SOFTWARE RELEASE NOTICE

01. SRN Number: CSPE-SRN-170

02. Project Title: Effect of Water Chemistry on Internal Corrosion of Pipeline | Project No. 20-8910-004

03. SRN Title: Installation of ESP V 6.0 and CSP V. 1.2 (OLI Systems, Inc.)

04. Originator/Requestor: N. Sridhar | Date: 04/08/98

05. Summary of Actions

- ■ Release of new software : Installation of acquired (leased) software.
- □ Release of modified software:
  - □ Enhancements made
  - □ Corrections made
- □ Change of access software
- □ Software Retirement

06. Persons Authorized Access

Name	RO/RW	A/C/D
N. Sridhar	RO	A
R. Pabalan	RO	A

07. Element Manager Approval: N. Sridhar Date: 4/8/98

08. Remarks: This software is currently being used in only one project. However, there maybe other projects in the future that may utilize this software.

SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE-SRN-170

2. Project Title: Effect of Water Chemistry on Internal Corrosion of Pipeline	Project No. 20.08910.004

3. SRN Title: Installation of ESP V.6.0 and CSP V.1.2 (OLI Systems, Inc.)

4. Originator/Requestor: Lietai Yang	Date: 9/28/2001

5. Summary of Actions

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

6. Validation Status

- ☐ Validated
- ☐ Limited Validation
- ☐ Not Validated Explain: _____

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete

8. Element Manager Approval: [signature] Date: 10/2/01

9. Remarks:

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 4/08/98	02. Summary prepared by (Name and phone) N. Sridhar (210)522-5538	03. Summary Action: NEW
04. Software Date: 12/01/97	05. Short Title: Installation of OLI Software ESP V 6.0 / CSP V 1.2	
06. Software Title: ESP V 6.0 and CSP V 1.2: Components of OLI Software		07. Internal Software ID:

08. Software Type:	09. Processing Mode:	10. Application Area
☐ Automated Data System	■ Interactive	A. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA
■ Computer Program	☐ Batch	☐ Subsystem PA ☐ Other
☐ Subroutine/Module	☐ Combination	B. Specific: Pipeline Corrosion

11. Submitting Organization and Address:	12. Technical Contact(s) and Phone:
CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78238	N. Sridhar (210)522-5538 R. Pabalan (210)522-5304

13. Narrative: This software predicts the speciation of an aqueous solution given some input chemistry. It also predicts stability diagrams.

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

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

23. Software Availability:	24. Documentation Availability:
☐ Available ■ Limited ☐ In-House ONLY	■ Available ☐ Inadequate ☐ In-House ONLY

It is required that OLI Systems be paid an annual fee to obtain a "Hardware Key" to allow access after 1 year's time.

Software Custodian: Steve Nolen Date: 4/8/98

42/42

Reissued To N. Sridhar NS
S/N No. 265 4/8/98
20-8910
20-1136

CNWRA
CO
CO 265 4/8/98

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INSTALLATION TESTS FOR
ESP SOFTWARE FROM
N. SRIDHAR SCIENTIFIC
NOTE BOOK No. 265
BEN 4/8/98

INSTALLATION TEST FOR ESP VERSION 5.3. 25/42

PRCI Project 15-9712 (chg. 20-8910-002) 4/8/98

Calculation of solution compositions using OLI V.5.3 ESP.

Case 1

$CaCl_2$: 166 g
Total : 3000 g
CO_2 : 1.0066 g (10 psi)
H_2S : 0.0566 g (0.5 psi)
Total P : 500 psia.
T : 60°F

~~Should be 1.677. So recalculate in following page.~~ Original result correct. 1/27/98

Precipitation point with respect to $CaCO_3$:
$NaHCO_3$: 0.94 g
pH : 5.78

To get pH = 6,

NaOH : 0.794 ~~g~~ mol (1/27)

The solution composition for this condition is given in the next page.

