SOFTWARE RELEASE NOTICE

01. SRN Number: SRN-246

02. Project Title: Evolution of Near-field Environment | Project No.: 20-1402-562

03. SRN Title: MULTIFLO V1.5

04. Originator/Requestor: Scott Painter | Date: 7/23/01

05. Summary of Actions

- ☐ Release of new 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
Scott Painter	RW	
Mohan Seth	RW	

07. Element Manager Approval: [signature] for ECP Date: 07/24/2001

08. Remarks:

CNWRA Form TOP-6 (06/95)

SOFTWARE SUMMARY FORM

01. Summary Date: 7/23/2001	02. Summary prepared by (Name and phone) **Scott Painter, 522-3348**	03. Summary Action: **New**
04. Software Date: 7/23/2001	05. Short Title: **MULTIFLO Version 1.5**	
06. Software Title: **MULTIFLO Version 1.5**		07. Internal Software ID: **NONE**

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: **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**
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: **~70,000**
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: ☐ Available ■ Limited ☐ In-House ONLY	24. Documentation Availability: ■ Available ☐ Inadequate ☐ In-House ONLY DRAFT

Software Developer: Scott Painter Date: 7-23-01

CNWRA Form TOP-4-1

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

Software Title/Name: MULTIFLO

Version: 1.5

Demonstration workstation: ~~Gargon~~ "Vulcan" – Room No. A209, Bldg 189

Operating System: UNIX ~~or NT~~ on Solaris

Developer: Scott Painter & Mohan Seth

Software Requirements Description (SRD) [TOP-018, Section 5.3]

SRD Version: Revision 2, November 2000

SRD Approval Date: 10/31/2000

SRD and any changes thereto reviewed in accordance with QAP-002 requirements?
Yes: ☒ No: ☐ N/A: ☐

Is a Software Change Report(s) (SCR) used for minor modifications (i.e., acquired code), problems or changes to a configured version of software?
Yes: ☒ No: ☐ N/A: ☐

Comments: SCR-350 is number of the SCR.

Software Development Plan (SDP) [TOP-018, Section 5.4]

SDP Version: for Multiflo 2.0 – dated 2/5/2001

SDP (EM) Approval Date: E. Pensky – 2/5/2001

The SDP addresses applicable sections of TOP-018, Appendix B, SDP Template?
Yes: ☒ No: ☐ N/A: ☐

Is the waiver (if used) in accordance with specified guidelines?
Yes: ☒ No: ☐ N/A: ☒

Comments: No waiver utilized. QA

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

Design and Development [TOP-018, Section 5.5.1 - 5.5.4]

Is code development in accordance with the conventions (i.e., coding conventions)described in the SDP/SCR?

Yes: ☒ No: ☐ N/A: ☐

Module(s) Reviewed: GEM & METRA

Comments:

Is code 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: METRA –

Comments:

Is development of the code and informal module/subroutine-level testing documented in scientific notebook and/or SCR?

Yes: ☒ No: ☐ N/A: ☐

SCR's and/or Scientific Notebook(s) Reviewed:
S/N No. 282E, Volume 9, & SCR 350

Comments:

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: Mon Jul 23 14:01:22 2001

Name/Version Displayed: METRA F.

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

Medium and Header Documentation [TOP-018, Section 5.5.6]

A program title block of main program contains: Program Title, Customer Name, Customer Office/Division, Customer Contact(s), Customer Phone Number, Associated Documentation, Software Developer and Phone Number, Date, and Disclaimer Notice?

Yes: ☒ No: ☐ N/A: ☐

Comments: NRC client is John Bradbury @ 301-415-6597

Source code module headers contain: Program Name, Client Name, Contract reference, Revision Number, Revision History, and Reference to SRD/SCR requirement(s)?

