SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE - SRN - 254	
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: [signature] Date: 8/17/01

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)

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 N Sridhar L. Yang Date: 08/18/01

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

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
➜ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: OLI Software ESP

Version: ESP V 6.5 & CSP V 2.2

Demonstration workstation: PC

Operating System: Windows NT 4.0

User: Lietai Yang

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system?

Yes: ■ No: ❒ N/A: ❒

Computer Platforms: PC Operating Systems: Windows NT 4.0

Location of Acceptance Test Results: Documented in S/N 430, page 115

Comments: The comparison with literature data is recorded in S/N 430, page 116-117. Copy included in QA software folder.

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version?

Yes: ❒ No: ■ N/A: ❒

Date and Time Displayed: ___
Name/Version Displayed: ___

Comments: Although runs are not uniquely identified by date, and name of software and version, this information is added on the spreadsheet header. See copies in QA software folder (pgs. 62, 69, and 133).

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?

Yes: ■ No: ❒ N/A: ❒

Comments: EXE file type

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ACQUIRED SOFTWARE NOT TO BE MODIFIED←

User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ■ No: ❒ N/A: ❒

User's Manual Version and Date: ESP V.6.5 & CSP V.2.2
Comments: 3rd Edition Manual

Are there basic instructions for the *installation* and *use* of the software?

Yes: ■ No: ❒ N/A: ❒

Location of Instructions: Documented in S/N 430, page 115
Comments:

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed?

Yes: ■ No: ❒ N/A: ❒

Date of Approval: 8/18/2001

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ■ No: ❒ N/A: ❒

Comments: Copies included from S/N 430

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ■ No: ❒ N/A: ❒

Location of Executable Code: On CD ROM

Comments: No source code available.

Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted.

Yes: ■ No: ❒ N/A: ❒

Location of executable files: QA software folder
Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
➔ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ■ No: ❒ N/A: ❒

SRN Number: CSPE-SRN-254

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ❒ No: ■ N/A: ❒

Version and Date of SVTP: ____

Date Reviewed and Approved via QAP-002: _____

Comments: Previous versions are classified as validation category III. Validation category for this version it to be determined.

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ❒ No: ■ N/A: ❒

Version and Date of SVTR: _____

Date Reviewed and Approved via QAP-002: _____

Comments: Previous versions are classified as validation category III. Validation category for this version it to be determined.

Additional Comments:

L. Yang 09/28/01 — Software Evaluator/User/Date

9/28/2001 — Software Custodian/Date

Maria J Padilla 9/28/01

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.

Template Reconcile Units LastResult Help

Sample: UZ-B

YM_WATER Study
YM_WATER Model
Concentrations

Values in mg/l

Cations	Input	Reconciled	Anions	Input	Reconciled
CA+2	49.9	51.[illegible]	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 7.68165

<PgDn>

~~SiO2: 143 mg/L = 0.00238 mol/kg~~ ; added ~1 mg/L Ca++ for reconciliation

S.y. 04/18/01

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

SiO_2: 89.8 mg/L = 1.495 E-3 mol/kg.

Sample DE-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.	488.9561
AL+3	13.8	13.79854	NO3-1	4.	3.999582
			SO4-2	28.	27.99708

<PgDn>

not included: SiO_2: 173 mg/L = 0.0[illegible] ~~29.8 mg/L = 1.49 E-3 mol/kg~~ 2.9 eq/l
added NO_3^- during reconciliation

Sample: NRG-A. Calculated pH = 7.43

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.	[illegible]	CL-1	185.	184.9998
MG+2	23.3	[illegible]	CO3-2		
NA+1	35.6	[illegible]	HCO3-1	34.	[illegible]
AL+3			NO3-1	32.	[illegible]
			SO4-2	159.	158.9996

1.6219 mol

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

Results: File Name: Darrell-Pb-Chem.xls in c:\w director.

