SOFTWARE RELEASE NOTICE

01. SRN Number: SRN- GHGC-270

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

03. SRN Title: MULTIFLO V1.5.1

04. Originator/Requestor: Scott Painter | Date: 6/20/02

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: L. C. Hamm Date: 6/20/2002

08. Remarks:

CNWRA Form TOP-6 (06/95)

SOFTWARE SUMMARY FORM

01. Summary Date: 6/13/2002	02. Summary prepared by (Name and phone) **Scott Painter, 522-3348**	03. Summary Action: **New**
04. Software Date: 6/13/2002	05. Short Title: **MULTIFLO Version 1.5.1**	
06. Software Title: **MULTIFLO Version 1.5.1**		07. Internal Software ID: **NONE**

08. Software Type:	09. Processing Mode:	10. APPLICATION AREA
☐ Automated Data System	☐ Interactive	a. General: ■ Scientific/Engineering ■ Auxiliary Analyses ☐ Total System PA
■ Computer Program	☐ Batch	☐ Subsystem PA ☐ Other
☐ Subroutine/Module	■ Combination	b. Specific: **Groundwater multiphase flow and reactive transport model**

11. Submitting Organization and Address:	12. Technical Contact(s) and Phone:
CNWRA **6220 Culebra Road** **San Antonio, TX 78228**	**Scott Painter, (210) 522-3348**

13. Narrative:
The code is used to model multiphase groundwater flow and reactive transport.

14. Computer Platform	15. Computer Operating System:	16. Programming Language(s):	17. Number of Source Program Statements:
SUN	**UNIX**	**Fortran 77**	**~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:	24. Documentation Availability:
☐ Available ■ Limited ☐ In-House ONLY	■ Available ☐ Inadequate ☐ In-House ONLY DRAFT

Software Developer: Scott Painter Date: 6-24-02

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

Software Title/Name: Multifb

Version: 1.5.1

Demonstration workstation: Spock

Operating System: Unix | Solaris

Developer: Scott Painter

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

SRD Version: 2.0

SRD Approval Date: 10/3/2000

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 #351 attached.

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

SDP Version: 2.0

SDP (EM) Approval Date: 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 required

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: bndcond.f, solve.f

Comments: bcond.f, init.f

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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: See above

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: SN282E

Comments: Test results on V. 1.5.1 CD.

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: Wed June 12 16:05:54 2002

Name/Version Displayed: Multiflo V. 1.5.1

Comments: See attached

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: See attached

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: bndcond.f solve.f
bcond.f init.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: Various file types – See SSF

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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

Comments: Performed by Painter.

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?

Yes: ☑ No: ☐ N/A: ☐

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

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: Solaris PC Operating Systems: NT Unix

Location of Acceptance Test Results: See enclosed CD.

Comments: Used same test suite used for version 1.5.

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

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: PC Solaris Operating Systems: NT Unix

Location of Acceptance Test Results: See enclosed CD.

Comments:

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: 1.5 Transmittal 12/13/01

Comments:

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

Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: Readme file on CD. for V. 1.5.

Comments: Located in user's manual

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: 6/24/02

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

Yes: ☑ No: ☐ N/A: ☐

Comments: See list.

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: See CD V. 1.5.1

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: See CD V. 1.5.1

Comments:

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: G HGC - 270

Comments:

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QA VERIFICATION REPORT
FOR
→DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE←

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: SVTP is targeted for ~~Aug. 9, 2002~~ June 14, 2002 6/21/02

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: Validation is targeted for Aug. 9, 2002

Additional Comments:

