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SOFTWARE RELEASE NOTICE

12/22/2000
PA -

01. SRN Number: SRN- 232		
02. Project Title: Evolution of Near-field Environment		Project No.: 20-1402-562
03. SRN Title: MULTIFLO V1.2.3		
04. Originator/Requestor: Scott Painter		Date: 12/7/00
05. Summary of Actions		
<input type="checkbox"/> Release of new software		
<input checked="" type="checkbox"/> Release of modified software:		
<input type="checkbox"/> Enhancements made (modest changes per NRC request)		
<input checked="" type="checkbox"/> Corrections made		
<input type="checkbox"/> Change of access software		
<input type="checkbox"/> Software Retirement		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
Scott Painter	RW	
Stefan Meyer	RW	
07. Element Manager Approval: E.C.R.		Date: 12/22/00
08. Remarks:		

SOFTWARE SUMMARY FORM

01. Summary Date: 12/21/2000		02. Summary prepared by (Name and phone) Scott Painter, 522-3348		03. Summary Action: New	
04. Software Date: 12/21/2000		05. Short Title: MULTIFLO Version 1.2.3			
06. Software Title: MULTIFLO Version 1.2.3				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 type="checkbox"/> Batch <input checked="" type="checkbox"/> Combination		10. APPLICATION AREA a. General: <input checked="" type="checkbox"/> Scientific/Engineering <input checked="" type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> Other b. Specific: Groundwater multiphase flow and reactive transport model	
11. Submitting Organization and Address: CNWRA 6220 Culebra Road San Antonio, TX 78228			12. Technical Contact(s) and Phone: Scott Painter, (210) 522-3348 Mohan Seth, (972) 699-3610		
13. Narrative: The code is used to model multiphase groundwater flow and reactive transport.					
14. Computer Platform SUN		15. Computer Operating System: UNIX		16. Programming Language(s): Fortran 77	
17. Number of Source Program Statements: ~80,000		18. Computer Memory Requirements: Problem Dependent		19. Tape Drives: N/A	
20. Disk/Drum Units: N/A		21. Graphics: ASCII plot data files		22. Other Operational Requirements Thermodynamic database required.	
23. Software Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY			24. Documentation Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY DRAFT		
Software Developer: <u>Scott Painter</u> Date: <u>12-22-2000</u>					

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

DEVELOPED SOFTWARE¹

Software Title/Name: MULTIFLO
Version: 1.2.3
Demonstration workstation: VULCAN
Operating System: UNIX-SOLARIS
Lead Developer: SCOTT PRINTER

1. Software Requirements Description: TOP-018, Section 5.3

Software Requirements Description (SRD) and any changes thereto reviewed in accordance with QAP-002 requirements?

Yes: ☒ No: ☐ N/A: ☐

SRD Version:

SRD Approval Date:

Notes:

2. Software Development Plan (SDP): TOP-018, Section 5.4

a) The Element Manager has approved the SDP and any changes?

Yes: ☐ No: ☐ N/A: ☐

b) The SDP addresses applicable section of TOP-018, Appendix B, Software Development Plan Template?

Yes: ☐ No: ☐ N/A: ☐

SDP Version:

SDP Approval Date:

Notes:

*MULTIFLO predates the requirement for a
Software Development Plan. Sd 12/21/2000*

¹ See TOP-018, Table 1 for criteria.

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**DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE**

3. Design and Development: TOP-018, Section 5.5.1, 5.5.2

- a) Is development and module/subroutine-level testing documented either in scientific notebooks and/or in Software Change Reports (SCR)?

Yes: ☒ No: ☐ N/A: ☐

Scientific Notebook(s): S/N 282 E.

SCR Number(s): SCR 342

Notes: N/A

- b) Is development and module/subroutine-level testing sufficiently documented so that an informed reviewer can follow the testing procedures and logic?

Yes: ☒ No: ☐ N/A: ☐

Notes: S. PINTER has used the same acceptance test for the past 2.5 years. Document in code.