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

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

Inputs	Case 1, 0.5 M NaCl, No solid above 80 oC					Case 2, 1 M NaCl, No solid above 80 oC					Case 3, 4 M NaCl, No solid above25 oC			
H2O (mol)	55.5					55.5					55.5			
NaCl (mol)	0.5					1					4			
LiCl (mol)	0					0					0			
HCl (mol)	0					0					0			
PbCl2 (mol)	4.00E-03					4.00E-03					4.00E-03			
Pb(CH3CO2)2 (mol)	0.004					0.004					0.004			
PbSO4 (mol)	0.001					0.001					0.001			
Total Pb (ppm)	**1808.6943**					**1774.34395**					**1602.585**			
Stream	T25oC	T25oC	T80oC	T100oC	T120oC	T25oC	T25oC	T80oC	T100oC	T120oC	T25oC	T80oC	T100oC	T120oC
Phase	Aqueous	Solid	Aqueous	Aqueous	Aqueous	Aqueous	Solid	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous	Aqueous
Temperature, C	25	25	80	100	120	25	25	80	100	120	25	80	100	120
Pressure, atm	1	1	1	1	2	1	1	1	1	2	1	1	1	2
pH	6.78395		6.04375	5.89688	5.78944	7.02567		6.28311	6.14	6.03875	7.95701	7.18945	7.0032	6.85401
Total mol/hr	56.5068	0.0027333	56.5096	56.5088	56.508	56.9907	0.002272	56.9927	56.9922	56.9913	59.7523	59.7523	59.7521	59.7519
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	55.4997		55.4994	55.4993	55.4992	55.0086		55.0085	55.0085	55.0084	52.2355	52.2355	52.2355	52.2355
ACETACID	4.03E-05		2.53E-04	3.79E-04	5.26E-04	1.89E-05		1.20E-04	1.76E-04	2.40E-04	9.34E-07	6.09E-06	9.60E-06	1.41E-05
ACET2	2.78E-17		5.06E-15	1.67E-14	4.41E-14	6.78E-18		1.25E-15	4.01E-15	1.02E-14	3.13E-20	6.11E-18	2.24E-17	6.63E-17
H2SO4	8.78E-27		1.15E-24	3.85E-24	1.10E-23	1.99E-27		1.88E-25	6.00E-25	1.61E-24	3.42E-30	2.74E-28	9.47E-28	2.77E-27
HCL	2.99E-14		3.81E-12	1.34E-11	3.76E-11	3.00E-14		3.79E-12	1.32E-11	3.63E-11	9.15E-15	1.18E-12	4.50E-12	1.38E-11
SO3	1.16E-30		4.16E-28	2.33E-27	1.17E-26			6.93E-29	3.69E-28	1.74E-27				3.39E-30
LIOH														
NAACET	0.001077		0.0012685	0.001437	0.001634	0.00170985		0.001997	0.002241	0.002526	0.0035208	0.003855	0.004154	0.004485
PBACET2	7.99E-06		2.39E-05	3.30E-05	4.44E-05	1.58E-06		4.76E-06	6.32E-06	8.09E-06	1.28E-09	4.68E-09	6.30E-09	7.82E-09
PBCL2	0.0018636	0.0025077	0.003267	0.003451	0.003593	0.00167755	0.002272	0.002876	0.002931	0.002909	5.19E-05	1.07E-04	1.16E-04	1.18E-04
PBO	6.05E-08		5.32E-07	9.25E-07	1.49E-06	4.33E-08		3.78E-07	6.50E-07	1.04E-06	3.57E-09	3.57E-08	5.45E-08	7.26E-08
LIACET														
OHION	8.44E-08		4.12E-07	6.82E-07	1.08E-06	1.42E-07		7.20E-07	1.22E-06	1.99E-06	6.67E-07	3.94E-06	6.48E-06	1.01E-05
CLION	0.493561		0.49393	0.493463	0.492971	0.977239		0.977376	0.977084	0.976599	3.73873	3.73909	3.73916	3.73921
HION	2.15E-07		1.25E-06	1.80E-06	2.37E-06	1.15E-07		6.86E-07	9.83E-07	1.28E-06	6.00E-09	4.47E-08	7.44E-08	1.14E-07
HPBO2ION	6.50E-12		1.10E-10	2.40E-10	4.73E-10	9.05E-12		1.53E-10	3.34E-10	6.64E-10	8.23E-12	1.57E-10	2.77E-10	4.15E-10