Scott Painter 6-24-02
Software Developer/Date

Software Custodian/Date 6/24/02

```
  1294     0 qtpa4000b  muller       qw    06/11/2002 18:06:01
  1295     0 qtpa4000c  muller       qw    06/11/2002 18:06:45
  1296     0 qtpa4000d  muller       qw    06/11/2002 18:07:06
  1309     0 fast_cSet4 jmench       qw    06/12/2002 09:31:05
  1310     0 fast_cSet5 jmench       qw    06/12/2002 09:31:19
  1311     0 fast_cSet6 jmench       qw    06/12/2002 09:31:37
  1312     0 fast_cSet7 jmench       qw    06/12/2002 09:31:51
  1313     0 fast_cSet8 jmench       qw    06/12/2002 09:32:04
idaho% pwd
/net/spock/home/spainter
idaho% ls
3dunstruct       bin              fird2            mflo-bmark       rgreen           test
CSIRO            browning         fort.52          mflo-timing      satzone          tmp.cshrc
Edwards          chandrika        goodluck         mflo.e937        silica           ventilation
GPI3             cmesh            gslib            mflo.o937        sisim            vladimir
Green            cshrc.20010816   hughson          mflotests        submit.e1176     workshop
SKB              dhughson         injection        mflotests2       submit.e1187     yconst.dat
Tecplot          env_for_painter  kquantiles.dat   multiflo         submit.o1176     ym
amesh            fird             marsflo          qtz              submit.o1187
idaho% cd multiflo/mflo1.5.1
idaho% ls
AcceptanceTests  gem              gem.o            mainmlti.o       metra.o
Makefile         gem-diff         gem.tar          metra            multiflo
Mflo.tar         gem.f            mainmlti.f       metra.f          mymetra
idaho% cd Acc*
idaho% cd Acc*1
idaho% ls
VA1d.dat         VA1dfldf7.xyp    VA1dvz6.xyp      dcm1_aqm5.xyp    dcm1_secf5.xyp   dcm1_srfm5.xyp
VA1d.int         VA1dfldf8.xyp    VA1dvz7.xyp      dcm1_gasf1.xyp   dcm1_secm1.xyp   dcm1_volf1.xyp
VA1d_errs        VA1dfldm1.xyp    VA1dvz8.xyp      dcm1_gasf2.xyp   dcm1_secm2.xyp   dcm1_volf2.xyp
VA1d_his.xyp     VA1dfldm2.xyp    dcm1.inp         dcm1_gasf3.xyp   dcm1_secm3.xyp   dcm1_volf3.xyp
VA1d_out         VA1dfldm3.xyp    dcm1.out         dcm1_gasf4.xyp   dcm1_secm4.xyp   dcm1_volf4.xyp
VA1d_press.xyp   VA1dfldm4.xyp    dcm1.scr         dcm1_gasf5.xyp   dcm1_secm5.xyp   dcm1_volf5.xyp
VA1d_rh.xyp      VA1dfldm5.xyp    dcm1_aqf1.xyp    dcm1_gasm1.xyp   dcm1_srff1.xyp   dcm1_volm1.xyp
VA1d_sat.xyp     VA1dfldm6.xyp    dcm1_aqf2.xyp    dcm1_gasm2.xyp   dcm1_srff2.xyp   dcm1_volm2.xyp
VA1d_tmp.xyp     VA1dfldm7.xyp    dcm1_aqf3.xyp    dcm1_gasm3.xyp   dcm1_srff3.xyp   dcm1_volm3.xyp
VA1dfldf1.xyp    VA1dfldm8.xyp    dcm1_aqf4.xyp    dcm1_gasm4.xyp   dcm1_srff4.xyp   dcm1_volm4.xyp
VA1dfldf2.xyp    VA1dvz1.xyp      dcm1_aqf5.xyp    dcm1_gasm5.xyp   dcm1_srff5.xyp   dcm1_volm5.xyp
VA1dfldf3.xyp    VA1dvz2.xyp      dcm1_aqm1.xyp    dcm1_secf1.xyp   dcm1_srfm1.xyp   fort.22
VA1dfldf4.xyp    VA1dvz3.xyp      dcm1_aqm2.xyp    dcm1_secf2.xyp   dcm1_srfm2.xyp   fort.8
VA1dfldf5.xyp    VA1dvz4.xyp      dcm1_aqm3.xyp    dcm1_secf3.xyp   dcm1_srfm3.xyp
VA1dfldf6.xyp    VA1dvz5.xyp      dcm1_aqm4.xyp    dcm1_secf4.xyp   dcm1_srfm4.xyp
idaho% vi dcm1.out
"dcm1.out" 24016 lines, 551785 characters (288 null)
 This file was created on: Wed Jun 12 16:05:54 2002

          _/      _/ _/     _/ _/   _/_/_/_/_/ _/   _/_/_/_/_/ _/        _/_/
         _/_/  _/_/ _/      _/ _/        _/     _/   _/         _/      _/    _/
        _/  _/ _/ _/       _/ _/        _/     _/   _/_/_/     _/      _/    _/
       _/      _/ _/       _/ _/        _/     _/   _/         _/      _/    _/
      _/       _/  _/_/_/   _/_/_/   _/       _/   _/         _/_/_/    _/_/

                    Developed for the U.S. NRC

                              VERSION 1.5.1

                              June 2002

                MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

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             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
```

```
 Metra: Total Number of Steps     =       291
 Metra: Total Newtonian Iters     =      1175
 Metra: Total Time-Step Cuts      =         3
-------------------------------------------------------------------
 GEM:    Read/Initialization      =      0.24      0.13           1
 GEM:    Stdyst                   =      0.91      0.48        6936
 GEM:    coefficients             =      0.00      0.00           0
 GEM:    solver                   =     66.99     35.53       63744
 GEM:    Update                   =      0.94      0.50        6657
 GEM:    kinrxns+ionex+monod      =     22.30     11.83       31184
 GEM:    outgem/graphs            =      1.32      0.70        6657
 GEM:    Transd                   =      0.00      0.00           0
 GEM:    calcpsi                  =     30.25     16.04       39152
 GEM:    calcdpsi                 =      0.00      0.00           0
 GEM:    factorization            =      0.00      0.00           0
 GEM:    bicgstb/gmres            =      0.00      0.00           0
 GEM:    nrtrans(x)(+solver)      =     81.49     43.22           0
 GEM:    react                    =     23.70     12.57       30153
 GEM:    GEM execution time       =    169.63     89.98           0

 GEM:    Number of Steps          =      6657
 GEM:    Newtonian Iters          =     20294
 GEM:    Time-Step Cuts           =      1311

 Total GEM + METRA CPU-Time       =    188.53    100.
-------------------------------------------------------------------
 normal stop - run completed in    6657 steps   total iters =  20294
 cpu time =    180.3772 secs     3.0063 min      0.0501 hours
-------------------------------------------------------------------

 Note: Nonstandard floating-point mode enabled
 (See the Numerical Computation Guide, ieee_sun(3M)
spock% ~/multiflo/mflo1.5.1/multiflo VA1dgvt1 dcm1tvd
--> read icode: (1-metra, 2-gem, 3-coupled, 4-coupled: steady-state) 3
 --> open input file dcm1tvd.inp
```

```
  _/      _/ _/     _/ _/   _/_/_/_/_/ _/   _/_/_/_/_/ _/        _/_/
 _/_/  _/_/ _/     _/ _/        _/      _/   _/         _/      _/    _/
_/  _/ _/ _/      _/ _/         _/      _/   _/_/       _/      _/    _/
_/      _/ _/     _/ _/         _/      _/   _/         _/      _/    _/
_/      _/  _/_/_/   _/_/_/    _/      _/   _/         _/_/_/    _/_/
```

Developed for the U.S. NRC

Version 1.5.1

June 2002

MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

```
 --> Initializatize METRA
 --> open input file VA1dgvt1.dat
-----------------------------------[ METRA ]---------------------------------
 --> Initializatize GEM
 --> read input file: icode =  3
 Notice: For ICODE > 3, IPOR must be negative, have reset IPOR = -1
     --> master species for time-step control: ALL
      --> finish reading input data


 ========================================================
  Total Work Space Required for [aa] in MULTIFLO  =      26638
                                       Assigned  =   10000000
 ========================================================
```

```
VA1dfldf2.xyp   VA1dvz1.xyp     dcm1_aqf5.xyp   dcm1_gasm5.xyp  dcm1_srff5.xyp  dcm1_volm5.xyp
VA1dfldf3.xyp   VA1dvz2.xyp     dcm1_aqm1.xyp   dcm1_secf1.xyp  dcm1_srfm1.xyp  fort.22
VA1dfldf4.xyp   VA1dvz3.xyp     dcm1_aqm2.xyp   dcm1_secf2.xyp  dcm1_srfm2.xyp  fort.8
VA1dfldf5.xyp   VA1dvz4.xyp     dcm1_aqm3.xyp   dcm1_secf3.xyp  dcm1_srfm3.xyp
VA1dfldf6.xyp   VA1dvz5.xyp     dcm1_aqm4.xyp   dcm1_secf4.xyp  dcm1_srfm4.xyp
idaho% vi dcm1.out
"dcm1.out" 24016 lines, 551785 characters (288 null)
 This file was created on: Wed Jun 12 16:05:54 2002

          _/      _/ _/    _/ _/   _/_/_/_/_/ _/   _/_/_/_/ _/       _/_/
          _/_/ _/_/ _/     _/ _/       _/      _/   _/       _/     _/    _/
          _/  _/ _/ _/     _/ _/       _/      _/   _/_/     _/     _/    _/
          _/     _/ _/     _/ _/       _/      _/   _/       _/     _/    _/
          _/     _/  _/_/_/  _/_/_/    _/      _/   _/       _/_/_/   _/_/

                        Developed for the U.S. NRC

                                VERSION 1.5.1

                                June 2002

                  MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

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             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
:quit!
idaho% cd ..
idaho% ls
AcceptanceTest1  AcceptanceTest2  AcceptanceTest3  AcceptanceTest4  AcceptanceTest5
AcceptanceTest6
idaho% cd ..
idaho% cd ..
idaho% ls
BetaVersions      forDStephens      mflo1.2.1         mflo1.2.3         mflo1.5.1
database          forDStephens.tar  mflo1.2.1old      mflo1.2.3.tar     mflo1.5big
forDOE            forFreitas        mflo1.2.2         mflo1.2QA         mflo1.5x
forDOE.tar.gz     mflo1.2           mflo1.2.2.tar     mflo1.5           mflo2.0
idaho% cd mflo1.5.1
idaho% ls
AcceptanceTests  gem              gem.o            mainmlti.o       metra.o
Makefile         gem-diff         gem.tar          metra            multiflo
Mflo.tar         gem.f            mainmlti.f       metra.f          mymetra
idaho% vi mainmlti.f
"mainmlti.f" 779 lines, 28260 characters
c*file mainmlti.f

c               Copyright 2000 Southwest Research Institute

c Program Name:          MULTIFLO
c File/Program Name:     mainmlti.f/MULTIFLO
c Other modules:         block data metragem
c                        cputim.f
c                        seconds.f
c                        lnblnk.f
c                        convert.f
c                        frfmt.f
c Release Date:          June 2002
c Release Version:       1.5.1
c Client Name:           USNRC
c Client Contact:        John Bradbury (301-415-6597)
```

