

## SOFTWARE RELEASE NOTICE

01. SRN Number: <b>GS-SRN-001</b>		
02. Project Title: <b>Geochemical Modeling of Aqueous System, CNWRA Version 1.1</b>		Project No.
03. SRN Title: <b>EQ3/6</b>		
04. Originator/Requester: <b>Thomas J. Ratchford</b>		Date: <b>12/14/93</b>
05. Summary of Actions <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Release of new code admitted to CM System</li> <li><input type="checkbox"/> Release of modified code:             <ul style="list-style-type: none"> <li><input type="checkbox"/> Enhancements made</li> <li><input type="checkbox"/> Corrections made</li> </ul> </li> <li><input checked="" type="checkbox"/> Change of access code</li> </ul>		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
07. Element Manager Approval:		Date:
08. Remarks:		

## SOFTWARE SUMMARY FORM

01. Summary Date: 6/25/93		02. Summary prepared by (Name and phone) Mark V. Muller, 522-3222		03. Summary Action: New	
04. Software Date: May 1993		05. Short Title: EQ3/6-93			
06. Software Title: EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems, CNWRA version 1.1				07. Internal Software ID: none	
08. Software Type:  <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module		09. Processing Mode:  <input type="checkbox"/> Interactive <input checked="" type="checkbox"/> Batch <input type="checkbox"/> Combination		10. APPLICATION AREA a. General: <input checked="" type="checkbox"/> Scientific/Engineering <input type="checkbox"/> Bibliographic/Textual <input type="checkbox"/> Process Control <input type="checkbox"/> Management Business <input type="checkbox"/> Computer Systems Support/Utility <input type="checkbox"/> Other b. Specific: Reaction Path Solver	
11. Submitting Organization and Address: CNWRA			12. Technical Contact(s) and Phone: Bill Murphy, 522-5263		
13. Narrative:  The primary codes EQPT, EQ3, and EQ6 effect database manipulation, equilibrium aqueous species distributions, and reaction path mass transfer.					
14. Keywords:  geochemistry, aqueous speciation, mass transfer					
15. Computer Model and Manufacturer  Cray/XMP		16. Computer Operating System:  UNICOS		17. Programming Language(s):  FORTRAN	
18. Number of Source Program Statements:  50,000 +		19. Computer Memory Requirements:  2 megabytes		20. Tape Drives:  N/A	
21. Disk/Drum Units:  N/A		22. Terminals:  N/A			
23. Other Operational Requirements  None					
24. Software Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY <input checked="" type="checkbox"/> Active <input type="checkbox"/> Inactive			25. Documentation Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY		
26. Submission Package Status: CCB Acceptance Criteria: Met <input checked="" type="checkbox"/> Not Met <input type="checkbox"/> Software QA Assessment: Successful <input checked="" type="checkbox"/> Unsuccessful <input type="checkbox"/>					
Code Custodian: <u>Mark V. Muller</u> Date: <u>7/13/93</u>					

CNWRA Form TOP-4-1 (11/91)

*Randley H. Johnson for CCB 7/12/93*  
*Chairman, CCB*

```
gemstone.49 ~/eq36/ver11 =>
gemstone.49 ~/eq36/ver11 => pwd
/u1/mmv/eq36/ver11
gemstone.50 ~/eq36/ver11 => ls -F
eq3/      eq6/      eqdata/  eqlib/
gemstone.51 ~/eq36/ver11 => ls -F *
```

```
eq3:
s.a.out      s.data1      s.eq3.com      s.eq3nrr125.f  s.eq3nrr125.o
s.input      s.input.dat   s.output        s.pickup        s.screen.out
```

```
eq6:
s.a.out      s.data1      s.eq6.com      s.eq6r121.f    s.eq6r121.o
s.input      s.input6.dat  s.output        s.pickup        s.screen.out
s.tab        s.tabx
```

```
eqdata:
s.a.out      s.data0      s.data0.com-r1  s.data1
s.data1f     s.eqpt.com    s.eqptr81.f     s.eqptr81.o
s.output     s.slist
```

```
eqlib:
s.eqlibr154.a  s.eqlibr154.f  s.eqlibr154.o
gemstone.52 ~/eq36/ver11 =>
```

134.20.1.1 05:12:26

EQ3/6 Software, Version 1.1  
MS-DOS 5.0 Backup Format  
File Listing  
Created 06/30/93