HSO4ION	2.21E-09		6.84E-08	1.69E-07	3.78E-07	9.91E-10		2.23E-08	5.30E-08	1.13E-07	2.13E-11	3.98E-10	9.35E-10	1.97E-09
LIION														
LISO4ION														
NAION	0.498868		0.498656	0.498495	0.498307	0.989354		0.989069	0.988835	0.988562	3.76111	3.7608	3.76052	3.7602
NASO4ION	5.25E-05		7.25E-05	6.59E-05	5.63E-05	8.25E-05		8.07E-05	7.07E-05	5.81E-05	8.87E-05	6.33E-05	4.85E-05	3.43E-05
ACETATEION	0.0065306		0.0060438	0.005752	0.0054	0.00610914		0.0057	0.005406	0.005061	0.0040076	0.003668	0.003366	0.00303
PBACET3ION	4.98E-06		1.07E-05	1.61E-05	2.46E-05	1.09E-06		2.39E-06	3.44E-06	5.05E-06	1.53E-09	4.03E-09	5.77E-09	8.02E-09
PBACETION	3.21E-04		3.54E-04	3.18E-04	2.78E-04	8.49E-05		9.52E-05	8.31E-05	7.01E-05	1.89E-07	2.70E-07	2.49E-07	2.14E-07
PBCL3ION	4.94E-04		8.37E-04	9.23E-04	0.001023	9.77E-04		0.001619	0.001724	0.001824	2.18E-04	4.33E-04	4.90E-04	5.33E-04
PBCL4ION	4.42E-04		4.50E-04	4.73E-04	5.24E-04	0.00243066		0.002349	0.002359	0.002468	0.0081882	0.007908	0.007841	0.007798
PBCLION	0.0024445		0.0032239	0.002971	0.002673	0.00128365		0.001696	0.00152	0.001316	1.19E-05	2.01E-05	1.95E-05	1.76E-05
PBION	6.48E-04		5.80E-04	4.35E-04	3.13E-04	1.73E-04		1.59E-04	1.17E-04	8.21E-05	1.66E-07	2.04E-07	1.62E-07	1.18E-07
PBOHION	4.03E-05		2.53E-04	3.78E-04	5.24E-04	1.88E-05		1.19E-04	1.75E-04	2.38E-04	2.66E-07	2.12E-06	3.09E-06	3.94E-06
SO4ION	7.22E-04		9.27E-04	9.34E-04	9.43E-04	9.09E-04		9.10E-04	9.20E-04	9.33E-04	8.52E-04	8.78E-04	8.93E-04	9.07E-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	1050.98	0.631813	1051.62	1051.62	1051.62	1163.62	1163.62	1163.62	1163.62
Volume, m3/hr	0.0010123	1.30E-07	0.0010391	0.001053	0.00107	0.0010129	1.08E-07	0.001041	0.001055	0.001071	0.0010204	0.001059	0.001071	0.001083
Enthalpy, cal/hr	-3.84E+06	-265.003	-3.79E+06	-3.77E+06	#######	-3.86E+06	-195.149	-3.80E+06	-3.78E+06	-3.76E+06	-3.93E+06	-3.88E+06	-3.87E+06	-3.85E+06
Density, g/m3	1.02E+06	5.89E+06	9.93E+05	9.80E+05	9.64E+05	1.04E+06	5.85E+06	1.01E+06	9.97E+05	9.82E+05	1.14E+06	1.10E+06	1.09E+06	1.07E+06
Vapor fraction														
Solid fraction		1					1							
Organic fraction														
Osmotic Pres, atm	22.8623		26.0598	26.9772	27.7647	46.6328		52.9188	54.8012	56.4493	231.494	258.729	268.568	278.325
Redox Pot, volts														
E-Con, 1/ohm-cm	0.0462659		0.0998507	0.11922	0.138152	0.0836697		0.179759	0.215077	0.249256	0.218002	0.474041	0.574753	0.677594
E-Con, cm2/ohm-mol	92.0167		204.141	247.075	290.735	84.7429		187.297	227.053	267.06	58.9564	133.018	163.196	194.602
Abs Visc, cP	0.933946		0.377935	0.301039	0.248232	0.97815		0.4002	0.319175	0.263346	1.37419	0.569755	0.458327	0.38248
Rel Visc	1.04853		1.06707	1.06912	1.07	1.09816		1.12993	1.13352	1.13515	1.54279	1.60865	1.62771	1.64867
Ionic Strength	0.504865		0.50569	0.504961	0.504279	1.00364		1.00376	1.00329	1.00287	4.00641	4.00582	4.00547	4.0051

