SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE-SRN-231	
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.6.2e and CSP V. 2.0e	
4. Originator/Requestor: L. Yang	Date: 11/29/00

5. Summary of Actions

- ■ Release of new software (New version)
- ☐ 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: 11/29/00

8. Remarks: Installation test was performed by N. Sridhar on 11/29/00 and the results compares with ESP6.0 (scientific Notebook #135, p. 10-11).

The comparison is documented by L. Yang (see enclosed) and recorded in Scientific Notebook #430, pages 30 through 35.

SOFTWARE RELEASE NOTICE

1. SRN Number: CSPE-SRN-231

2. Project Title: Evolution of Near Field Environment and Container Life Source Term	Project No. 20.01402.561 & 20.01402.571

3. SRN Title: OLI ESP V.6.2e and CSP V.2.0e

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:
  - ☐ Enhancements made
  - ☐ Corrections made
- ■ Software Retirement

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:

SOFTWARE SUMMARY FORM

01. Summary Date: 11/07/00	02. Summary prepared by (Name and phone) L. Yang (210)522 2483	03. Summary Action: Updating
04. Software Date: 01/17/2000	05. Short Title: OLI Software ESP V 6.2e /CSP V 2.0e	
06. Software Title: ESP V 6.2e and CSP V 2.0e: Components of OLI Software		07. Internal Software ID:

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

11. Submitting Organization and Address:	12. Technical Contact(s) and Phone:
CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228	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	15. Computer Operating System:	16. Programming Language(s):	17. Number of Source Program Statements:
PC	Windows NT/95	N/A	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:	24. Documentation Availability:
☐ Available ■ Limited ☐ In-House ONLY	■ 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

N Sridhar 12/5/00

Software User: N. Sridhar and L. Yang Date: 11/29/00

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

12/5/2000

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE

ACQUIRED CODE - NOT TO BE MODIFIED[1]

Software Title/Name: OLI Software ESP

Version: ESP V6.2e/CSP V2.0e

Demonstration workstation: Krull

Operating System: Windows NT/95

Developer: Microsoft

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1. Output: TOP-018, Section 5.5.4

Software designed so that individual runs are uniquely identified by Date, Time, Name of software and version?

Yes: ☐ No: ☐ N/A: ☑

Date and time of run: N/A

Name and version: N/A

Notes: Acquired code that is not to be modified is accepted as is.

2. Medium and Header Documentation: TOP-018, Section 5.5.6

The physical labeling of software medium (tapes, disks, etc.) contain required information?

Yes: ☑ No: ☐ N/A: ☐

Program Name: OLI Software

Module/Name/Title: ESP/CSP

Module Revision: ESP V6.2e/CSP V2.0e

File Type (ASCII, OBJ, EXE): EXE

Recording Date: 12/5/2000

Operating System of Supporting Hardware: Windows NT

Notes: Acquired code that is not to be modified may not have all above elements.

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[1] See TOP-018. Table 1 for criteria.

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
ACQUIRED CODE - NOT TO BE MODIFIED

3. User's Manual: TOP-018, Section 5.5.5

a) Is there a Users' Manual for the software?

Yes: ☑ No: ☐ N/A: ☐

User's Manual Version and Date: _____

Notes:

b) Are there basic instructions for the use of the software?

Yes: ☑ No: ☐ N/A: ☐

Location of Instruction: QA records room.

Notes:

4. Acceptance Testing: TOP-018, Section 5.6

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

Yes: ☑ **No:** ☐ N/A: ☐

Platform(s): PC

Operating System(s): Windows NT

Location of Test Results: ~~OK~~ [illegible] 12/5/2000 Contained in Scientific Notebook #430.

Notes:

5. Configuration Control: TOP-018, Section 5.7

a) Is the Software Summary Form completed and signed?

Yes: ☑ No: ☐ N/A: ☐

Software Summary Form Approval Date: _____

Notes:

b) Is a software technical description prepared, documenting the essential mathematical and numerical basis?

Yes: ☐ No: ☐ N/A: ☑ [illegible] 12/5/2000

Location Technical Description: N/A

Notes:

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

Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: OLI File

Notes:

DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
ACQUIRED CODE - NOT TO BE MODIFIED

6. Configuration Control, continued: TOP-018, Section 5.7

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

Yes: ☑ No: ☐ N/A: ☐

Location of Script/Make Files: in this folder on CD

Notes:

7. Software Release: TOP-018, Section 5.9

Upon acceptance of the software as verified above, has a Software release Notice, Form TOP-6 been issued?

Yes: ☑ No: ☐ N/A: ☐

Version number on software (1.0 for 1st issue): ESP/CSP

Version number on SRN: V6.2e/2.0e

Notes:

8. Software Validation: TOP-018, Section 5.10

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

Yes: ☒ (met) No: ☐ N/A: ☑

Version/Date of SVTP: ~~29 November 2000~~ (rev)

Date reviewed and approved via QAP-002: N/A

Notes:

b) 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/Date of SVTR: N/A

Date reviewed and approved via QAP-002: N/A

Notes:

Additional Remarks:

N. Sridhar

CNWRA Software ~~Developer~~ User/Date 12/5/00

12/5/2000

CNWRA Software Custodian/Date

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

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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

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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

From Notebook #135

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

$Fe^{II}Cl_2$ = 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~~ 1M. 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

N. Sridhar
9/17/98

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

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

CRIIICL3IN lmoles	PH lmoles	CRIIICLION lmoles	CRIIIION lmoles	CRIIICL2ION lmoles	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

N Fridlak 9/18/98