- c) Is development in accordance with the conventions described in the SDP/SCR, i.e. coding convention?

Yes: ☒ No: ☐ N/A: ☐

Notes: See SCR 342.

4. Internal Documentation: TOP-018, Section 5.5.3

Software internally documented to allow a user to understand the function(s) being performed and to follow the flow of execution of individual routines?

Yes: ☒ No: ☐ N/A: ☐

Module(s) Reviewed: MULTIFLO/GEM - KINRXN.F

MULTIFLO/GEM - COEFIMP.F

MULTIFLO/GEM - UPDTGEM.F

Notes: 6 modules were changed. Copies made of some changes (attached).

5. 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: Changed on Dec 7, 2000

Name and version: MULTIFLO Version 1.2.3

Notes: Runs made 12/7/2000, copies made 12/21/2000

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**DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE**

6. Code Reviews: TOP-018, Section 5.5.5

Are code reviews (if implemented) documented in a scientific notebook or in another format that allows others to understand the code review process and results?

Yes: ☒ No: ☐ N/A: ☐

Scientific Notebook: 282E - Acceptance Testing documented

Notes: Acquired code that is not to be modified is accepted as is. No code reviews required.

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

a) Program title block of main program contains required information?

Yes: ☒ No: ☐ N/A: ☐

Program Title: MULTIFLO

Customer Name: U.S. NRC

Customer Office/Division: DWM

Customer Contact(s): Barry Leslie

Customer Phone Number: 301-415-6652

Associated Documentation: Revision History included.

Disclaimer Notice: yes - in 2 part

Notes:

b) Source code module header contains required information provides Program Name, Client Name, Contract Reference, Revision Number, and Revision History?

Yes: ☒ No: ☐ N/A: ☐

Module Reviewed: updtgem.f

Module Reviewed: KINRXN.f

Module Reviewed: COE.fmp.f

Notes: SEE ATTACHED PRINT OUTS

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**DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE**

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

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

Yes: ☒ No: ☐ N/A: ☐

Program Name: MULTIFLO
Module/Name/Title: " 1.2.3
Module Revision: " 1.2.3
File Type (ASCII, OBJ, EXE): ASCII
Recording Date: 12/22/2000
Operating System of Supporting Hardware: SOLARIS

Notes: provided to CNWRA QA 12/22/2000.

8. 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: MULTIFLO Rev 2 Chg 1 - Feb 2000

Notes: These changes do not require manual change. &c

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

Yes: ☒ No: ☐ N/A: ☐

Location of Instruction: MULTIFLO User's Manual

Notes:

9. Acceptance Testing: TOP-018, Section 5.6

- a) Does the acceptance testing demonstrate whether or not requirements in the SRD and/or SCR have been fulfilled?

Yes: ☒ No: ☐ N/A: ☐

Location of Test Results: _____

Notes: Acceptance Test demonstrates capability to meet the SRD and these "bug fixes" are relatively minor.

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DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE

9. Acceptance Testing, continued: TOP-018, Section 5.6

- b) Has acceptance testing been conducted for each intended computer platform and operating system?

Yes: ☒ No: ☐ N/A: ☐

Platform(s): SOLARIS

Operating System(s): UNIX

Location of Test Results: WITH THE CODE ON THE CD.

Notes:

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

Yes: ☐ No: ☐ N/A: ☒

Platform(s): _____

Operating System(s): _____

Location of Test Results: _____

Notes: S. PRINTER will install it on an NT platform, but that is not required.

10. 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: 12/22/2000

Notes:

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

Yes: ☒ No: ☐ N/A: ☐

Location Technical Description: The multiflo users manual

Notes: has this.

- 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: In The QA Records Room

Notes: Also, Dr. PRINTER will have a copy on The Vulcan Server.

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**DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE
DEVELOPED SOFTWARE**

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

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

Yes: ☒ No: ☐ N/A: ☐

Location of Script/Make Files: QA Records Room

Notes: MAKE FILES ON CD.

12. 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): 1.2.3

Version number on SRN: 1.2.3

Notes: SRN signed by E. Penney.

