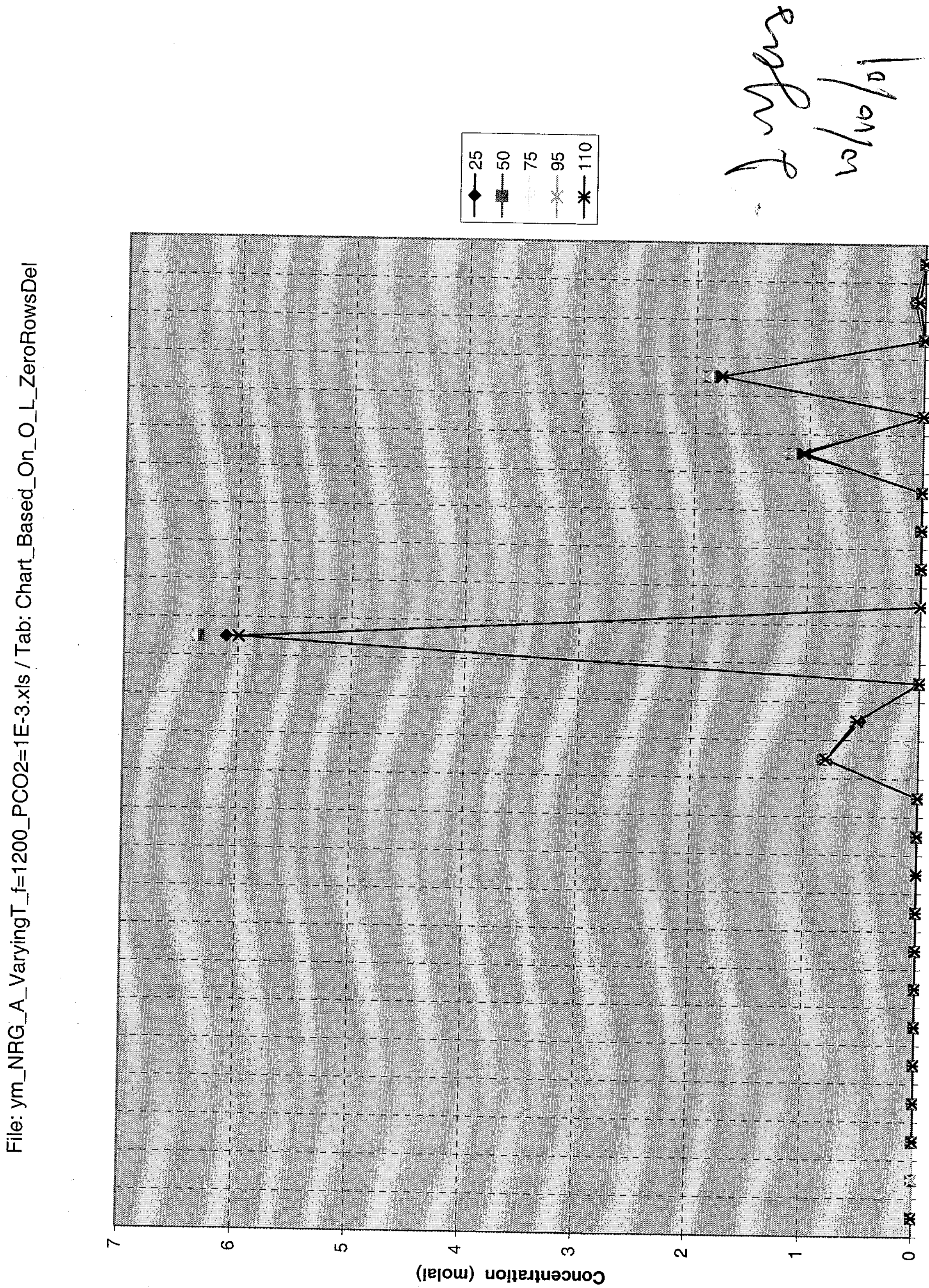
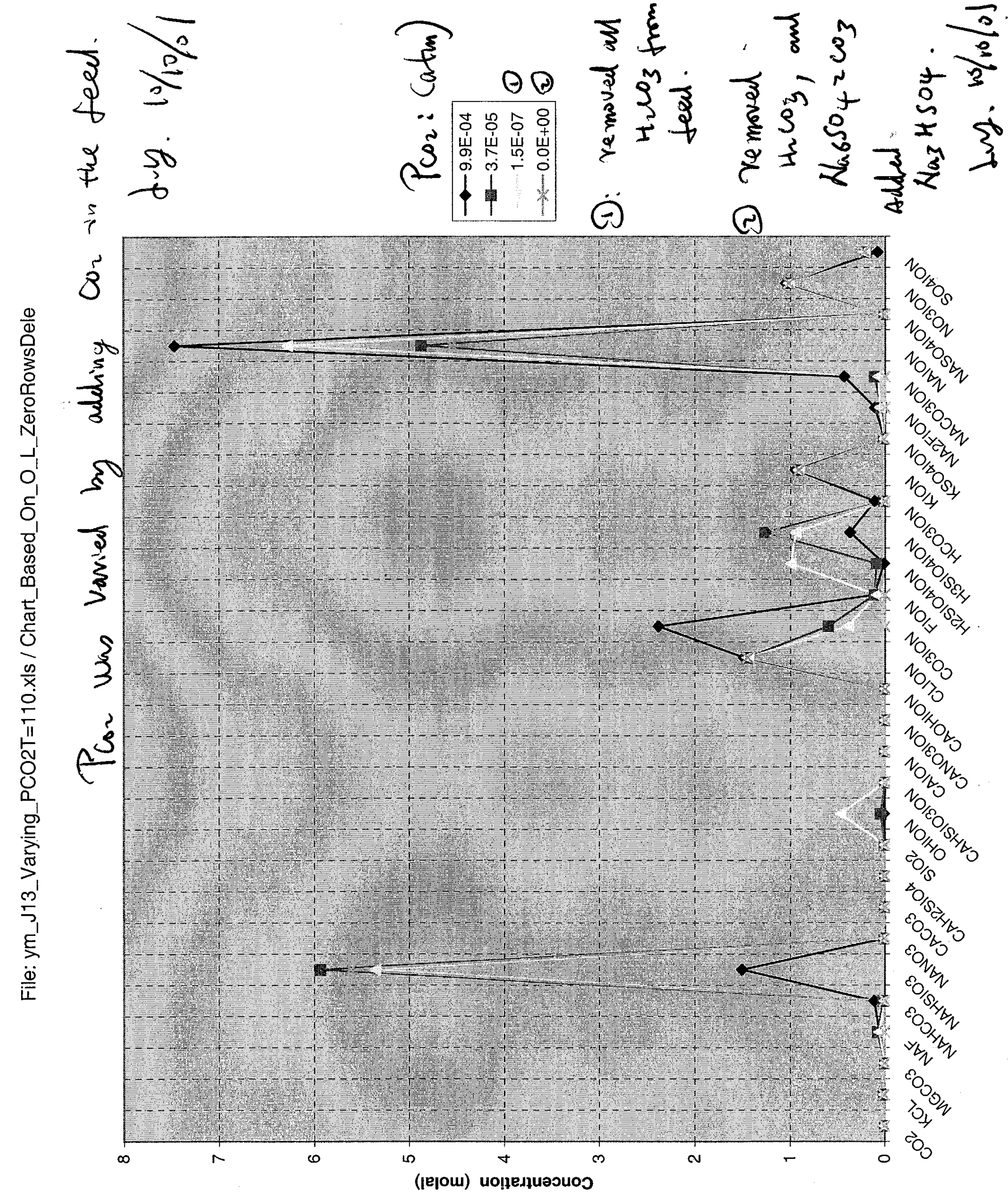
25
50
75
95
110
Concentration (molal)
0
1
2
3
4
5
6
7
8
9
10
CO2
KCL
MGCO3
MGH2SIO4
MGSO4
NAF
NAHCO3
NAHSIO3
NANO3
CACO3
SIO2
OHION
CLION
CO3ION
FION
H2SIO4ION
H3SIO4ION
HCO3ION
KION
KSO4ION
MGHCO3ION
MGHSIO3ION
MGION
MGOHION
NA2FION
NACO3ION
NAION
NASO4ION
NO3ION
SO4ION


File: ym_NRG_A_VaryingT_f=1200_PCO2=1E-3.xls / Tab: Chart_Based_On_O_L_ZeroRowsDel
Concentration (molal)
0 1 2 3 4 5 6 7
25
50
75
95
110
CO2 MGCO3 MGSO4 NAHCO3 NAHSIO3 NANO3 CACO3 CASO4 SIO2 OHION CAHCO3ION CAHSIO3ION CAION CANO3ION CAOHION CLION H3SIO4ION HCO3ION MGHCO3ION MGHSIO3ION MGION MGOHION NAION NASO4ION NO3ION SO4ION
10/10/01


File: ym_J13_Varying_PCO2T=110.xls / Chart_Based_On_O_L_ZeroRowsDele
Concentration (molal)
0 1 2 3 4 5 6 7 8
9.9E-04
3.7E-05
1.5E-07
0.0E+00
CO2 KCL MGCO3 NAF NAHCO3 NAHSIO3 NANO3 CACO3 CAH2SIO4 SIO2 OHION CAHSIO3ION CAION CANO3ION CAOHION CLION CO3ION FION H2SIO4ION H3SIO4ION HCO3ION KION KSO4ION NA2FION NACO3ION NAION NASO4ION NO3ION SO4ION