Yes: ☒ No: ☐ N/A: ☐

Module(s) Reviewed: MATRA.f

Comments:

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: Example shown meets minimum TOP-018 Requirements.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

Code Reviews [TOP-018, Section 5.5.6]

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: ☐

Documented in Scientific Notebook No.: 282E, Volume 9

Comments:

Acceptance and Installation Testing [TOP-018, Section 5.6]

Does *acceptance testing* demonstrate whether or not requirements in the SRD and/or SCR(s) have been fulfilled?

Acceptance Testing provided "physically Reasonable results"

Yes: ☒ No: ☐ N/A: ☐

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

→ "Gorgon"

Both NT & "Vulcan"

Yes: ☒ No: ☐ N/A: ☐

Computer Platforms: Solaris → Operating Systems: NT & Solaris

Location of Acceptance Test Results: Results will be on the CD.

Comments: Input & output files.

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

"Gorgon" &

Yes: ☒ No: ☐ N/A: ☐

Computer Platforms: "Vulcan" Operating Systems: NT & Solaris

Location of Acceptance Test Results: 282E, Volume 9

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

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: _____

Comments: There will be an updated users' manual provided to the NRC at CNWRA approximately in November 2001.

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

Yes: ☒ No: ☐ N/A: ☐

Location of Instructions: In a Readme File with the code on the CD, There are additional installation instructions and information on multi-user use.

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: 7/23/2001

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

Yes: ☒ No: ☐ N/A: ☐

Comments: See SSF Attachment.

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: QA Records Room and on the CNWRA Server Vulcan.

Comments:

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

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
DESIGN VERIFICATION REPORT
FOR
→ *DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE* ←

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: 246

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: Expected in CY 2002 per B. Sagar Code Validation Schedule.

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: Expected in CY2002 per B. Sagar Code Validation schedule.

Additional Comments:

7-23-2001
Software Developer/Date

Software Custodian/Date 2/23/2001

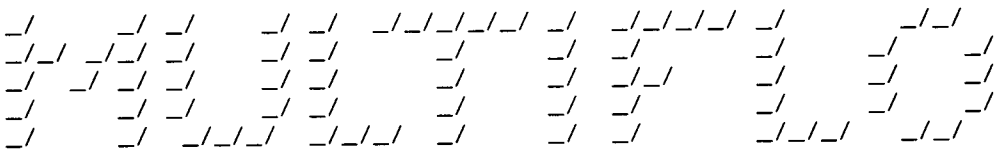
```
bigmetra1.5b4  metra1.5b3     multiflo       mymflo
vulcan% rm metra1.5b3
vulcan% rm metra1.5b4
vulcan% rm metra15beta
vulcan% ls
amesh          bigmetra1.5b4  metra          mygem          mymflo
bigmetra       gem            multiflo       mymetra        vmetra
vulcan% ls -l
total 2656
-rwxr-xr-x   1 spainter sunuser   180224 Apr 18 14:13 amesh
lrwxrwxrwx   1 spainter sunuser       59 Feb 20 16:25 bigmetra ->
/net/vulcan/home/spainter/multiflo/mflo1.2.3/bigmetra/metra
-rwxr-xr-x   1 spainter sunuser  1148284 Jul 11 17:25 bigmetra1.5b4
lrwxrwxrwx   1 spainter sunuser       52 Dec 19  2000 gem ->
/net/vulcan/home/spainter/multiflo/mflo1.2.3/gem/gem
lrwxrwxrwx   1 spainter sunuser       56 Dec 19  2000 metra ->
/net/vulcan/home/spainter/multiflo/mflo1.2.3/metra/metra
lrwxrwxrwx   1 spainter sunuser       53 Dec 29  2000 multiflo ->
/net/vulcan/home/spainter/multiflo/mflo1.2.3/multiflo
lrwxrwxrwx   1 spainter sunuser       50 Mar  7 08:46 mygem ->
/net/vulcan/home/spainter/multiflo/mflo1.5/gem/gem
lrwxrwxrwx   1 spainter sunuser       54 Feb  7 09:34 mymetra ->
/net/vulcan/home/spainter/multiflo/mflo1.5/metra/metra
lrwxrwxrwx   1 spainter sunuser       51 Mar  1 14:42 mymflo ->
/net/vulcan/home/spainter/multiflo/mflo1.5/multiflo
lrwxrwxrwx   1 spainter sunuser       55 Mar 23 15:50 vmetra ->
/net/vulcan/home/spainter/multiflo/mflo1.5/vmetra/metra
vulcan% ls
amesh          bigmetra1.5b4  metra          mygem          mymflo
bigmetra       gem            multiflo       mymetra        vmetra
vulcan% pwd
/net/vulcan/home/spainter/bin
vulcan% ls
amesh          bigmetra1.5b4  metra          mygem          mymflo
bigmetra       gem            multiflo       mymetra        vmetra
vulcan% cd
vulcan% cd multiflo/mflo1.5/metra
vulcan% ls *.f
accm.f      ecmtbl.f    inpmetra.f  pproc.f     recdat.f    update.f
allot.f     emip.f      iter.f      prints.f    rstart.f    updtpsk.f
bcond.f     emipmnc.f   itermnc.f   pvt.f       setbc.f     updtvpk.f
blkdtmet.f  equil.f     mainmtra.f  pvtfunc.f   slv1p.f     util.f
coefmnc.f   griddat.f   openfls.f   pvth2o.f    solve.f     watsolv.f
coefs.f     init.f      outmetra.f  pvtmnc.f    source.f
cond.f      initmnc.f   pckr.f      pvtvp.f     thomas.f
dtstep.f    inpifv.f    plots.f     pvtvpmnc.f  trans.f
vulcan% cd ..
vulcan% cd gem
vulcan% ls *.f
allotgem.f  elechem.f   graph3d.f   linmonod.f  read1.f     startup.f
blkdtgem.f  eqjac.f     gunits.f    luslv.f     read2.f     stdyst.f
bndcond.f   eqlib.f     implicit.f  maingem.f   setbcon.f   stepgem.f
calcpsi.f   eqres.f     imret.f     massbal.f   setconn.f   textab.f
coefimp.f   flogk.f     initgem.f   masstran.f  solprd.f    transd.f
coeftvd.f   gameq.f     interpf.f   opsplit.f   solprodt.f  updtgem.f
dataall.f   gamextd.f   ionexc.f    outgem.f    solve1d.f   util.f
database.f  graph1d.f   kinrxnaq.f  pecletnr.f  speciate.f  watsolv.f
derives.f   graph2d.f   kinrxns.f   pprcgem.f   srcgem.f    zonek.f
vulcan% cd ..
vulcan% ls *.f
gem.f       mainmlti.f  metra.f
vulcan% cd metra
vulcan% ls *.h
add.h       impl.h      para1.h     pvtfunc.h   title.h
com.h       metragem.h  paramtrs.h  pvttbl.h    units.h
frfmt.h     minc.h      pckr.h      scalars.h   watsolv.h
vulcan% cd ..
vulcan% cd gem
vulcan% ls *.h
addgem.h    debye.h     gmfwt.h     metragem.h  scalgem.h   title.h
comgem.h    fields.h    impl.h      minrl.h     scratch.h   units.h
```

```
comprs.h    frfmt.h     iounits.h   ofiles.h    surfkin.h   watsolv.h
cxkin.h     gas.h       kinetic.h   paramtrs.h  tdconst.h
vulcan%
```

```
c*file  metra.f

c Program Name:           MULTIFLO/METRA
c File/Subroutine Names: metra.f/metra.f

c Release Date:          July 2001
c Release Version:       1.5
c Client Name:           USNRC
c Client Contact:        John Bradbury (301-415-6597)
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
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c VERSION/REVISION HISTORY

c $Id$
c $Log$

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

c  April  97          Mohan S. Seth         Initial Implementation
c                     Peter C. Lichtner