If NaOH is added without CO_2 & H_2S, the pH will be : 11.5. There will be no solids precipitated.

If CO_2 & H_2S are present, then $CaCO_3$ will be precipitated as shown in the next page.

N Sridhar 1/27/98

26/42

ESP V-5.3 STREAM:prci 01/27/98 PAGE 1

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	5.9865			
Total mol/hr	161.43	5.7773E-03	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2814.5	0.0	0.0	0.0
CO2	0.37938	0.0	0.0	0.0
H2S	3.0778E-02	0.0	0.0	0.0
HCL	1.5037E-19	0.0	0.0	0.0
NAHCO3	4.7156E-02	0.0	0.0	0.0
CACO3	9.1327E-10	0.57823	0.0	0.0
OHION	4.0119E-07	0.0	0.0	0.0
CAION	56.002	0.0	0.0	0.0
CAOHION	1.6944E-06	0.0	0.0	0.0
CLION	116.57	0.0	0.0	0.0
CO3ION	1.0755E-04	0.0	0.0	0.0
HCO3ION	0.39193	0.0	0.0	0.0
HION	3.3130E-06	0.0	0.0	0.0
HSION	3.4524E-03	0.0	0.0	0.0
NACO3ION	1.3033E-05	0.0	0.0	0.0
NAION	11.489	0.0	0.0	0.0
CAHCO3ION	7.3581E-03	0.0	0.0	0.0
SION	2.0920E-09	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	2999.4	0.57823	0.0	0.0
Volume, L/hr	2.8513	2.1335E-04	0.0	0.0
Enthalpy, cal/hr	-1.1038E+07	-1667.	0.0	0.0
Density, g/L	1052.0	2710.2		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.0000	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, psia	638.64			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	7.2475E-02			
E-Con, cm2/ohm-mol	107.62			
Ionic Strength	1.6670			

N. Smith 1/27/98

[redacted]

1/27/98 PRCI Project

Case 2:

P : 500 psia
CO_2 : 1.677 g [10 psi]
H_2S : 0.0366 g [0.5 psi]

Head space (gas phase) in autoclave is 48.33 cu.in or 791.98 cm^3.

Total moles of gas assuming ideal gas = $\frac{\left(\frac{500}{14.7}\right) \times 791.98}{(8.31)(288.6)}$ at 15.6°C

$= \frac{1.1565}{}$ moles.

CO_2 moles = 0.0231 moles = 1.012 gms
H_2S moles = 0.0012 moles = 0.0393 gms

Total = 3000 gm
$MgCl_2$ = 235 gm
For pH = 6, add NaOH = 0.778 mol = 31.12 gm 1/27
No solids are expected to form [See print out next page] in the autoclave.

When preparing outside the autoclave and adding 31.12 gm NaOH, pH = 5.95
Also 2[illegible] gm $Mg(OH)_2$ will form.

1/27/98

When preparing outside the autoclave and adding 0.778 gm NaOH, 0.5 gm $Mg(OH)_2$ will form.

N. Sridhar
1/27/98

28/42

ESP V-5.3 STREAM:prci 01/27/98 PAGE 1

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	6.0000			
Total mol/hr	160.73	0.0	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2755.6	0.0	0.0	0.0
CO2	7.8818E-02	0.0	0.0	0.0
H2S	3.2351E-02	0.0	0.0	0.0
HCL	2.2796E-19	0.0	0.0	0.0
NAHCO3	1.0096E-02	0.0	0.0	0.0
OHION	4.7006E-07	0.0	0.0	0.0
CLION	177.47	0.0	0.0	0.0
CO3ION	4.1110E-05	0.0	0.0	0.0
HCO3ION	9.0817E-02	0.0	0.0	0.0
HION	2.6132E-06	0.0	0.0	0.0
HSION	3.6369E-03	0.0	0.0	0.0
MGHCO3ION	1.5120	0.0	0.0	0.0
MGION	54.673	0.0	0.0	0.0
MGOHION	3.1734E-05	0.0	0.0	0.0
NACO3ION	3.8692E-06	0.0	0.0	0.0
NAION	11.284	0.0	0.0	0.0
SION	3.8233E-09	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	3000.8	0.0	0.0	0.0
Volume, L/hr	2.8033	0.0	0.0	0.0
Enthalpy, cal/hr	-1.0954E+07	0.0	0.0	0.0
Density, g/L	1070.4			
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, psia	1163.7			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	9.0952E-02			
E-Con, cm2/ohm-mol	91.705			
Ionic Strength	2.6335			