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

L.Y. 04/19/01

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

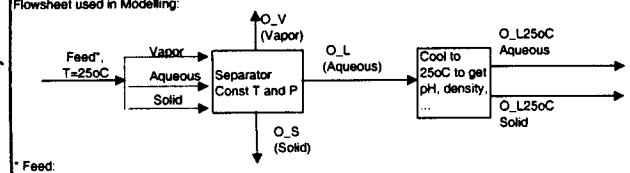
Summary of Modeling Results with OLI ESP 6.5

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,atm	0.479577			877.248
189	RedoxPot,volts				
190	E-Con,1/ohm-cm	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

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 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

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

$P^{o}_{H_2O}$

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		

P_{H_2O}

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

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~~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$_2$. The error is $\frac{35.1 - 30.5}{30.5} = 0.15$ which $= 15\%$ is quite significant.

J. Yang 08/17/01

SOFTWARE VALIDATION TEST PLAN FOR ENVIRONMENTAL SIMULATION PROGRAM (ESP) VERSION 6.5/CORROSION SIMULATION PROGRAM (CSP) VERSION 2.2, ENVIRONMENTAL SIMULATION PROGRAM FOR CONCENTRATED BRINES (ESPCB) VERSION 7.0 ALFA, AND STREAMANALYZER 1.1

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

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May 2002

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5/29/02
Date

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1 SCOPE OF THE VALIDATION

This document establishes the Software Validation Test Plan for validating the functionality of the OLI Systems' simulation packages, Environment Simulation Program (ESP) Version 6.5/ Corrosion Simulation Program (CSP) 2.2, StreamAnalyser 1.1, and Environment Simulation Program for Concentrated Brines (ESPCB) Version 7.0 Alfa, through comparisons of calculated results with published data available in the literature.

ESP/CSP, StreamAnalyzer, and ESPCB are different packages of the OLI simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). ESP is for evaluating the thermodynamic properties of different streams in a chemical process in industrial and environmental applications. ESP has a larger database of thermodynamic parameters and represents standard-state properties using the Helgeson-Kirkham-Flowers (Helgeson, et. al., 1981) equation-of-state and excess properties using the aqueous activity coefficient expressions developed by Bromley (1972) and Pitzer (1973, 1991). These models enable simulation of aqueous chemical systems using ESP for temperatures to 300 °C, pressures to 1,500 atm, and ionic strengths up to 30 molal. CSP is for evaluating the thermodynamic properties that are related to the characteristics of corrosion and the corrosion rate of a metal in a given solution system. A regular ESP/CSP package contains both the ESP and CSP components. StreamAnalyzer is essentially a component of the ESP and packaged as a stand-alone software for evaluating the thermodynamic properties of a single aqueous stream. StreamAnalyzer has been added with a friendly graphic-user interface. The ESPCB is a special version of ESP specifically developed for Southwest Research Institute®. The ESPCB contains an additional Mixed Solvent Electrolyte Model and some added new data bank. The ESPCB is suitable for use in highly concentrated salts (close to or above 30 molal). The scope of this test will be within the following ranges:

Temperature:	0 to 300 °C
Pressure:	0 to 1500 atm (saturation pressure of water)
Ionic Strength:	0 to 30 molal for the ESP 6.5, CSP 2.2 and StreamAnalyzer 1.1
	0 to 50 molal for ESPCB 7.0 Alfa

2 REFERENCES

The following documents are referenced in this Software Validation Test Plan.

Bromley, L.A. "Approximate Individual Ion Values of β (or B) in Extended Debye-Huckel Theory for Uni-Univalent Aqueous Solutions at 298.15 K." *Journal of Chemical Thermodynamics.* Vol. 4. p. 669. 1972.

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3 ENVIRONMENT

3.1 Software

The family of the OLI simulation packages ESP Version 6.5/CSP Version 2.2, StreamAnalyser Version 1.1, and ESPCB Version 7.0 Alfa run in Windows environment (95, 98, 2000, Me and NT). The validation test will be conducted in NT 4.0.