Header Information

```
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        Peter C. Lichtner      Initial Implementation
c                   Mohan S. Seth
c  May 98                                  Beta Release
c  February 2000    Peter C. Lichtner      1.2 Release
c                   Mohan S. Seth
c                   Scott Painter
c  May 2000                               V1.2.1 Minor Bug fixes
c  August 2000                            V1.2.2 Fix bug related to water
c                                           density calculation and
c                                           phase change test
c  December 2000                          V1.2.3 Fix bug related to dryout
c                                           in GEM. Also change surface
c                                           area update in GEM, which
c                                           was bypassed for secondary
c                                           minerals. Minor fix to printing
c                                           errors.
c
c  July 2001                              V1.5 Section 5,7,8 of V2.0 SRD
c                                           Also assorted minor fixes
c  June 2002                              SCR351
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c DISCLAIMER/NOTICE

c This computer code/material was developed 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
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c usefulness of any information, apparatus, product or process
c disclosed, or represent that its use would not infringe on
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c IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW WILL THE SPONSORS
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c INABILITY TO USE (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA
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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 routine is the main program for the MULTIFLO driver which
c  couples METRA and GEM.

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Header Information

MULTIFLO, 1.5.1 LIST OF FILES, June 21, 2002

```
 Volume in drive R is 020619_1112
 Volume Serial Number is 8658-EF75


 Directory of R:\

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/19/02  11:12a        <DIR>          mflo1.5.1
               3 File(s)              0 bytes

 Directory of R:\mflo1.5.1

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/19/02  11:12a        <DIR>          AcceptanceTests
06/19/02  11:12a        <DIR>          gem
02/21/02  02:08p                20,740 gem.f
06/12/02  05:02p                20,267 gem.obj
06/12/02  02:53p                28,260 mainmlti.f
06/12/02  05:02p                18,787 mainmlti.obj
02/21/02  05:20p                 2,470 Makefile
06/19/02  11:12a        <DIR>          metra
02/21/02  02:08p                24,168 metra.f
06/12/02  05:02p                11,750 metra.obj
06/12/02  04:05p             8,512,440 multiflo
06/12/02  05:02p             8,299,777 multiflo.exe
06/12/02  05:02p               116,203 multiflo.map
              15 File(s)     17,054,862 bytes

 Directory of R:\mflo1.5.1\AcceptanceTests

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/19/02  11:12a        <DIR>          AcceptanceTest1
06/19/02  11:12a        <DIR>          AcceptanceTest2
06/19/02  11:12a        <DIR>          AcceptanceTest3
               5 File(s)              0 bytes

 Directory of R:\mflo1.5.1\AcceptanceTests\AcceptanceTest1

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/12/02  04:11p                 8,075 dcm1_aqf5.xyp
06/12/02  04:08p                 8,075 dcm1_aqm3.xyp
06/12/02  04:06p                 3,371 dcm1_srfm2.xyp
06/12/02  04:06p                 3,371 dcm1_srfm1.xyp
06/12/02  04:09p                 8,075 dcm1_aqm4.xyp
06/12/02  04:06p                 3,371 dcm1_srff2.xyp
06/12/02  04:06p                 3,371 dcm1_srff1.xyp
06/12/02  04:08p                 5,803 dcm1_secm3.xyp
06/12/02  04:06p                 5,803 dcm1_secm2.xyp
06/12/02  04:06p                 5,803 dcm1_secm1.xyp
06/12/02  04:06p                 8,075 dcm1_aqm1.xyp
06/12/02  04:11p                 8,075 dcm1_aqm5.xyp
```

```
06/12/02  04:06p             8,075 dcm1_aqm2.xyp
06/12/02  04:06p             3,530 dcm1_gasm2.xyp
06/12/02  04:06p             3,530 dcm1_gasm1.xyp
06/12/02  04:11p             3,371 dcm1_srfm5.xyp
06/12/02  04:09p             3,371 dcm1_srfm4.xyp
06/12/02  04:08p             3,371 dcm1_srfm3.xyp
06/12/02  04:11p             3,371 dcm1_srff5.xyp
06/12/02  04:09p             3,371 dcm1_srff4.xyp
06/12/02  04:08p             3,371 dcm1_srff3.xyp
06/12/02  04:11p             5,803 dcm1_secm5.xyp
06/12/02  04:09p             5,803 dcm1_secm4.xyp
06/12/02  04:11p             5,803 dcm1_secf5.xyp
06/12/02  04:06p             5,483 dcm1_volm1.xyp
06/12/02  04:06p             5,483 dcm1_volm2.xyp
06/12/02  04:11p             5,483 dcm1_volf5.xyp
06/12/02  04:11p             3,530 dcm1_gasm5.xyp
06/12/02  04:09p             3,530 dcm1_gasm4.xyp
06/12/02  04:08p             3,530 dcm1_gasm3.xyp
06/12/02  04:11p             3,530 dcm1_gasf5.xyp
06/12/02  04:11p             5,483 dcm1_volm5.xyp
06/12/02  04:08p             5,483 dcm1_volm3.xyp
06/12/02  04:09p             5,483 dcm1_volm4.xyp
05/31/02  03:41p             6,094 dcm1.inp
06/12/02  04:11p           551,785 dcm1.out
06/12/02  04:11p           430,857 dcm1.scr
06/12/02  04:06p             8,075 dcm1_aqf1.xyp
06/12/02  04:06p             8,075 dcm1_aqf2.xyp
06/12/02  04:08p             8,075 dcm1_aqf3.xyp
06/12/02  04:09p             8,075 dcm1_aqf4.xyp
06/12/02  04:06p             3,530 dcm1_gasf1.xyp
06/12/02  04:06p             3,530 dcm1_gasf2.xyp
06/12/02  04:08p             3,530 dcm1_gasf3.xyp
06/12/02  04:09p             3,530 dcm1_gasf4.xyp
06/12/02  04:06p             5,803 dcm1_secf1.xyp
06/12/02  04:06p             5,803 dcm1_secf2.xyp
06/12/02  04:08p             5,803 dcm1_secf3.xyp
06/12/02  04:09p             5,803 dcm1_secf4.xyp
06/12/02  04:06p             5,483 dcm1_volf1.xyp
06/12/02  04:06p             5,483 dcm1_volf2.xyp
06/12/02  04:08p             5,483 dcm1_volf3.xyp
06/12/02  04:09p             5,483 dcm1_volf4.xyp
05/06/02  05:18p               345 fort.22
05/06/02  05:18p               345 fort.8
02/21/02  03:22p            15,089 VA1d.dat
02/21/02  03:22p             9,049 VA1d.int
06/12/02  04:06p            14,460 VA1dfldf1.xyp
06/12/02  04:06p            14,460 VA1dfldf2.xyp
06/12/02  04:08p            14,460 VA1dfldf3.xyp
06/12/02  04:09p            14,460 VA1dfldf4.xyp
06/12/02  04:06p            13,405 VA1dvz1.xyp
06/12/02  04:06p            13,405 VA1dvz2.xyp
06/12/02  04:08p            13,405 VA1dvz3.xyp
06/12/02  04:09p            13,405 VA1dvz4.xyp
06/12/02  04:11p            13,405 VA1dvz5.xyp
05/06/02  05:19p            13,405 VA1dvz6.xyp
05/06/02  05:19p            13,405 VA1dvz7.xyp
05/06/02  05:20p            13,405 VA1dvz8.xyp
```