c
c
c  May 98                                   Beta Release
c  February 2000      Mohan S. Seth         1.2 Release
c                     Peter C. Lichtner
c                     Scott Painter
c  May 2000                                 minor bug fixes
c
c  July 2001                                V1.5 add capability for
c                                             nonzero start time
c                                           Minor changes to accomodate
c                                             changed argument list for
c                                             some routines
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c DISCLAIMER/NOTICE

c This computer code/material was prepared as an account of work
c performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA)
c for the Division of Waste Management of the Nuclear Regulatory
c Commission (NRC), an independent agency of the United States
c Government. The developer(s) of the code nor any of their sponsors
c make any warranty, expressed or implied, or assume any legal
c liability or responsibility for the accuracy, completeness, or
c usefulness of any information, apparatus, product or process
c disclosed, or represent that its use would not infringe on
c privately-owned rights.

c IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW WILL THE SPONSORS
c OR THOSE WHO HAVE WRITTEN OR MODIFIED THIS CODE, BE LIABLE FOR
c DAMAGES, INCLUDING ANY LOST PROFITS, LOST MONIES, OR OTHER SPECIAL,
c INCIDENTAL OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OR
c INABILITY TO USE (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA
c BEING RENDERED INACCURATE OR LOSSES SUSTAINED BY THIRD PARTIES OR A
```

```
c FAILURE OF THE PROGRAM TO OPERATE WITH OTHER PROGRAMS) THE PROGRAM,
c EVEN IF YOU HAVE BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES,
c OR FOR ANY CLAIM BY ANY OTHER PARTY.

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c  PURPOSE:

c     This is main driver program for the metra code. Essentially
c     no computations are performed by this module, but it controls
c     the flow of computations. Upon completing a time step, it
c     returns to mainmlti.f.

c     This module is replaced my mainmetra.f when METRA is run in
c     standalone mode.

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c  INTERFACING ARGUMENTS:

c  Variable name       Type                    Description
c  =============       =====                   ============

c    aa                array(maxax), real*8    work array
c    delt              scalar, real*8          time-step size of metra
c    dnew              scalar, real*8          time-step size
c    ttime             scalar, real*8          metra target time
c    tplot             scalar, real*8          target time if icode =3
c    maxax             scalar, integer*4       aa-array size

c-------------------------------------------------------------------------
c   Externals
c   =========

c   accm        computes accumulatin terms in the jacoby in the absence
c               of vapor pressure lowering
c   accmvp      computes accumulatin terms in the jacoby in the presence
c               of vapor pressure lowering
c   coefs       computes jacobain coefs arising from flux terms in the
c               absence of vapor pressure lowering
c   coefsvp     computes jacobain coefs arising from flux terms in the
c               presence of vapor pressure lowering
c   updtpsk     update primary variables after each newtonian iteration
c               in the absence of vapor pressure lowering
c   updtvpk     update primary variables after each newtonian iteration
c               in the presence of vapor pressure lowering
c   pvth2ox     pvth2o, This is made external to be able to
c                       use different pvt packages. Currently
c                       only one is used.
c   pvt         calc pvt properties fo fluid in the absence of vapor
c               pressure lowering.
c   pvtvp       calc pvt properties fo fluid in the presence of vapor
c               pressure lowering.

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c   INTERFACING ROUTINES

c     Calling routines
c     ================
```