3.2 Hardware Requirements

The family of the OLI simulation packages ESP Version 6.5/CSP Version 2.2, StreamAnalyzer Version 1.1, and ESPCB Version 7.0 Alfa run on the IBM PC family of microcomputers or compatible systems. According to the license agreement for PC users, the software can be installed in many computers. However, a hardware key is required on the microcomputer that runs the program. With only one hardware key issued to a license holder, only one user is allowed to use the software at a given time. The family of the OLI simulation packages also run

on network system. With a license for network system, the program can be used by multiusers at the same time. The validation test will be conducted with a Pentium II PC.

The input and output parameters can be printed to either a printer or a text spreadsheet file. The CSP and StreamAnalyzer also support graphical output to printers.

4 PREREQUISITES

Running the OLI simulation packages and output the results as an spreadsheet file requires presence of a spreadsheet software, such as MS Excel 97 present in the system.

5 ASSUMPTIONS AND CONSTRAINTS

The user of OLI packages is assumed to be familiar with chemical thermodynamics.

The ESP 6.5/CSP2.2 and StreamAnalyser 1.1 are based on the standard-state properties using the Helgeson-Kirkham-Flowers (1981) equation-of-state and excess properties using the aqueous activity coefficient expressions developed by Bromley (1972) and Pitzer (1973,1991). The software has the following limitations:

Water content: > 65 percent (Molar basis)
Temperature: -50 to 300 °C
Ionic Strength: 0 to 30 molal
Pressure: 0 to 1500 atm

The limitations for the ESPCB 7.0 Alfa are:

Water content: up to 100 percent (Molar basis)
Temperature: -50 to 300 °C
Ionic Strength: up to fused salts
Pressure: 0 to 1,500 atm

6 TEST CASES

The test cases described in this section involve calculations of mineral solubilities and vapor pressures of salt solutions and salt mixtures in the temperature range of 0 to 300 °C.

6.1 Test Case 1—NaCl Solubility as a Function of Temperature

The solubility of NaCl(s) will be calculated from 25 to 300 °C and compared with experimental data. The test will determine the ability of the ESP6.5/CSP2.2, StreamAnalyzer 1.1, and ESPCB 7.0 to accurately calculate the solubility of a single salt at different temperature conditions.

6.1.1 Test Input

Input temperatures will be 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C, the input pressure will be 1.0 atm. At 100 °C and above, the input pressures will be the vapor saturation pressure at the temperature of interest.

6.1.2 Test Procedure

The test will be run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point calculation at temperatures equal or above 100 °C.

6.1.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1 and ESPCB7.0 Alfa will be saved to three files named ESP_Case1.xls, StreamAnalyser_Case1.xls, and EXPCB_Case1.xls respectively. These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and Cl^-. The calculated Na^+ (or Cl^-) concentrations will be compared with experimental data given in Liu and Lindsay (1972) and Linke (1965). The test results will be considered acceptable if within ±10 percent of experimental data.

6.2 Test Case 2—NaCl and/or KCl Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl and/or KCl will be calculated at different temperatures and compared with experimental data. The test will determine the ability of the OLI software to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

6.2.1 Test Input

Input temperatures will be 40, 100, and 120 °C. Below 100 °C, the input pressure will be 1.0 atm. At 100 °C and above, the input pressure will be the vapor saturation pressure at the temperature of interest. When the solubility of NaCl is calculated, a fixed value of K^+ concentration will be input and an extra amount of NaCl will be specified in the input stream. On the other hand, when the solubility of KCl is calculated, a fixed value of Na^+ concentration will be input and an extra amount of KCl will be specified in the input stream. The solubilities of the two salts in the eutonic solution of NaCl and KCl will be calculated by specifying extra amount of both NaCl and KCl in the input stream.

6.2.2 Test Procedure

The test will be run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point calculation at temperatures equal or above 100 °C.

6.2.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1, and ESPCB7.0 Alfa will be saved to three files named ESP_Case2.xls, StreamAnalyser_Case2.xls, and EXPCB_Case2.xls, respectively. These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ and Cl^-. The calculated Na^+, K^+, (or Cl^-) concentrations will be compared with experimental data given in Linke (1965). The test results will be considered acceptable if within ±10 percent of experimental data. The value of ±10 percent is arbitrarily set in this report because ±10 percent variation in concentration would not significantly affect the performance of the engineered barrier system in the repository system.