13. 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: ☐ No: ☒ N/A: ☐

Version/Date of SVTP: _____

Date reviewed and approved via QAP-002: _____

Notes: Software Validation has NOT yet been accomplished. IT will be in the future.

- 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: _____

Date reviewed and approved via QAP-002: _____

Notes: NOT A THIS TIME.

Additional Remarks:

David Paine 12-22-2000
CNWRA Software Developer/Date

Sharon Mahesh /12/22/2000
CNWRA Software Custodian/Date

c*file updtgem.f

c Program Name: MULTIFLO/GEM
 c File/Subroutine Name: updtgem.f
 c Release Date: February 2000
 c Release Version: 1.2.3
 c Client Name: USNRC
 c Contract Number: NRC 02-97-009
 c CNWRA Contact: Scott Painter (210-522-3348)
 c Center for Nuclear Waste Regulatory Analyses
 c*file updtgem.f

c Program Name: MULTIFLO/GEM
 c File/Subroutine Name: updtgem.f
 c Release Date: December 2000
 c Release Version: 1.2.3
 c Client Name: USNRC
 c Contract Number: NRC 02-97-009
 c CNWRA Contact: Scott Painter (210-522-3348)
 c Center for Nuclear Waste Regulatory Analyses
 c San Antonio, Texas 78238-5166
 c spainter@swri.edu
 ccc

c VERSION/REVISION HISTORY

c \$Id\$
 c \$Log\$

c-----
 c Date Author(s) Comments/Modifications
 c-----

c April 97 Peter C. Lichtner Initial Implementation
 c Mohan S. Seth
 c December 2000 fixed surface area update.
 c was bypassed
 c for secondary minerals
 c

cc

c-----update surface area
 if (isurf.eq.1) then
 do 10 n = 1, nmax
 if(por(n).le.zero) go to 10
 fac = one
 c sp make porosity update happen in coupled mode
 if (ipor .eq. 1) fac = (por(n)/por0(n))*twthrds
 do nr = 1, nkin
 surf(nr,n) = surf0(nr,n)*fac ! sp 11.29.00
 if (pphik(nr,n) .eq. zero) phik0(nr,n) = zero
 if (phik0(nr,n) .gt. zero) then
 c surf(nr,n) = surf0(nr,n)*fac* ! sp 11.29.00
 surf(nr,n) = surf(nr,n)* ! sp 11.29.00
 (pphik(nr,n)/phik0(nr,n))*twthrds

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c*file kinrxns.f

c Program Name: MULTIFLO/GEM
c File/Subroutine Name: kinrxn.f ✓
c Release Date: December 2000
c Release Version: 1.2.3
c Client Name: USNRC
c Contract Number: NRC 02-97-009
c CNWRA Contact: Scott Painter (210-522-3348)
c Center for Nuclear Waste Regulatory Analyses
c San Antonio, Texas 78238-5166
c spainter@swri.edu
cc

c VERSION/REVISION HISTORY

c \$Id\$
c \$Log\$

c-----
c Date Author(s) Comments/Modifications
c-----
c April 97 Peter C. Lichtner Initial Implementation
c Mohan S. Seth
c December 2000 modified by scott painter. Do not shut down kinetic ✓
c precipitation during
c dryout
cc

do 200 n = n1b,n2b
if(iconvrg(n).gt.0) go to 200
c sp v1.2.3 the following not needed. allow precipitation to continue
c if supersaturated with respect to mineral
c-----check for zero saturation
c if (isat.eq.0 .and. icksat.eq.1) then
c if (iwet(n).eq.0) then
c do nr = 1, nkin
c do lp = npar1(nr), npar2(nr)
c rkin(lp,n) = zero
c enddo
c enddo
c goto 200
c endif
c endif

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```
c  kinrxn.f
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

``` c INCLUDE FILES ```

Name	Description
impl.h	-Declares real variables to real*8 and sets frequently used constants in common.
metragem.h	-Variables which are common to both metra and gem codes.
paramtrs.h	-Sets dimension limits for all variables.
scalgem.h	-Scalars in common.
kinetic.h	-Common block for kinetic rate parameters.
comgem.h	-General common block.
iounits.h	-Input/output units.

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