This file was created on: Mon Jul 23 14:01:22 2001



Developed for the U.S. NRC

VERSION 1.5

July, 2001

MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

dcm demonstration with YM parameters
Aug 27, 1999

*GRID---> Co-ordinate Geometry : DCMXYZ

Number of Elements in I-direction.....	NX =	1	
Number of Elements in J-direction.....	NY =	1	
Number of Elements in K-direction.....	NZ =	80	
Total Number of Elements.....	NB =	160	
Frequency of Short screen output.....IFRQS	=	10	
Index for Amount of Output	IPRINT =	0	
Index for Warning Messages	IWARN =	0	
Index for Debugging	IDEBUG =	0	
Debugging Nodes Range.....IBG1-IBG2	=	1	3
Increments for Node-Debugging.....	IBGINC =	1	

*DBAS database: D:\multiflo\database\mastertemp.V8.R5

*OPTS Parameters Specifying Options Invoked

Index for Formulation-Method.METHOD	=	2
Index for OS Algorithm.....IOPS	=	1
Index for Finite-Differencing..IFOR	=	0
Flux Limitor Algorithm.....IFLXLIM	=	0
Maximum Newtonian Iterations..ITMAX	=	32
Maximum Time-Step Cuts.....IHALMAX	=	16
No of constant dt after cut..NDTCMX	=	1
Index for LOG/LINEAR .....LOGLIN	=	0
Index for DELT size calcs...ISTEPDT	=	3
Index for BCOND flux in OS ...IBCOS	=	0
Index for Mineral Surf. area..ISURF	=	0
Index for Activity Coefs.....IACT	=	0
Stationary state.....ISST	=	-1
Upstream weight factor.....WTUP	=	0.000
Courant Number.....COURNR	=	5.0000E+05
DELT Reduction Factor.....DTCUTF	=	5.000E-01
Conc. change for auto-step .DELCMAX	=	1.000E+00
log(activity change).....QKMAX	=	5.000E+02
wt.factor: rate split in OS...WTKIN	=	0.000E+00

```
This file was created on: Mon Jul 23 14:01:22 2001

        HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
        H
H
        H       Multi-Component Unsaturated Fluid Flow Simulator
H
        H
H
        H                METRA  Version Number: 1.5
H
        H
H
        H       Developed By  Mohan S. Seth,  TS&E, July  2001
H
        H       with Peter Lichtner and Scott Painter,  CNWRA
H
        H
H
        H       CNWRA - Southwest Research Institute (2000)
H
        HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
H
```



```
            METRA-DCM, 1-D
              8-31-99


*RSTART           Run started from Restart File #  0
                  Run restart time (secs)       #  0.000000E+00


                  Total Number of Nodes          =   160
                  Total Number of Connections    =   238
                  Max nodes connected to a node  =     3


Mass and Energy in place at Time =    0.00000     [s]    step #     0

component-1 (kgm) =    73744.7       component-2 (kgm) =    49.3952
total mass  (kgm) =    73794.1       total energy (MJ) =    42082.3
Average gas sat   =  0.372425        Avergage Liq Sat. =  0.627575

Pore Volume (m3) =  0.117868E+03   Bulk Volume (m3)   =  0.726900E+03

------------------------------------------------------------------------
-----------------------------------------------------

                                    HHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
                                    H                            H
                                    H  Initialization Completed  H
                                    H                            H
                                    HHHHHHHHHHHHHHHHHHHHHHHHHHHHHH
```

README File for MULTIFLO V1.5
July 2001.

This directory contains the MULTIFLO source code, and executable for Windows NT 4, and MAKEFILES for compiling the code on Solaris operating system.

The directory structure looks like this:

Multiflo
  database
  METRA
  GEM
  AcceptanceTestsNT
    AcceptanceTest1
    AcceptanceTest2
    AcceptanceTest3
  AcceptanceTestsSolaris
    AcceptanceTest1
    AcceptanceTest2
    AcceptanceTest3

Installation Instructions:

To Compile on Windows (Lahey comiler) :

(1) In GEM directory, type

    lf95 *.f -O3 -out gem

(2) Remove util.obj, maingem.obj, and watsolv.obj from gem subdirectory.

(3) In metra subdirectory, type

    lf95 *.f -O3 -out metra

(4) Remove mainmtra.obj from metra subdirectory.

(5) In multiflo directory type.

    lf95 -O3 gem*.obj metra*.obj *.f -out multiflo

To Compile on Solaris :

(1) In gem directory type "make"

(2) In metra directory type "make"

(3) In multiflo directory type "make"

To run Acceptance Tests:

(1) Add toplevel multiflo directory to path. Change location of database in *.inp files to match location of the database directory.