N. Smith
1/27/98

[redacted]

1/27/98

Case 3: Same as case 2 (p 18) but add $NaHCO_3$ to make pH = 6

Amount of $NaHCO_3$ needed: 18.266 gm ~~mol (1534 gms)~~ NB 1/27

~~This is a large amount~~

NB 1/27 See print out on p ~~28~~ 23

Case 4 Half the amount

Not necessary

NB 1/27

Case 5 Same as case 1, but

CO_2 = 1.012 g

H_2S = 0.0393 g

NaOH to get pH = 6 : ~~0.821 mol = 32.8 g~~ 0.821 gm NB 1/27 (808 ~~NB 1/27~~ ~~32.8~~ NB 1/27)

(See table on p 21 for strict)

If NaOH (32.8 g) added w/o CO_2 & H_2S:

pH = 12.21

A lot of $Ca(OH)_2$ will be precipitated [20 gm]

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	6.0000			
Total mol/hr	161.47	6.6190E-03	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2815.2	0.0	0.0	0.0
CO2	0.35683	0.0	0.0	0.0
H2S	3.2949E-02	0.0	0.0	0.0
HCL	1.4580E-19	0.0	0.0	0.0
NAHCO3	4.5887E-02	0.0	0.0	0.0
CACO3	9.1353E-10	0.66248	0.0	0.0
OHION	4.1386E-07	0.0	0.0	0.0
CAION	55.983	0.0	0.0	0.0
CAOHION	1.7474E-06	0.0	0.0	0.0
CLION	116.60	0.0	0.0	0.0
CO3ION	1.0761E-04	0.0	0.0	0.0
HCO3ION	0.38025	0.0	0.0	0.0
HION	3.2126E-06	0.0	0.0	0.0
HSION	3.8126E-03	0.0	0.0	0.0
NACO3ION	1.3079E-05	0.0	0.0	0.0
NAION	11.526	0.0	0.0	0.0
CAHCO3ION	7.1352E-03	0.0	0.0	0.0
SION	2.3826E-09	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	3000.2	0.66248	0.0	0.0
Volume, L/hr	2.8520	2.4444E-04	0.0	0.0
Enthalpy, cal/hr	-1.1041E+07	-1910.	0.0	0.0
Density, g/L	1052.0	2710.2		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.0000	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, psia	638.60			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	7.2478E-02			
E-Con, cm2/ohm-mol	107.58			
Ionic Strength	1.6667			

1/22/98

To verify the previous calculation, an isothermal calculation using NaOH = 0.521

Case 5:

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	5.9898			
Total mol/hr	161.43	6.0678E-03	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2814.5	0.0	0.0	0.0
CO2	0.37387	0.0	0.0	0.0
H2S	3.3022E-02	0.0	0.0	0.0
HCL	1.4926E-19	0.0	0.0	0.0
NAHCO3	4.6867E-02	0.0	0.0	0.0
CACO3	9.1328E-10	0.60731	0.0	0.0
OHION	4.0415E-07	0.0	0.0	0.0
CAION	55.991	0.0	0.0	0.0
CAOHION	1.7067E-06	0.0	0.0	0.0
CLION	116.57	0.0	0.0	0.0
CO3ION	1.0756E-04	0.0	0.0	0.0
HCO3ION	0.38911	0.0	0.0	0.0
HION	3.2885E-06	0.0	0.0	0.0
HSION	3.7318E-03	0.0	0.0	0.0
NACO3ION	1.3048E-05	0.0	0.0	0.0
NAION	11.501	0.0	0.0	0.0
CAHCO3ION	7.3038E-03	0.0	0.0	0.0
SION	2.2779E-09	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	2999.4	0.60731	0.0	0.0
Volume, L/hr	2.8513	2.2408E-04	0.0	0.0
Enthalpy, cal/hr	-1.1038E+07	-1751.	0.0	0.0
Density, g/L	1052.0	2710.2		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.0000	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, psia	638.64			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	7.2476E-02			
E-Con, cm2/ohm-mol	107.60			
Ionic Strength	1.6669			