``` c SYSTEM LIBRARY ROUTINES ```

Name	Description
none	

```
c  none
```

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

``` c OUTPUT UNIT(s) ```

Unit Name(Number)	Description	file name
iunit2 (8)	normal run output	masout

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

``` c REFERENCES ```

```
c  none
```

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

```
subroutine kinrxns (nc,ncx,nk,np,r,qk,qf,qb,affin,rrkin,rkin,
. pot,cc,cx,phik,surf,gam,gamx,cdl,eqkinr,iflgerr,index,aa,n1b,n2b)
```

```
include 'impl.h'
include 'addgem.h'
include 'paramtrs.h'
include 'metragem.h'
include 'kinetic.h'
include 'iounits.h'
include 'scalgem.h'
include 'comgem.h'
include 'comprs.h'
```

```
dimension r(nc,*),qk(nk,*),qf(nk,*),qb(nk,*),affin(nk,*),
. rrkin(np,*),rkin(np,*),phik(nk,*),surf(nk,*),
. cc(nc,*),cx(ncx,*),gam(nc,*),gamx(ncx,*),cdl(nc,nc,*),
. eqkinr(nk,*),pot(*)
```

```
/sp
```

```
c-----index = 0 - normal call (all reaction rates)
c              1 - electrochemical reaction rates only
```

```
iflgerr = 0
rgast0 = one/(rgaskj*tk0)
```

```
do 200 n = n1b,n2b
```

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no	type-curve	swirm	m-mtx	alpham	swext (phim	sgc phif	fkm
fkf)							
1	VAN	1.300E-01	2.310E-01	1.150E-06	-1.000E+08	0.000E+00	
2	VAN	1.000E-02	6.670E-01	2.370E-03	6.000E-02	0.000E+00	
3	VAN	1.300E-01	2.447E-01	2.010E-06	-1.000E+08	0.000E+00	
4	VAN	1.000E-02	6.690E-01	2.370E-03	6.000E-02	0.000E+00	
5	VAN	3.300E-01	4.548E-01	3.740E-06	3.800E-01	0.000E+00	
6	VAN	1.000E-02	6.690E-01	9.120E-04	6.000E-02	0.000E+00	
7	VAN	1.000E-01	2.531E-01	3.980E-05	-1.000E+08	0.000E+00	
8	VAN	1.000E-02	6.690E-01	1.100E-03	6.000E-02	0.000E+00	
9	VAN	1.400E-01	4.925E-01	7.940E-06	1.900E-01	0.000E+00	
10	VAN	1.000E-02	6.690E-01	1.850E-03	6.000E-02	0.000E+00	
11	VAN	1.700E-01	3.002E-01	5.440E-05	2.200E-01	0.000E+00	
12	VAN	1.000E-02	6.670E-01	3.450E-03	6.000E-02	0.000E+00	
13	VAN	1.000E-01	3.859E-01	3.430E-05	1.500E-01	0.000E+00	
14	VAN	1.000E-02	6.670E-01	9.130E-04	6.000E-02	0.000E+00	
15	VAN	1.000E-01	3.195E-01	1.810E-04	1.500E-01	0.000E+00	
16	VAN	1.000E-01	3.200E-01	1.810E-04	1.500E-01	0.000E+00	
17	VAN	1.100E-01	2.304E-01	5.840E-05	-1.000E+08	0.000E+00	
18	VAN	1.000E-02	5.660E-01	1.440E-04	6.000E-02	0.000E+00	
19	VAN	6.000E-02	2.479E-01	6.210E-06	-1.000E+08	0.000E+00	
20	VAN	1.000E-02	6.670E-01	1.730E-03	6.000E-02	0.000E+00	
21	VAN	8.000E-02	1.983E-01	4.010E-06	-1.000E+08	0.000E+00	
22	VAN	1.000E-02	6.670E-01	1.260E-03	6.000E-02	0.000E+00	
23	VAN	1.800E-01	5.138E-01	2.272E-06	2.300E-01	0.000E+00	
24	VAN	1.000E-02	6.670E-01	1.320E-03	6.000E-02	0.000E+00	
25	VAN	5.000E-01	3.709E-01	7.386E-06	5.500E-01	0.000E+00	
26	VAN	1.000E-02	6.590E-01	1.190E-03	6.000E-02	0.000E+00	
27	VAN	4.000E-02	1.592E-01	7.600E-05	-1.000E+08	0.000E+00	
28	VAN	1.000E-02	6.690E-01	1.180E-03	6.000E-02	0.000E+00	
29	VAN	6.000E-02	2.291E-01	4.120E-05	-1.000E+08	0.000E+00	
30	VAN	1.000E-02	6.670E-01	1.180E-03	6.000E-02	0.000E+00	
31	VAN	2.000E-01	2.119E-01	2.160E-05	-1.000E+08	0.000E+00	
32	VAN	1.000E-02	6.540E-01	1.120E-03	6.000E-02	0.000E+00	
33	VAN	3.300E-01	4.322E-01	1.030E-06	3.800E-01	0.000E+00	