6-29-1993 10:22:44

001 \SPACESYS\M2\EQ36\EQDATA\DATA1F  
001 \SPACESYS\M2\EQ36\EQDATA\SLIST  
001 \SPACESYS\M2\EQ36\EQDATA\EQPTR81.F  
001 \SPACESYS\M2\EQ36\EQDATA\A.OUT  
002 \SPACESYS\M2\EQ36\EQDATA\A.OUT  
002 \SPACESYS\M2\EQ36\EQDATA\DATA0.COM  
003 \SPACESYS\M2\EQ36\EQDATA\DATA0.COM  
003 \SPACESYS\M2\EQ36\EQDATA\DATA1  
004 \SPACESYS\M2\EQ36\EQDATA\DATA1  
004 \SPACESYS\M2\EQ36\EQDATA\EQPTR81.O  
004 \SPACESYS\M2\EQ36\EQDATA\EQPT.COM  
004 \SPACESYS\M2\EQ36\EQDATA\DATA0  
005 \SPACESYS\M2\EQ36\EQDATA\DATA0  
005 \SPACESYS\M2\EQ36\EQDATA\OUTPUT  
005 \SPACESYS\M2\EQ36\EQLIB\EQLIBR15.O  
006 \SPACESYS\M2\EQ36\EQLIB\EQLIBR15.O  
006 \SPACESYS\M2\EQ36\EQLIB\EQLIBR15.F  
006 \SPACESYS\M2\EQ36\EQLIB\EQLIBR15.A  
006 \SPACESYS\M2\EQ36\EQ6\PICKUP  
006 \SPACESYS\M2\EQ36\EQ6\SCREEN.OUT  
006 \SPACESYS\M2\EQ36\EQ6\TAB  
006 \SPACESYS\M2\EQ36\EQ6\TABX  
006 \SPACESYS\M2\EQ36\EQ6\A.OUT  
007 \SPACESYS\M2\EQ36\EQ6\A.OUT  
008 \SPACESYS\M2\EQ36\EQ6\A.OUT  
008 \SPACESYS\M2\EQ36\EQ6\EQ6R121.O  
009 \SPACESYS\M2\EQ36\EQ6\EQ6R121.O  
009 \SPACESYS\M2\EQ36\EQ6\DATA1  
009 \SPACESYS\M2\EQ36\EQ6\INPUT  
009 \SPACESYS\M2\EQ36\EQ6\OUTPUT  
009 \SPACESYS\M2\EQ36\EQ6\EQ6.COM  
009 \SPACESYS\M2\EQ36\EQ6\EQ6R121.F  
010 \SPACESYS\M2\EQ36\EQ6\EQ6R121.F  
010 \SPACESYS\M2\EQ36\EQ6\INPUT6.DAT  
010 \SPACESYS\M2\EQ36\EQ3\EQ3NRR12.F  
011 \SPACESYS\M2\EQ36\EQ3\EQ3NRR12.F  
011 \SPACESYS\M2\EQ36\EQ3\INPUT.DAT  
011 \SPACESYS\M2\EQ36\EQ3\PICKUP  
011 \SPACESYS\M2\EQ36\EQ3\SCREEN.OUT  
011 \SPACESYS\M2\EQ36\EQ3\EQ3NRR12.O  
011 \SPACESYS\M2\EQ36\EQ3\EQ3.COM  
011 \SPACESYS\M2\EQ36\EQ3\A.OUT  
012 \SPACESYS\M2\EQ36\EQ3\A.OUT  
012 \SPACESYS\M2\EQ36\EQ3\DATA1  
013 \SPACESYS\M2\EQ36\EQ3\DATA1  
013 \SPACESYS\M2\EQ36\EQ3\INPUT  
013 \SPACESYS\M2\EQ36\EQ3\OUTPUT  
013 BACKUP.LOG

December 14, 1993

MEMORANDUM

TO: H.L. M<sup>c</sup> Kaque

FROM: T.J. Ratchford

SUBJECT: Software Release Notice (SRN)

TOP-18 requires the Element Manager to be notified when a software code has been placed under configuration management. The attached Software Release Notices are to advise you of the placement of EQ3/6 and SEISM1 under configuration management and to request a listing of persons authorized access to EQ3/6 and SEISM1. Please complete the form for each program and return it to me at your conveniences. If there are any questions please feel free to call me at 3083.

Block 06, Persons Authorized Access.

Under "Name":

Persons name and cray User Name.


Under "RO/RW":

Assign access permission for each person.

RO = Read only access

RW = Read and Write access

Block 07: Element Manager Approval and date.

Thank You  
  
Thomas J. Ratchford  
Code Custodian

*The Geochemical Modeling Group  
L-219, Lawrence Livermore National Laboratory  
P.O. Box 808  
Livermore, CA 94550*

*Telephone: (415) 423-2970 FTS 543-2970*

*FAX: (415) 423-1997 Confirm: (415) 423-0672*

December 26, 1990

Dr. William Murphy  
Center for Nuclear Waste Regulatory Analysis  
South West Research Institute  
6220 Culebra Road  
San Antonio, TX 78284

Dear Bill:

I am writing this letter to you in connection with the transfer to you from LLNL of EQ3/6, Version 3245.1090. This transfer was made to fulfill a request from the NRC to the U.S. DOE. The software has been provided to you for use in your work for the NRC, and in that connection you need take no further action.

Copyright to the software is held by the Regents of the University of California, with the U.S. Government retaining a nonexclusive right to its use. Distribution or usage of the software outside this purview requires the execution of a license/collaboration agreement. If you or a colleague at your institution wish to use the software for work done for other than the U.S. government, please contact me to arrange such an agreement. For your convenience, a blank copy of the non-profit version of the standard agreement is enclosed. Such an agreement can be executed at no cost, as long as the package does not have to be retransmitted from LLNL.