```
05/06/02  05:20p                 121 VA1d_errs
06/12/02  04:11p               5,849 VA1d_his.xyp
06/12/02  04:11p             147,995 VA1d_out
06/12/02  04:11p              14,567 VA1d_press.xyp
06/12/02  04:11p              14,567 VA1d_rh.xyp
06/12/02  04:11p              14,567 VA1d_sat.xyp
06/12/02  04:11p              14,567 VA1d_tmp.xyp
05/06/02  05:19p              14,460 VA1dfldf7.xyp
05/06/02  05:20p              14,460 VA1dfldf8.xyp
06/12/02  04:11p              14,460 VA1dfldf5.xyp
05/06/02  05:19p              14,460 VA1dfldf6.xyp
06/12/02  04:08p              14,460 VA1dfldm3.xyp
05/06/02  05:19p              14,460 VA1dfldm7.xyp
06/12/02  04:09p              14,460 VA1dfldm4.xyp
05/06/02  05:20p              14,460 VA1dfldm8.xyp
06/12/02  04:11p              14,460 VA1dfldm5.xyp
06/12/02  04:06p              14,460 VA1dfldm1.xyp
05/06/02  05:19p              14,460 VA1dfldm6.xyp
06/12/02  04:06p              14,460 VA1dfldm2.xyp
              90 File(s)      1,827,017 bytes

 Directory of R:\mflo1.5.1\AcceptanceTests\AcceptanceTest2

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/12/02  04:18p                8,075 dcm1_aqf5.xyp
06/12/02  04:16p                8,075 dcm1_aqm3.xyp
06/12/02  04:17p                8,075 dcm1_aqm4.xyp
06/12/02  04:16p                5,803 dcm1_secm3.xyp
06/12/02  04:13p                5,803 dcm1_secm2.xyp
06/12/02  04:13p                5,803 dcm1_secm1.xyp
06/12/02  04:13p                8,075 dcm1_aqm1.xyp
06/12/02  04:18p                8,075 dcm1_aqm5.xyp
06/12/02  04:13p                8,075 dcm1_aqm2.xyp
06/12/02  04:13p                3,530 dcm1_gasm2.xyp
06/12/02  04:13p                3,530 dcm1_gasm1.xyp
06/12/02  04:18p                5,803 dcm1_secm5.xyp
06/12/02  04:17p                5,803 dcm1_secm4.xyp
06/12/02  04:18p                5,803 dcm1_secf5.xyp
06/12/02  04:13p                5,483 dcm1_volm1.xyp
06/12/02  04:13p                5,483 dcm1_volm2.xyp
06/12/02  04:18p                5,483 dcm1_volf5.xyp
06/12/02  04:18p                3,530 dcm1_gasm5.xyp
06/12/02  04:17p                3,530 dcm1_gasm4.xyp
06/12/02  04:16p                3,530 dcm1_gasm3.xyp
06/12/02  04:18p                3,530 dcm1_gasf5.xyp
06/12/02  04:18p                5,483 dcm1_volm5.xyp
06/12/02  04:16p                5,483 dcm1_volm3.xyp
06/12/02  04:17p                5,483 dcm1_volm4.xyp
02/21/02  03:22p                6,084 dcm1.inp
06/12/02  04:18p              578,664 dcm1.out
06/12/02  04:18p              472,998 dcm1.scr
06/12/02  04:13p                8,075 dcm1_aqf1.xyp
06/12/02  04:13p                8,075 dcm1_aqf2.xyp
06/12/02  04:16p                8,075 dcm1_aqf3.xyp
06/12/02  04:17p                8,075 dcm1_aqf4.xyp
06/12/02  04:13p                3,530 dcm1_gasf1.xyp
```

```
06/12/02  04:13p                3,530 dcm1_gasf2.xyp
06/12/02  04:16p                3,530 dcm1_gasf3.xyp
06/12/02  04:17p                3,530 dcm1_gasf4.xyp
06/12/02  04:13p                5,803 dcm1_secf1.xyp
06/12/02  04:13p                5,803 dcm1_secf2.xyp
06/12/02  04:16p                5,803 dcm1_secf3.xyp
06/12/02  04:17p                5,803 dcm1_secf4.xyp
06/12/02  04:13p                5,483 dcm1_volf1.xyp
06/12/02  04:13p                5,483 dcm1_volf2.xyp
06/12/02  04:16p                5,483 dcm1_volf3.xyp
06/12/02  04:17p                5,483 dcm1_volf4.xyp
02/26/02  11:44a                  345 fort.22
02/26/02  11:44a                  345 fort.8
02/21/02  03:22p                9,049 VA1d.int
02/21/02  03:22p               15,114 VA1dgvt.dat
02/25/02  04:09p                  121 VA1dgvt_errs
06/12/02  04:13p               14,460 VA1dgvtfldf1.xyp
06/12/02  04:18p              148,883 VA1dgvt_out
06/12/02  04:13p               14,460 VA1dgvtfldf2.xyp
06/12/02  04:16p               14,460 VA1dgvtfldf3.xyp
06/12/02  04:17p               14,460 VA1dgvtfldf4.xyp
06/12/02  04:18p               18,987 VA1dgvt_sat.xyp
06/12/02  04:13p               14,460 VA1dgvtfldm2.xyp
06/12/02  04:16p               14,460 VA1dgvtfldm3.xyp
06/12/02  04:13p               14,460 VA1dgvtfldm1.xyp
06/12/02  04:18p               18,987 VA1dgvt_tmp.xyp
06/12/02  04:18p               18,987 VA1dgvt_rh.xyp
06/12/02  04:18p                7,617 VA1dgvt_his.xyp
02/25/02  04:09p               14,460 VA1dgvtfldm6.xyp
02/25/02  04:09p               14,460 VA1dgvtfldm7.xyp
06/12/02  04:17p               14,460 VA1dgvtfldm4.xyp
06/12/02  04:18p               14,460 VA1dgvtfldm5.xyp
02/25/02  04:09p               14,460 VA1dgvtfldf6.xyp
02/25/02  04:09p               14,460 VA1dgvtfldf7.xyp
06/12/02  04:18p               14,460 VA1dgvtfldf5.xyp
02/25/02  04:09p               14,460 VA1dgvtfldm8.xyp
02/21/02  03:22p               14,460 VA1dgvtfldm9.xyp
02/25/02  04:09p               14,460 VA1dgvtfldf8.xyp
02/21/02  03:22p               14,460 VA1dgvtfldf9.xyp
06/12/02  04:13p               13,405 VA1dgvtvz2.xyp
06/12/02  04:13p               13,405 VA1dgvtvz1.xyp
02/25/02  04:09p               13,405 VA1dgvtvz6.xyp
06/12/02  04:18p               13,405 VA1dgvtvz5.xyp
06/12/02  04:17p               13,405 VA1dgvtvz4.xyp
06/12/02  04:16p               13,405 VA1dgvtvz3.xyp
02/21/02  03:22p               13,405 VA1dgvtvz9.xyp
02/25/02  04:09p               13,405 VA1dgvtvz8.xyp
02/25/02  04:09p               13,405 VA1dgvtvz7.xyp
06/12/02  04:18p               18,987 VA1dgvt_press.xyp
              83 File(s)      1,925,003 bytes