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```
*THERM      Thermal and Diffusion Parameters for Rocks
=====
```

i	Rhocpr	Ckdry	Cksat	Crp	Crt	Tau	Cdiff	Cexp	
	enbd	emisvt							
1	1	1	48	48	9.66014E+04	109.1541	1.0000E+00	3.9846E-03	1.3855E+05
1.0915E+02	3.4185E-01	0.0000E+00							
1	1	1	49	49	9.66111E+04	109.6488	1.0000E+00	4.1934E-03	1.4083E+05
1.0965E+02	3.5182E-01	0.0000E+00							
1	1	1	50	50	9.66178E+04	109.3347	1.0000E+00	4.3973E-03	1.3947E+05
1.0933E+02	3.4048E-01	0.0000E+00							
1	1	1	51	51	9.66246E+04	109.0126	1.0000E+00	4.6216E-03	1.3811E+05
1.0901E+02	3.2746E-01	0.0000E+00							
1	1	1	52	52	9.66342E+04	108.5669	1.0000E+00	4.9914E-03	1.3624E+05
1.0857E+02	3.0779E-01	0.0000E+00							
1	1	1	53	53	9.66478E+04	107.9405	1.0000E+00	5.6437E-03	1.3364E+05
1.0794E+02	2.7957E-01	0.0000E+00							
1	1	1	54	54	9.66696E+04	106.8952	1.0000E+00	6.7702E-03	1.2920E+05
1.0690E+02	4.4365E-01	0.0000E+00							
1	1	1	55	55	9.66993E+04	105.4285	1.0000E+00	8.4609E-03	1.2315E+05
1.0543E+02	3.8868E-01	0.0000E+00							
1	1	1	56	56	9.67344E+04	103.7255	1.0000E+00	1.1220E-02	1.1648E+05
1.0373E+02	3.3092E-01	0.0000E+00							
1	1	1	57	57	9.67778E+04	101.6689	1.0000E+00	1.6354E-02	1.0900E+05
1.0167E+02	2.6494E-01	0.0000E+00							
1	1	1	58	58	9.68312E+04	99.2134	1.0000E+00	2.7488E-02	1.0111E+05
9.9213E+01	1.8811E-01	0.0000E+00							

This file was created on: Thu Dec 7 10:55:59 2000

```
H HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
H                                                                    H
H      Multi-Component Unsaturated Fluid Flow Simulator              H
H                                                                    H
H           METRA   Version Number: 1.2.3                           H
H                                                                    H
H      Developed By  Mohan S. Seth, TSE, December 2000             H
H with Peter Lichtner and Scott Painter, CNWRA                      H
H                                                                    H
H      CNWRA - Southwest Research Institute (2000)                  H
H HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
```

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*RSTART Run started from Restart File # 0