6.3 Test Case 3—Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

The solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions will be calculated at 0 and 50 °C and compared with experimental data. The test will determine the ability of OLI packages to accurately calculate the solubility of minerals in a solution containing multicomponent dissolved salts.

6.3.1 Test Input

The input temperature will be 0 and 50 °C and the input pressure will be 1.0 atm. The concentration of Ca^{2+}, Na^+ and K^+ will be varied, and the saturated concentration of Mg^{2+} will be calculated with slightly excess $MgCl_2$ in the solid phase.

6.3.2 Test Procedure

The test will be run by specifying the calculation type as isothermal calculation.

6.3.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser 1.1 and ESPCB7.0 Alfa will be saved to three files named ESP_Case3.xls, StreamAnalyser_Case3.xls, and EXPCB_Case3.xls respectively. These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+}, Na^+, K^+, Mg^{2+}, and Cl^-. The calculated Mg^{2+} concentrations will be compared with solubility data given by Korin and Roy (1988). The test results will be considered acceptable if within ±10 percent of experimental data.

6.4 Test Case 4—Vapor Pressure of KCl Solutions at 300 °C as a Function of Concentration

The vapor pressure of KCl solutions as a function of concentration will be calculated and compared with experimental data. The test will determine the ability of the OLI packages to accurately calculate the vapor pressures of single alkaline-chloride solutions.

6.4.1 Test Input

The input temperature will be 300 °C and the input pressure will be the vapor saturation pressure at the temperature of interest. The input KCl concentrations will be varied.

6.4.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation.

6.4.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1, and ESPCB7.0 Alfa will be saved to three files named ESP_Case4.xls, StreamAnalyser_Case4.xls, and EXPCB_Case4.xls, respectively. These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of K^+ and Cl^-. The calculated KCl solution vapor pressure will be compared with vapor pressure data from Zarembo, et al. (1976). The test results will be considered acceptable if within ±10 percent of experimental data.

6.5 Test Case 5—Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C as a Function of Concentration

The vapor pressure of $CaCl_2$ solutions as a function of concentration will be calculated and compared with experimental data. The test will determine the ability of the OLI packages to accurately calculate the vapor pressures of alkaline-earth-metal chloride solutions.

6.5.1 Test Input

The input temperature will be 100 °C and the input pressure will be the vapor saturation pressure. The input $CaCl_2$ concentrations will be varied.

6.5.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation.

6.5.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1, and ESPCB7.0 Alfa will be saved to three files named ESP_Case5.xls, StreamAnalyser_Case5.xls and EXPCB_Case5.xls respectively. These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+} and Cl^-. The calculated $CaCl_2$ solution vapor pressure will be compared with vapor pressure data from handbook (Weast, 1984). The test results will be considered acceptable if within ±10 percent of experimental data.

6.6 Test Case 6—Lowering of Vapor Pressure by $NaNO_3$, NaOH, $NaHSO_4$, and $NaHCO_3$ in Aqueous Solutions at 100 °C

The vapor pressures of $NaNO_3$, NaOH, $NaHSO_4$, and $NaHCO_3$ solutions will be calculated and compared with experimental data. The test will determine the ability of the OLI packages to accurately calculate the vapor pressures of nitrate, hydroxide, bisulphate, and bicarbonate solutions.

6.6.1 Test Input

The input temperature will be 100 °C and the input pressure will be the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH, $NaHSO_4$, and $NaHCO_3$ will be varied.

6.6.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation.

6.6.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1, and ESPCB7.0 Alfa will be saved to three files named ESP_Case6.xls, StreamAnalyser_Case6.xls, and EXPCB_Case6.xls, respectively. These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions. The calculated solution vapor pressures will be compared with vapor pressure data from handbook (Weast, 1984). The test results will be considered acceptable if within ±10 percent of experimental data.

6.7 Test Case 7—Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

The mutual deliquescence point of mixed NaCl-$NaNO_3$-KNO_3 salts will be calculated and compared with experimental data. The test will determine the ability of the OLI Packages to accurately calculate the mutual deliquescence point of mixed salts.

6.7.1 Test Input

The input temperature to be used will be 86 °C. The input concentrations of $NaNO_3$, NaCl, and KNO_3 will be specified such that undissolved $NaNO_3$, NaCl, and KNO_3 will be all present in the output streams.

6.7.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation.