Case 3:

1/27/98 $MgCl_2 + NaHCO_3 + CO_2 + H_2S$ (see Top of p. 20

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	6.0000			
Total mol/hr	160.96	0.0	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2755.6	0.0	0.0	0.0
CO2	0.93483	0.0	0.0	0.0
H2S	3.2241E-02	0.0	0.0	0.0
HCL	2.2074E-19	0.0	0.0	0.0
NAHCO3	0.16831	0.0	0.0	0.0
OHION	4.5261E-07	0.0	0.0	0.0
CLION	177.47	0.0	0.0	0.0
CO3ION	4.5208E-04	0.0	0.0	0.0
HCO3ION	1.0932	0.0	0.0	0.0
HION	2.5956E-06	0.0	0.0	0.0
HSION	3.7438E-03	0.0	0.0	0.0
MGHCO3ION	16.842	0.0	0.0	0.0
MGION	50.306	0.0	0.0	0.0
MGOHION	2.9855E-05	0.0	0.0	0.0
NACO3ION	6.3521E-05	0.0	0.0	0.0
NAION	15.793	0.0	0.0	0.0
SION	3.8036E-09	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	3018.3	0.0	0.0	0.0
Volume, L/hr	2.8181	0.0	0.0	0.0
Enthalpy, cal/hr	-1.1000E+07	0.0	0.0	0.0
Density, g/L	1071.0			
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, psia	1163.9			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	9.1763E-02			
E-Con, cm2/ohm-mol	86.828			
Ionic Strength	2.5743			

1/27/98

Case 6 :

$CaSO_4$: 29.8 gm

Calculation done to get pH=6 showed that $CaSO_4$ is essentially insoluble at this pH.

Hence set point pH=7 was tried
NaOH needed = 1.179 gm

Both $CaCO_3$ & $CaSO_4$ precipitated (see table on p.25)

Without CO_2 & H_2S for same addition of NaOH
pH = 12.13
$CaSO_4$ ppt. (24.15 gm)

Case 7 :

$CaSO_4$: 15.0 gm (everything same)
NaOH needed for pH = 6 = 0.372 gm
Some ppt of $CaSO_4$ noted
Same as without acid gases.