Sincerely yours,

*Tom*

Thomas J. Wolery

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enclosure: blank non-profit license/collaboration agreement

# SOFTWARE PROBLEM/CHANGE REPORT

CNWRA

SPCR Number:		3704-SPCR-001	
Project Title: Geochemistry		Project Number: 20-3704-012	
SPCR Title: Implementation of EQ3/6 source codes at SwRI CTC VAX			
AFFECTED SOFTWARE AND/OR DOCUMENTATION			
Among the EQ3/6 package affected software is: EQ3NR, EQ6, EQIB, EQPT source codes from EQ3/6 92 package. LLNL versions 3245R-x. <i>WMP 6/3/92</i>			
DESCRIPTION OF PROBLEM/CHANGE			
Comment out LLNL system dependent clock routines; implement SwRI VAX routines. Implement read only restriction on data base file open statement in EQIB to permit multiple users at CNWRA. <i>WMP 6/3/92</i>			
PROBLEM SOLUTION/NEED FOR CHANGE			
Minor code changes.			
Originator: W. Murphy		Title: Senior Research Scientist	
		Date: 06/03/92	
PROJECT			
Need By Date: 06/03/92		Approved <input checked="" type="checkbox"/>	
Disapproved <input type="checkbox"/>			
Element Manager: <i>John J. Kinsler</i>		Date: <i>6/5/92</i>	
CCB/Quality Assurance Engineer: <i>Robert D. Smith</i>		Date: <i>6/3/92</i>	
IMPLEMENTED SOLUTION			
Required changes made: SwRI clock calls implement in source codes. Read only limitation implemented in EQIB data base open. New versions designated as: EQ3NR.3245R124xWM <i>WMP 6/3/92</i> EQPT.3245xR80xMYR <i>WMP 6/3/92</i> EQ6.3245R119xWMM <i>WMP 6/3/92</i> EQLIB.3245R153xMYR <i>WMP 6/3/92</i> Reference controlled notebook 037 (Murphy).			
Implemented By: W. Murphy		Date: 06/03/92	

**Memorandum**

To: EQ3/6 Users at CNWRA  
cc: J.L. Russell, B. Sagar, W.C. Patrick, B.E. Mabrito, J.E. Latz

From: W. M. Murphy

Date: May 29, 1992

Re: Controlled use of EQ3/6

(version EQ3/6-92) JLB 5/31/92

Controlled versions of the EQ3/6 software exist on the CTCVAX in the directory user3:[wmm.eq36control]. All CNWRA users may access these files. If users have no requirement to make modifications to these versions, then they need not retain copies of the codes and data bases in their individual accounts. Command files can be constructed to access the executable versions of the programs and the data files directly from the controlled account. A sample command file is attached to this memorandum. Files in the eq36control directory are:

DATA0.DAT	(=DATA0.COM.R12)
DATA0.HMW	(=DATA0.HMW.R12)
DATA0.PIT	(=DATA0.PIT.R12)
DATA1.COMP	(=DATA1 version of DATA0.DAT)
DATA1.HMW	(=DATA1 version of DATA0.HMW)
DATA1.PIT	(=DATA1 version of DATA0.PIT)
EQ3NR.FSC	(=EQ3NR version 3245R124xWM)
EQ3NR.OBJ	(=object version of EQ3NR.FSC)
EQ3NR.EXE	(=executable version of EQ3NR.FSC)
EQ6.FSC	(=EQ6 version 3245R119xWMM)
EQ6.OBJ	(=object version of EQ6.FSC)
EQ6.EXE	(=executable version of EQ6.FSC)
EQLIB.FSC	(=EQLIB version 3245R153xMUR)
EQLIB.OBJ	(=object version of EQLIB.FSC)
EQPT.FSC	(=EQPT version 3245R80xMUR)
EQPT.OBJ	(=object version of EQPT.FSC)
EQPT.EXE	(=executable version of EQPT.FSC)

Documentation in support of these files is in CNWRA controlled notebook 037 in my possession. Please contact me with any questions.



```

$!
$!
$!      EQ6
$!
$ set def [user.directory]
$!
$ assign      [user.directory]EQ6.OUT      OUTPUT
$ assign      user3:[wmm.eq36control]DATA1.comp  DATA1
$ assign      [user.directory]PICKUP.DAT      PICKUP
$ assign      [user.directory]TAB.DAT          TAB
$ assign      [user.directory]TABS.DAT         TABS
$ assign      [user.directory]TABX.DAT         TABX
$ assign      [user.directory]INPUT.DAT        INPUT
$ assign      [user.directory]INPUTS.DAT       INPUTS
$!
$ run user3:[wmm.eq36control]eq6
$!
$ deassign    OUTPUT
$ deassign    DATA1
$ deassign    PICKUP
$ deassign    TAB
$ deassign    TABS
$ deassign    TABX
$ deassign    INPUT
$ deassign    INPUTS
$ exit

```