6.7.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2, StreamAnalyser1.1, and ESPCB7.0Alfa will be saved to three files named ESP_Case7.xls,

StreamAnalyser_Case7.xls, and EXPCB_Case7.xls, respectively. These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and NO_3^-, Cl^-, and K^+. The calculated deliquescence points which is the ratio between the vapor pressure of the saturated three salts and the vapor pressure of water or the activity of water directly reported in the StreamAnalyzer. The calculated values will be will be compared with the deliquescence point measured in the experiments (Yang, et al., 2001). The test results will be considered acceptable if within ±10 percent of experimental data. The error is set at ±10 percent because there should not be much variation among the different databases.

6.8 Test Case 8—Stability Diagram for Nickel-Water System

The stability diagram of nickel-water system at 25 °C will be calculated and compared with published stability diagram. The test will determine the ability of the OLI ESP6.5/CSP2.2 to accurately calculate the stability diagram of metals in solution.

6.8.1 Test Input

The input temperature to be used will be 25 °C. HCl and NaOH will be used as the acid and base titrants respectively for pH adjustment. Only water will be specified in the input stream. The concentration of Ni^{2+} will be set at the trace species amount (1E–6 M) which is specified in the Option menu under Trace Species Amount submenu.

6.8.2 Test Procedure

The test will be run in the pH range of 0 to 14 and the potential range of -1.0 to 2.0. An E–pH will be produced.

6.8.3 Test Results

A hard copy of the output stability diagram (E–pH diagram) from the run with ESP6.5/CSP2.2 will be printed. Comparisons will be made between the calculated and the published potential and pH values (Pourbaix, 1974) for selected solid lines that represent the boundaries between stability areas of a solid and an aqueous species or two aqueous species. The results will be considered acceptable if the errors are within ±0.15 V for potentials and ±0.3 for pH from values showing on the published E–pH diagrams unless there are significant uncertainties in the source data used by the published E–pH diagrams.

6.9 Test Case 9—Solubility of $NaNO_3$ and NaOH at Concentrations Beyond 30 M

The solubility of $NaNO_3$ and NaOH salts will be calculated and compared with experimental data. The test will determine the ability of the ESPCB software to accurately calculate the solution properties of extremely concentrated aqueous solutions.

6.9.1 Test Input

The input temperature to be used will be from 94 to 202 °C. The input concentrations of $NaNO_3$ and NaOH will be specified such that undissolved $NaNO_3$ and NaOH will be present in the output streams.

6.9.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation.

6.9.3 Test Results

The results of the calculation outputs from the runs with ESPCB7.0 Alfa will be saved to EXPCB_ Case9.xls. The file lists the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, NO_3^-, and OH^-. The calculated solubility values will be compared with the published solubility data (Linke, 1965). The test results will be considered acceptable if within ±10 percent of experimental data.

6.10 Test Case 10—Lowering of Vapor Pressure by $NaNO_3$, NaOH, $NaHSO_4$, and $NaHCO_3$ in Aqueous Solutions at 100 °C Using Private Databases

In addition to the public database, OLI simulation packages contain several private databases such as Geochem, Ceramic, and Corrosion. In most simulations, the public database contains all the thermodynamic data that are required. However, there cases some species that are required in a simulation cannot be found in the public database. In this case, one or more private databases that contain the required species must be activated by the user. The OLI engine will search the private databases first (according to the sequence appeared in the activated private list) for all the species involved in the simulation. If there are still species that are not found in the specified private databases, the public database will be activated. This case is the same to Case 6 except the private databases (Geochem, Ceramic, and Corrosio) will be activated during the simulation to test the effect of databases on the simulation results

6.10.1 Test Input

The input temperature to be used will be 100 °C and the input pressure will be the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH, $NaHSO_4$, and $NaHCO_3$ will be varied.

6.10.2 Test Procedure

The test will be run by specifying the calculation type as bubble point calculation. The chemistry model will be regenerated with the Geochem, Ceramic, and Corrosio databases being activated.

6.10.3 Test Results

The results of the calculation outputs from the runs with ESP6.5/CSP2.2 will be saved to a file named ESP_Case10.xls. This file list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions. The calculated solution vapor pressures will be compared with the results obtained in Case 6. The test results will be considered acceptable if within ±5 percent of experimental data.