Case 8

1/27/98

Because $CaSO_4$ solubility increases at this pH,

Case 6

34/42

ESP V-5.3 STREAM:prci 01/27/98 PAGE 1

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	7.0000			
Total mol/hr	164.15	0.14211	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2935.7	0.0	0.0	0.0
CO2	8.0170E-02	0.0	0.0	0.0
H2SO4	3.9436E-23	0.0	0.0	0.0
H2S	1.8241E-02	0.0	0.0	0.0
HCL	2.3925E-21	0.0	0.0	0.0
SO3	3.6749E-27	0.0	0.0	0.0
NAHCO3	0.11974	0.0	0.0	0.0
CASO4	1.4471	0.0	0.0	0.0
CACO3	1.1793E-09	0.81491	0.0	0.0
OHION	3.4300E-06	0.0	0.0	0.0
CAION	2.4766	0.0	0.0	0.0
CAOHION	9.2819E-07	0.0	0.0	0.0
CLION	17.837	0.0	0.0	0.0
CO3ION	8.4069E-04	0.0	0.0	0.0
HCO3ION	0.67885	0.0	0.0	0.0
HION	3.9554E-07	0.0	0.0	0.0
HSION	1.9678E-02	0.0	0.0	0.0
HSO4ION	1.3324E-05	0.0	0.0	0.0
NACO3ION	2.0896E-04	0.0	0.0	0.0
NAION	12.155	0.0	0.0	0.0
NASO4ION	0.29013	0.0	0.0	0.0
CAHCO3ION	6.5954E-04	0.0	0.0	0.0
SION	4.6174E-08	0.0	0.0	0.0
SO4ION	6.4849	0.0	0.0	0.0
CASO4.2H2O	0.0	23.065	0.0	0.0
==========	==========	==========	==========	==========
Total g/hr	2977.3	23.880	0.0	0.0
Volume, L/hr	2.9447	9.2095E-03	0.0	0.0
Enthalpy, cal/hr	-1.1236E+07	-6.7206E+04	0.0	0.0
Density, g/L	1011.1	2593.0		
Vapor fraction	0.0	0.0	0.0	0.0
Solid fraction	0.0	1.0000	0.0	0.0
Organic fraction	0.0	0.0	0.0	0.0
Osmotic Pres, psia	116.14			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	1.6809E-02			
E-Con, cm2/ohm-mol	78.730			
Ionic Strength	0.26625			

N. Smith 4/17/98

1/27/98 Case 8:

NaCl : 30 gm

CO_2 : 10 psi

H_2S : 0.5 psi

P : ~~3000~~ 500

pH = 6 ; $NaHCO_3$: 1.2~~32~~ 89 g

See print out on p 27

Case 9:

Same as case 8, but pH = 8.

See print out on p.28

NaOH = 0.95 g

N. Srinivas
1/27/98

Case 8

36/42

ESP V-5.3 STREAM:prci 01/27/98 PAGE 1

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	6.0000			
Total mol/hr	165.89	0.0	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2969.3	0.0	0.0	0.0
CO2	1.0064	0.0	0.0	0.0
H2S	3.5112E-02	0.0	0.0	0.0
HCL	2.4914E-20	0.0	0.0	0.0
NAHCO3	0.15530	0.0	0.0	0.0
OHION	3.3029E-07	0.0	0.0	0.0
CLION	18.013	0.0	0.0	0.0
CO3ION	8.6536E-05	0.0	0.0	0.0
HCO3ION	0.81656	0.0	0.0	0.0
HION	3.7432E-06	0.0	0.0	0.0
HSION	3.6732E-03	0.0	0.0	0.0
NACO3ION	2.5398E-05	0.0	0.0	0.0
NAION	11.991	0.0	0.0	0.0
SION	7.3025E-10	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	3001.3	0.0	0.0	0.0
Volume, L/hr	2.9784	0.0	0.0	0.0
Enthalpy, cal/hr	-1.1339E+07	0.0	0.0	0.0
Density, g/L	1007.7			
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, psia	116.97			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	1.4619E-02			
E-Con, cm2/ohm-mol	79.554			
Ionic Strength	0.17566			

N. Siddiqui
1/27/98

[redacted]

Case 9 :

ESP V-5.3 STREAM:prci 01/27/98 PAGE 1

STREAM: prci
POINT :