 Directory of R:\mflo1.5.1\AcceptanceTests\AcceptanceTest3

06/19/02  11:12a        <DIR>          .
06/19/02  11:12a        <DIR>          ..
06/12/02  04:40p                8,075 dcm1tvd_aqm1.xyp
06/12/02  04:46p                8,075 dcm1tvd_aqm5.xyp
```

```
06/12/02  04:44p               8,075 dcm1tvd_aqm4.xyp
06/12/02  04:43p               8,075 dcm1tvd_aqm3.xyp
06/12/02  04:40p               8,075 dcm1tvd_aqm2.xyp
06/12/02  04:46p               8,075 dcm1tvd_aqf5.xyp
06/12/02  04:40p               5,803 dcm1tvd_secf1.xyp
06/12/02  04:46p               5,803 dcm1tvd_secf5.xyp
06/12/02  04:44p               3,530 dcm1tvd_gasf4.xyp
06/12/02  04:44p               3,530 dcm1tvd_gasm4.xyp
06/12/02  04:44p               5,483 dcm1tvd_volf4.xyp
06/12/02  04:40p               5,803 dcm1tvd_secf2.xyp
06/12/02  04:40p               3,530 dcm1tvd_gasf1.xyp
06/12/02  04:40p               3,530 dcm1tvd_gasm1.xyp
06/12/02  04:46p               3,530 dcm1tvd_gasf5.xyp
06/12/02  04:46p               3,530 dcm1tvd_gasm5.xyp
06/12/02  04:40p               5,483 dcm1tvd_volf1.xyp
06/12/02  04:46p               5,483 dcm1tvd_volf5.xyp
06/12/02  04:43p               5,803 dcm1tvd_secf3.xyp
06/12/02  04:40p               3,530 dcm1tvd_gasf2.xyp
06/12/02  04:40p               3,530 dcm1tvd_gasm2.xyp
06/12/02  04:40p               5,483 dcm1tvd_volf2.xyp
06/12/02  04:44p               5,803 dcm1tvd_secf4.xyp
06/12/02  04:43p               3,530 dcm1tvd_gasf3.xyp
06/12/02  04:43p               3,530 dcm1tvd_gasm3.xyp
06/12/02  04:43p               5,483 dcm1tvd_volf3.xyp
06/12/02  04:40p               5,803 dcm1tvd_secm1.xyp
06/12/02  04:46p               5,803 dcm1tvd_secm5.xyp
06/12/02  04:44p               5,483 dcm1tvd_volm4.xyp
06/12/02  04:40p               5,803 dcm1tvd_secm2.xyp
06/12/02  04:40p               5,483 dcm1tvd_volm1.xyp
06/12/02  04:46p               5,483 dcm1tvd_volm5.xyp
06/12/02  04:43p               5,803 dcm1tvd_secm3.xyp
06/12/02  04:40p               5,483 dcm1tvd_volm2.xyp
06/12/02  04:44p               5,803 dcm1tvd_secm4.xyp
06/12/02  04:43p               5,483 dcm1tvd_volm3.xyp
02/21/02  03:22p               6,063 dcm1tvd.inp
06/12/02  04:46p             574,989 dcm1tvd.out
06/12/02  04:46p             465,403 dcm1tvd.scr
06/12/02  04:40p               8,075 dcm1tvd_aqf1.xyp
06/12/02  04:40p               8,075 dcm1tvd_aqf2.xyp
06/12/02  04:43p               8,075 dcm1tvd_aqf3.xyp
06/12/02  04:44p               8,075 dcm1tvd_aqf4.xyp
02/21/02  03:22p               9,049 VA1d.int
02/21/02  03:22p              15,211 VA1dgvt1.dat
02/21/02  03:22p                 121 VA1dgvt1_errs
06/12/02  04:40p              14,460 VA1dgvt1fldf1.xyp
06/12/02  04:46p             148,883 VA1dgvt1_out
06/12/02  04:40p              14,460 VA1dgvt1fldf2.xyp
06/12/02  04:43p              14,460 VA1dgvt1fldf3.xyp
06/12/02  04:44p              14,460 VA1dgvt1fldf4.xyp
06/12/02  04:46p               7,617 VA1dgvt1_his.xyp
06/12/02  04:46p              18,987 VA1dgvt1_tmp.xyp
06/12/02  04:46p              18,987 VA1dgvt1_rh.xyp
06/12/02  04:40p              13,405 VA1dgvt1vz2.xyp
02/21/02  03:22p              13,405 VA1dgvt1vz6.xyp
06/12/02  04:43p              13,405 VA1dgvt1vz3.xyp
02/21/02  03:22p              13,405 VA1dgvt1vz7.xyp
06/12/02  04:46p              18,987 VA1dgvt1_sat.xyp
```

```
06/12/02  04:44p                13,405 VA1dgvt1vz4.xyp
02/21/02  03:22p                13,405 VA1dgvt1vz8.xyp
06/12/02  04:40p                13,405 VA1dgvt1vz1.xyp
06/12/02  04:45p                13,405 VA1dgvt1vz5.xyp
02/21/02  03:22p                13,405 VA1dgvt1vz9.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldf6.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldf7.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldf8.xyp
06/12/02  04:45p                14,460 VA1dgvt1fldf5.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldf9.xyp
06/12/02  04:40p                14,460 VA1dgvt1fldm2.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldm6.xyp
06/12/02  04:46p                18,987 VA1dgvt1_press.xyp
06/12/02  04:43p                14,460 VA1dgvt1fldm3.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldm7.xyp
06/12/02  04:44p                14,460 VA1dgvt1fldm4.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldm8.xyp
06/12/02  04:40p                14,460 VA1dgvt1fldm1.xyp
06/12/02  04:45p                14,460 VA1dgvt1fldm5.xyp
02/21/02  03:22p                14,460 VA1dgvt1fldm9.xyp
              81 File(s)      1,913,119 bytes