(2) In AcceptanceTest1 directory type "multiflo VA1d dcm1"

(3) In AcceptanceTest2 directory type "multiflo VA1dgvt dcm1"

(4) In AcceptanceTest3 directory type "multiflo VA1dgvt1 dcm1tvd"

Software Development Plan

SOFTWARE DEVELOPMENT PLAN FOR MULTIFLO VERSION 2.0

January 2001

This software development plan (SDP) describes the approach to be followed in implementing the modifications to MULTIFLO in going from Version 1.2.3 to Version 2.0. The design specifications for the MULTIFLO Version 2.0 code are outlined in the Software Requirements Description (SRD) for MULTIFLO Version 2.0.

1.0 SCOPE

The scope of the software development effort is described in detail in the SRD. The GEM and METRA components of the code will both be modified. In addition, a set of utility routines for manipulating input and output data will be developed.

2.0 BASELINE ITEMS

Release of MULTIFLO V2.0 will be staged. The total variation diminishing (TVD) algorithm, the gravity drainage boundary condition, and improved fracture-to-matrix flow representation will be released in Version 1.5. Remaining capabilities described in the SRD will be released with V2.0. Utility routines will be under a separate release. The specific products to be delivered from this software development project include: (1) source code for MULTIFLO V1.5, (2) source code for MULTIFLO V2.0, (3) source code for utility programs: (4) updated *make* files for each release; and (5) revised User Manual for each release.

3.0 PROJECT MANAGEMENT

3.1 Work Breakdown Structure

Task 1 TVD algorithm (Seth and Painter, 5 days)

Task 2 Gravity drainage boundary condition (Seth and Mayer, 2 days)

Task 3 Improved representation of fracture-to-matrix flow (Seth and Painter, 2 Days)

Task 4 Final Testing for Version 1.5 (Painter, Seth, and Mayer, 5 days)

Task 5 Revise User Manual for Version 1.5 (Painter and support staff, 1 day)

Task 6 Pumping wells (Seth and Painter, 20 days)

Task 7 Hydrodynamic Dispersion (Painter and Mayer, 15 days)

Task 8 Final Testing for Version 2.0 (Painter, Seth, and Mayer, 5 days)

Task 9 Revise User Manual for Version 2.0 (Painter, Seth, and support staff, 5 days)

Task 10 Utility Routines (Painter, 15 days)

Task 11 Prepare New Appendix to User Manual Describing Utility Routines (Painter, 5 days)

3.2 Schedules

The following schedule is preliminary. As of this writing, there are no formal delivery dates imposed by the client. Tasks 1.5 will be completed by March 31, 2001. Tasks 6-9 will be completed by November 31, 2001, and tasks 10-11 will be completed by January 31, 2002.

3.3 Staff

Work for Version 2.0 will be performed primarily by M. Seth working under the supervision of S. Painter, and by S. Painter. S. Mayer will contribute to tasks 2, 5, 7 and 8.

4.0 DEVELOPMENT PROCEDURES

4.1 Hardware and Software resources

All code development will be done on SUN workstations or servers running the SOLARIS operating system, or on Microsoft Windows compatible PCs. The SUN FORTRAN 77 Version 5.0 will be used on the UNIX platform and Lahey Fortran 90 (LF90) Version 4.5 or ABSOFT (?) will be used on the PC platform.

4.2 Coding

Coding for MULTIFLO will be done in FORTRAN 77. Coding style will be consistent with that of MULTIFLO V1.2. Utility routines will be coded in ANSI C, following the style and conventions of Press et al.

4.3 Acceptance testing and Analysis

The results of testing will be recorded in scientific notebook 282E. In addition, results of the

standard MULTIFLO acceptance test and variants will be included with the source code for all releases.

5.0 CONFIGURATION MANAGEMENT PLAN

The working version of the code will be maintained by S Painter on the SUN server named VULCAN. New or modified modules will be tested and reviewed by S. Painter before the changes are incorporated with the working code. A description of the changes and locations of the working directories will be recorded in scientific notebook 282E. Baselined versions (i.e. Version 1.2.3) are kept in the QA records vault.

5.1 Tools

Unix utilities *diff*, *filemerge* and *make* will be used to perform the code manipulations required to maintain the official version of the working code.