Phases---------->	Aqueous	Solid	Vapor	Organic
Temperature, C	15.600	15.600	15.600	15.600
Pressure, psia	500.00	500.00	500.00	500.00
pH	8.0000			
Total mol/hr	165.88	0.0	0.0	0.0
----------	g/hr----------	g/hr----------	g/hr----------	g/hr----------
H2O	2969.3	0.0	0.0	0.0
CO2	1.4607E-02	0.0	0.0	0.0
H2S	3.2969E-03	0.0	0.0	0.0
HCL	2.4875E-22	0.0	0.0	0.0
NAHCO3	0.22821	0.0	0.0	0.0
OHION	3.3061E-05	0.0	0.0	0.0
CLION	18.013	0.0	0.0	0.0
CO3ION	1.2641E-02	0.0	0.0	0.0
HCO3ION	1.1871	0.0	0.0	0.0
HION	3.7467E-08	0.0	0.0	0.0
HSION	3.4547E-02	0.0	0.0	0.0
NACO3ION	3.7381E-03	0.0	0.0	0.0
NAION	12.163	0.0	0.0	0.0
SION	6.9029E-07	0.0	0.0	0.0
	==========	==========	==========	==========
Total g/hr	3001.0	0.0	0.0	0.0
Volume, L/hr	2.9779	0.0	0.0	0.0
Enthalpy, cal/hr	-1.1339E+07	0.0	0.0	0.0
Density, g/L	1007.8			
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, psia	115.87			
Redox Pot, volts	0.0			
E-Con, 1/ohm-cm	1.4725E-02			
E-Con, cm2/ohm-mol	78.908			
Ionic Strength	0.17824			

N Sridhar 4/27/98

INSTALLATION TEST
For ESP Version 6.0

2/25/98 PRCI - New Test 4/8/98 38/42

Additional chemical compositions were received from Dari DesNoyer (Consumers Energy). OLI Systems was used to calculate the test conditions.

Software used: ESP version 6.0
Bench mark run to compare to previous version:

Problem same as on p. 18 (Case 2)

NaOH required to maintain pH = 6 was 0.7711 gms. This value is close, but slightly different from that shown on p. 18 [0.778 gms]. It appears that the value is a slight function of how the problem is set up. For example, if water inflow is set up as 30000 gm & the Total inflow is set up as 30000 g, then calculated NaOH = 0.7711. If water inflow is set up ~~close to the final~~ as 30000 g, but Total inflow is NOT Specified 2/27 then NaOH = 0.832 gm. Perhaps a convergence problem.

N. Sridhar
2/27/98

2/27/98

Case 10:

Total : 3000 gm

Consumer sample W-292

pH = 5.5

$CaCl_2$: (from 34,300 ppm Ca) = 285 gm.

$MgCl_2$: (from 8700 ppm Mg) = 102 gm

KCl : (from 1,350 ppm K) = 7.7 gm

NaCl : (from 46,400 ppm Na) = 351.0 gm.

Total H_2S ppm : 4.05 + 4.06 = 8.11 ppm

$= 2.43 \times 10^{-2}$ gm.

This is less than what we have added, so we continue 0.5 psia H_2S as before (see p. 18)

CO_2 = 10 psia = 1.012 gm (see p. 18)

H_2S = 0.5 psi = 0.0393 gm (see p. 18)

Total pressure = 500 psia.

To make pH = 5.5, NaOH to be added = 0.639 gm

No solids were predicted.

Printed to file : case10.lis

Case 11:

Same as Case 10 but total pressure = 800 psi.

NaOH needed for pH 5.5 = 0.638 gm.

N. Tribble

2/27/98

40/42

Case #: 12 N7

Consumer sample W = 333

pH = 4.3

Total H_2S = 16.7 ppm = 5.01×10^{-2} gm. = 0.64 psia

NaOH = 0.209 gm to make pH = 4.3
No solids.

Printed to case12.lis file.

N. Smith
2/27/98

3/4/98 Case #13

same as Case #12 except :

30 g : NaCl
0 g : $MgCl_2$
0 g : $CaCl_2$
0 g : $CaSO_4$
0 g : KCl

10 psi CO_2 = 0.012 g
0.5 psi H_2S = 0.0393

No oxygen purge.

OLI calculation : NaOH to be added = 0.346 g

Case #14

Same as case 13, but no H_2S

OLI calculation : NaOH to be added = 0.340

Case #15

Same as Case 13, but no chloride.

NaOH = 0.28274 g

N. Smith
3/4/98