 Directory of R:\mflo1.5.1\gem

06/19/02  11:12a        <DIR>           .
06/19/02  11:12a        <DIR>           ..
02/21/02  02:07p                 2,005 addgem.h
02/21/02  02:06p                17,693 allotgem.f
06/12/02  04:57p                13,260 allotgem.obj
02/21/02  02:06p                 7,080 blkdtgem.f
06/12/02  04:57p             6,252,470 blkdtgem.obj
05/31/02  01:19p                15,212 bndcond.f
06/12/02  04:57p                14,411 bndcond.obj
02/21/02  02:06p                15,482 calcpsi.f
06/12/02  04:57p                18,459 calcpsi.obj
02/21/02  02:06p                24,264 coefimp.f
06/12/02  04:57p                29,383 coefimp.obj
02/21/02  02:06p                24,739 coeftvd.f
06/12/02  04:57p                27,683 coeftvd.obj
02/21/02  02:07p                 4,821 comgem.h
02/21/02  02:07p                   289 comprs.h
02/21/02  02:07p                   714 cxkin.h
02/21/02  02:06p                13,174 dataall.f
06/12/02  04:57p                12,487 dataall.obj
02/21/02  02:06p                44,989 database.f
06/12/02  04:57p                68,272 database.obj
02/21/02  02:07p                   142 debye.h
02/21/02  02:06p                15,646 derives.f
06/12/02  04:57p                22,662 derives.obj
02/21/02  02:06p                11,434 elechem.f
06/12/02  04:57p                 8,450 elechem.obj
02/21/02  02:06p                11,122 eqjac.f
06/12/02  04:57p                12,682 eqjac.obj
02/21/02  02:06p                39,442 eqlib.f
06/12/02  04:57p                45,271 eqlib.obj
02/21/02  02:06p                12,108 eqres.f
06/12/02  04:57p                 9,850 eqres.obj
```

```
02/21/02  02:07p                310 fields.h
02/21/02  02:06p              4,419 flogk.f
06/12/02  04:57p                754 flogk.obj
02/21/02  02:07p                503 frfmt.h
02/21/02  02:06p              9,638 gameq.f
06/12/02  04:57p              7,778 gameq.obj
02/21/02  02:06p              8,997 gamextd.f
06/12/02  04:57p              7,585 gamextd.obj
02/21/02  02:07p                 72 gas.h
06/12/02  03:39p          7,590,376 gem
06/12/02  04:58p          7,617,249 gem.exe
06/12/02  04:58p            102,880 gem.map
02/21/02  02:07p                114 gmfwt.h
02/21/02  02:06p             23,231 graph1d.f
06/12/02  04:57p             35,587 graph1d.obj
02/21/02  02:06p             29,790 graph2d.f
06/12/02  04:57p             42,376 graph2d.obj
02/21/02  02:06p             22,176 graph3d.f
06/12/02  04:57p             28,859 graph3d.obj
02/21/02  02:06p              7,493 gunits.f
06/12/02  04:57p              4,601 gunits.obj
02/21/02  02:07p                179 impl.h
02/21/02  02:06p             23,613 implicit.f
06/12/02  04:57p             24,145 implicit.obj
02/21/02  02:06p             31,117 imret.f
06/12/02  04:57p             36,183 imret.obj
05/31/02  03:04p             49,595 initgem.f
06/12/02  04:58p             73,182 initgem.obj
02/21/02  02:06p             10,142 interpf.f
06/12/02  04:58p             11,203 interpf.obj
02/21/02  02:06p              9,403 ionexc.f
06/12/02  04:58p             11,820 ionexc.obj
02/21/02  02:07p                210 iounits.h
02/21/02  02:07p                716 kinetic.h
02/21/02  02:06p             24,904 kinrxnaq.f
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```

SOFTWARE VALIDATION TEST PLAN FOR MULTIFLO VERSION 1.5.1

Prepared by

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Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

July 2002

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1.0 SCOPE OF THE VALIDATION

This software validation is for MULTIFLO V1.5.1 which comprises the METRA and GEM modules. Details of the software and its functioning can be found in the MULTIFLO User Manual. This validation covers the major capabilities of the code that are to be used in regulatory activities. These include:

(1) Nonisothermal multiphase flow and phase-change phenomena in partially saturated porous media

(2) Flow in composite fractured/porous media using a dual continuum formulation

(3) Flow in saturated porous media including compressibility effects

(4) Advective and diffusive transport of chemicals in the aqueous and gaseous phase

(5) Equilibrium speciation of aqueous and gaseous phase constituents

(6) Kinetically controlled mineral formation and dissolution, and resulting effects on porosity, permeability, and flow

(7) Unstructured grid configuration with arbitrary interblock connectivity

2.0 REFERENCES

J. Bear, Dynamics of Fluids in Porous Media, Dover Publications, New York, 1972.

P. A. Domenico and F. W. Schwartz, Physical and Chemical Hydrogeology, John Wiley, New York, 1990.

C. Doughty and K. Pruess, Journal of Geophysical Research, Vol 97, No. B2, Feb 10, 1992, pg. 1821-1838.

P.C. Lichtner, *Continuum Formulation of Multicomponent-multiphase Reactive Transport in* Reactive Transport in Porous Media, Edited by P.C Lichter, C.I. Steefel and E.H. Oelkers, Mineralogical Society of America, 1996.

S. Painter, P.C. Lichtner, and M. S. Seth, MULTIFLO User's Manual: Two-phase Nonisothermal Coupled Thermal-hydrological-chemical Flow Simulator, MULTIFLO Version 1.5, Center for Nuclear Waste Regulatory Analyses, 2001.

B. Sagar, Dispersion in three dimension: Approximate analytical solutions: American Society of Civil Engineers, Journal of Hydraulics Division, v 108, 1982.

E. Wexler, Analytical Solutions for 1-, 2-, and 3-Dimensional Solute Transport in Ground-Water Systems with Uniform Flow, USGS TWRI 3-B7, 1991.

3.0 ENVIRONMENT

Validation is to be performed on the SUN server known as Spock, which uses the Solaris 5.8 operating system. The commercial program Mathematica 4.1, running on the Windows NT (version 4) workstation Brahma, will be used for comparisons. No special peripherals are required.

4.0 PREREQUISITES, ASSUMPTIONS AND CONSTRAINTS

Requires the chemical reaction databases, which are controlled as part of the MULTIFLO system.

5.0 TEST CASES

5.1 Multiphase Simulations of Doughty and Pruess

These simulations are designed to test METRA's representation of nonisothermal flow, phase-change phenomena, and heat transport under transient conditions with and without vapor pressure lowering (major capability 1 in Section 1.0). The geometry is one-dimensional cylindrical with a line heat source in the center. These test cases correspond to Figure 6 of Doughty and Pruess (1992) and are described in more detail in Scientific Notebook 282E Vol 4 pg 9 and Scientific Notebook 282E Vol 5 pg 5.