5.2 Configuration Identification

The configuration identification scheme will be as follows: the first phase release will be Version 1.5.0. Subsequent minor bug fixes will be released as Version 1.5.1, 1.5.2, etc. Similarly, the second phase release will be initially be denoted Version 2.0, and will supersede the Version 1.5 series. Subsequent revisions will be numbered Version 2.*i.j*, where *i* is incremented for a major revision and *j* is incremented for a minor bug fix.

5.3 Configuration Procedures

The standard SCR change request form will be used for all significant changes to the controlled source code.

6.0 REFERENCES

W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, "Numerical Recipes in C, Second Edition", Cambridge University Press, 1996.

APPROVED:

P. C. P. 2/5/2001

Signature of Element Manager Date

Software Change Reports

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): **SCR-350**	2. Software Title and Version: **Multiflo V.1.5**	3. Project No: **20.01402.562**

4. Affected Software Module(s), Description of Problem(s):

The following are changes in the code modifications planned for Version 1.5. Version 1.5 is an interim release, as described in SDP for V2.0.

(1) Client requested that surface complexation (SRD for V2.0 Section 9) not be implemented. See attached letter.

(2) Need capability to make start time > 0.

(3) Excessive time step cutting in GEM.

(4) Convergence criteria in METRA is based on change in change in state variable, instead of change in state variable.

(5) Number of connections is currently limited to <10.

(6) Move assorted utility routines to separate file for code maintenance considerations.

5. Change Requested by: **Scott Painter** Date: **July 6, 2001**	6. Change Authorized by (*Software Developer*): **Scott Painter** Date: **July 6, 2001**

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

(2) Added tstart variable to mainmtra.f, setbc.f and source.f to address item (2).

(3) Change in stepgem.f to make limit concentration change twice the target concentration change.

(4) change to iter.f, updtpsk.f and updtvpk.f to implement item (4).

(5) change argument list in call to pproc() and inpifv() to allow more flexible dimensioning of nndcon array. Affects pproc.f and inpifv.f and addresses item (5).

(6) Created util.f, which resides in duplicate in gem and metra directory. Moved routines radcord.f, seconds.f, range.f, dcmfrac.f, frfmt.f, convert.f to this file.

8. Implemented by: **Mohan Seth/Scott Painter**	Date: **July 10, 2001**

9. Description of Acceptance Tests: **Ran the acceptance tests described in the SDP for V2.0. Tests will be repeated before final release. Output and input for the acceptance test problems are with the code, as always.**	
10. Tested by: **Scott Painter**	Date: **July 23, 2001**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): **SCR-351**	2. Software Title and Version: **Multiflo V.1.5**	3. Project No: **20.01402.562**

4. Affected Software Module(s), Description of Problem(s):

The following are changes needed for Version 1.5. Version 1.5 is an interim release, as described in SDP for V2.0.

(1) remove MINC coding, which is no longer needed and not completed.

(2) Fix problem with boundary blocks versus boundary regions for type 5,6 boundary condition.

(3) Fix problem with failure to print negative velocities to the _out file.

(4) symfac stops instead of returns when initial memory estimates are too small.

(5) need new calculation for reactive surface area in gem, as described in SN282E Vol 11.

(6) Dip angle not applied to boundary connections when using constant dip option in METRA.

(7) isothermal flag and single phase flag in GEM are not consistent with coupled mode. Need to be reset upon entering coupled mode.

5. Change Requested by: **Scott Painter** Date: **July 25, 2001**	6. Change Authorized by (*Software Developer*): **Scott Painter** Date: **July 25, 2001**

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

All changes implemented. New version to be released as V1.5.1.

8. Implemented by: **Mohan Seth/Scott Painter** Scott Painter	Date: 6-12-02

9. Description of Acceptance Tests:

Ran the same acceptance tests as for V1.5 (see SN282E). Output and input for the acceptance test problems are with the code, as always.

10. Tested by: Scott Painter	Date: 6-12-02