5.1.1 *Test Input*

Test input files are on the accompanying disk: *TestCase1\Run2\novpl.dat* and *TestCase1\Run2\vpl.dat*

5.1.2 *Test Procedure*

The test procedure is as follows:

(1) Run the case without vapor pressure lowering by typing *MULTIFLO novpl.*

(2) Enter 1 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Plot results for liquid saturation at 1 year versus the dimensionless similarity variable and compare with the "no vapor pressure lowering" case from Figure 6 of Doughty and Pruess (1992).

(5) Run the case with vapor pressure lowering by typing *MULTIFLO vpl.*

(6) Enter 1 at the command prompt.

(7) Verify that the code runs to completion without error.

(8) Plot results for liquid saturation and temperature at 1 year versus the dimensionless similarity variable and compare with Figure 6 of Doughty and Pruess.

5.1.2 *Expected Results*

Calculated temperature should be within 5% of the results shown in Figure 6 of Doughty and Pruess (1992). Saturation profiles should have the same shape as those in Figure 6 of Doughty and Pruess. Exact agreement is not to be expected because of numerical discretization error. Because of minor details between the two models, localized large deviations may also occur in regions where the saturation changes rapidly.

5.2 Infiltration in Dual Permeability Media

These simulations are designed to test METRA's representation of unsaturated flow in dual permeability media (major capability 2 in Section 1.0). The geometry is one dimensional vertical with specified saturation at the top and bottom boundaries. Details of the simulation can be found in Scientific Notebook 282E Vol 1 pg 16 and Scientific Notebook 282E Vol 5 pg 8.

5.2.1 *Test Input*

Test input file is on the accompanying disk: *TestCase2\sstate1.dat*

5.2.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing *MULTIFLO sstate1.*

(2) Enter 1 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Plot steady state results for liquid saturation in fractures and matrix versus depth, and compare with Mathematica solution as calculated by the script *Richards-DKM.nb.*

5.2.3 *Expected Results*

Richards equation provides an adequate approximation to the physical situation. A dual-permeability solution to Richard's equation was implemented in Mathematica, as described in Scientific Notebook 282E Vol 1 pg 16. The Mathematica script *Richards-DKM.nb* is on the attached disk. Small discrepancies (<5%) between the Mathematica and MULTIFLO solutions are to be expected. These may be caused, for example, by numerical discretization error and neglect of the air-phase in Richards approximation.

5.3 Drawdown in Infinite Confined Aquifer

This simulation is designed to test METRA's representation of saturated flow including compressibility effects (major capability 3 in Section 1.0). The geometry is one dimensional radial with specified withdrawal from the center.

5.3.1 *Test Input*

Details of the simulation can be found in Scientific Notebook 282E Vol 4 pg 12. The test input file is on the accompanying disk: *TestCase3\theis.dat.*

5.3.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing *MULTIFLO theis.*

(2) Enter 1 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Extract results for pressure at 1.e-4 years, convert to equivalent drawdown in meters, and compare with the well-known analytical solution of Theis.

5.3.3 *Expected Results*

This configuration has a well-known analytical solution by Theis (see Domenico and Schwartz, 1990), which is implemented in the Mathematica script (*Theis.nb*) on the attached disk. Small discrepancies (<10%) between the analytical and MULTIFLO solution are to expected because of numerical discretization error.

5.4 Equilibrium Speciation in GEM

This simulation is designed to test GEM's representation of equilibrium speciation for aqueous and gaseous species at 25 °C (major capability 5 in Section 1.0). The reaction system is written in MULTIFLO form as:

$$\emptyset \Leftrightarrow oh^- + h^+ - h_2o$$

$$\emptyset \Leftrightarrow -co_2(aq) + h^+ + hco_3^- - h_2o$$

$$\emptyset \Leftrightarrow -co_3^{2-} - h^+ + hco_3^-$$

$$\emptyset \Leftrightarrow -caco_3(aq) + ca^{2+} - h^+ + hco_3^-$$

$$\emptyset \Leftrightarrow -co_2(g) + h^+ + hco_3^- - h_2o$$

In addition, the solution is set to be in equilibrium with calcite mineral. The geometry is one dimensional with two blocks. Transport is by diffusion only and the initial and boundary conditions are identical. Under these assumptions, the system is started in steady state and should remain in steady state. The initial and boundary conditions are described in Scientific Notebook 282E, Vol 3, pg 9.

5.4.1 *Test Input*

The test input file is on the accompanying disk: *TestCase4\eq3compare.inp*

5.4.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing *MULTIFLO eq3compare.*

(2) Enter 2 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Using the reported initial concentrations and activity coefficients for primary and secondary species, verify by hand calculation that the mass action equations are satisfied and that the activity coefficients as calculated by the extended Debye-Huckel representations are correct.

(5) Verify that the concentrations for primary and secondary species are identical to the initial concentrations and that the calculated concentrations for interior nodes remain unchanged.

5.4.3 *Expected Results*

Left and right sides of the mass action equation should agree. Activity coefficients should agree with hand calculations. Initial and boundary concentrations should agree. In each case, the quantities should agree to four significant digits. Exact agreement is not to be expected because of finite precision in the MULTIFLO output.

5.5 Solute Transport in Dual Permeability Media

This simulation is designed to test GEM's representation of advective/diffusive transport in dual permeability media (major capability 4 in Section 1.0). The configuration involves constant flow in one dimension with flow in both the fractures and matrix. Transport is by advection and diffusion with first order mass exchange between the fracture and matrix system. At t=0, the inlet concentration for matrix and fractures is set to 10 times the initial concentration.

5.5.1 *Test Input*

The test input file is on the accompanying disk: *TestCase5\masin1.inp*

5.5.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing MULTIFLO masin1.

(2) Enter 2 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Verify that the concentrations agree with those of the semi-analytical solutions described in Scientific Notebook 282E Vol 1, page 26.

5.5.3 *Expected Results*

Results should agree with the semi-analytical solution described in Appendix A and Scientific Notebook 282E Vol 1, page 26, which is implemented in the Mathematica notebook *FloThruDCM.nb.* Small discrepancies (<5%) are to be expected because of discretization error.

5.6 Three-Dimensional Advective/Dispersive Transport in GEM

The test case tests the transport in GEM in three dimensions (major capability 4 in Section 1.0). The velocity field is uniform and constant with flow directed in the x direction. The initial concentration is 0.0008. At t=0, the concentration on a small "patch" at the inlet was increased by a factor of ten, and the system is allowed to evolve for 1 year. A constant darcy velocity of 1 m/yr in the x direction and a diffusion coefficient of 3.15 m^2/yr is used. The system size is 40 × 11 × 11 cells, with a nonuniform spacing in each direction. More details can be found in Scientific Notebook 282E Vol 1, page 29.

5.6.1 Test Input

The test input file is on the accompanying disk: *TestCase6\masin21.inp*

5.6.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing *MULTIFLO masin21.*

(2) Enter 2 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Verify that the spatial profiles of concentration at 1 year agree with the analytical solution of Sagar (1982), which is described in Scientific Notebook 282E Vol 1, page 29.

5.6.3 *Expected Results*

Results should agree, to within 10%, with the analytical solution of Sagar (1982) as summarized in Wexler (1991). Exact agreement is not to be expected because of numerical discretization error.

5.7 Fully Coupled Flow/Transport with Mineral Dissolution and Permeability Modification

This simulation tests the coupling between METRA and GEM and kinetically controlled mineral reactions in GEM (major capability 6 in Section 1.0). The geometry is a one-dimensional "flow through" configuration with constant pressure drop across the modeled region. The system contains only quartz initially in equilibrium with $sio_2(aq)$. At t=0, the concentration at the inlet is decreased by a factor of 10. The pressure drop across the system is held constant. As the mineral dissolves, both the permeability and velocity increase as a result. Details can be found in Scientific Notebook 282E Vol 4, pg 14.

Three scenarios are considered. In the first scenario, the simulation ends before the mineral is dissolved fully at the inlet, transport is by a combination of advection and diffusion, and a power-law relationship with exponent of 2 is used to relate permeability to porosity, as described in the MULTIFLO Users Manual. The second scenario is similar to the first except that the simulation time is longer, thereby allowing full dissolution of the mineral at the inlet, and transport is by advection only. The third scenario is the same as the second, except that no permeability modification is allowed.

5.7.1 *Test Input*

The test input file is on the accompanying disk. For Scenario 1, the METRA and GEM input files are *TestCase7\multi92.inp* and *TestCase7\masin92.inp*, respectively. For Scenario 2, the input files are *TestCase7\multi81.inp* and *TestCase7\masin81.inp.* For Scenario 3, the input files are *TestCase7\multi80.inp* and *TestCase7\masin80.inp.*

5.7.2 *Test Procedure*

The test procedure is as follows:

(1) Run the first scenario by typing *MULTIFLO multi92 masin92.*

(2) Enter 3 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Verify that the spatial profile of quartz volume fraction at 30,000 years agrees with the analytical solution (Scientific Notebook 282E Vol 4, page 14).

(5) Run the second scenario by typing *MULTIFLO multi81 masin81.*

(6) Enter 3 at the command prompt.

(7) Verify that the code runs to completion without error.

(8) Verify that the spatial profile of quartz volume fraction at 40,000 years agrees with the analytical solution (Scientific Notebook 282E Vol 4, page 15).

(9) Run the third scenario by typing *MULTIFLO multi80 masin80*

(10) Enter 3 at the command prompt.

(11) Verify that the code runs to completion without error.

(12) Verify that the spatial profile of quartz volume fraction at 40,000 years agrees with the analytical solution (Scientific Notebook 282E Vol 4, page 15).

5.7.3 *Expected Results*

Results should agree with the analysis described in Appendix B and Scientific Notebook 282E Vol 4, page 14-16, and implemented in the Mathematica notebook, *FloThruCoupled.nb*, which is on the attached disk. Results should be within 5% of the analytical results for the case with no permeability modification. For the cases with permeability modification, the analytical results are approximate and exact agreement is not to be expected. For these cases, the position of the dissolution front should agree with the analytical model to within 10%.

5.8 Tests of the Unstructured Grid Capability

The test case tests the unstructured grid capability (major capability 7 in Section 1.0). The test case is the same as Test Case 3 of Section 5.3, but implemented as an unstructured grid.

5.8.1 *Test Input*

The test input file is on the accompanying disk: *TestCase8\unstruct.inp*

5.8.2 *Test Procedure*

The test procedure is as follows:

(1) Execute MULTIFLO by typing *MULTIFLO unstruct.*

(2) Enter 1 at the command prompt.

(3) Verify that the code runs to completion without error.

(4) Verify that the drawdown agrees with that Test Case 3.

5.8.3 *Expected Results*

Results should be within 5% of the results of Test Case 3.

APPENDIX A: SEMI-ANALYTICAL SOLUTION FOR TEST CASE 5

The configuration involves constant flow in the z direction with flow in both the fractures and matrix. Transport is by advection and diffusion, with first order mass exchange between the fracture and matrix system. The inlet concentration for matrix and fractures is set to 10 times the initial concentration at t=0.

A semi-analytical approach was developed and implemented in Mathematica. The mass balance equations in one-dimension are,

$$\frac{\partial}{\partial t}[\varphi SC] = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - \alpha[C - C_F]$$

$$\frac{\partial}{\partial t}[\varepsilon_F \varphi_F S_F C_F] = D_F\frac{\partial^2 C_F}{\partial x^2} - V_F \varepsilon_F \frac{\partial C_F}{\partial x} + \alpha[C - C_F]$$

where φ is the porosity, S the saturation, C the concentration, D the diffusion coefficient, and V the velocity. The subscript F denotes the fracture system. The symbol ε refers to the fracture volume fraction. The ε multiplying the fracture velocity comes from the way block areas are calculated in GEM. The diffusion coefficient for the fracture system is $D_F = \varphi_F S_F \varepsilon_F D_0$ where the tortuosity has been set to 1. The diffusion coefficient for the matrix is the same except that it is missing the ε factor.

The diffusional coupling term is $\alpha \approx \frac{\varphi SD2A}{d}$ where A is the fracture/matrix interfacial area per unit volume, and d is the matrix block size (presumed constant). This expression neglects the fracture aperture relative to the grid block size. For constant properties, this system becomes,

$$\frac{\partial C}{\partial t} = D_0\frac{\partial^2 C}{\partial x^2} - \frac{V}{\varphi S}\frac{\partial C}{\partial x} - \alpha_1[C - C_F]$$

$$\frac{\partial C_F}{\partial t} = D_0\frac{\partial^2 C_F}{\partial x^2} - \frac{V_F}{\varphi_F S_F}\frac{\partial C_F}{\partial x} + \alpha_2[C - C_F]$$

$$\alpha_1 = \frac{2DA}{d}$$

$$\alpha_2 = \frac{2DA}{d}\frac{\varphi S}{\varphi_F S_F \varepsilon_F}$$

Taking the Laplace transform of the above, and applying the initial condition $C(0)=C_F(0)=0.$,

$$s\hat{C} = D\frac{\partial^2 \hat{C}}{\partial x^2} - V^* \frac{\partial \hat{C}}{\partial x} - \alpha_1\left[\hat{C} - \hat{C}_F\right]$$

$$s\hat{C}_F = D\frac{\partial^2 \hat{C}_F}{\partial x^2} - V_F^* \frac{\partial \hat{C}}{\partial x} + \alpha_2\left[\hat{C} - \hat{C}_F\right]$$

with initial conditions $\hat{C}(0) = C_0/s$ and $\hat{C}_F(0) = C_{F0}/s$ and bounded at positive infinity. This system has the solution,

$$\vec{\xi}(x;s) = c_1\mathbf{v}_1 \exp\left[\lambda_1 x\right] + c_2\mathbf{v}_2 \exp\left[\lambda_2 x\right]$$

where $\vec{\xi}(x;s) = \left(C, \frac{\partial C}{\partial x}, C_F, \frac{\partial C_F}{\partial x}\right)^T$, λ_1 and λ_1 are the negative eigenvalues, and $\mathbf{v}_1$ and $\mathbf{v}_2$ the corresponding eigenvectors of the matrix

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ \frac{s+\alpha_1}{D} & \frac{V}{D} & \frac{-\alpha_1}{D} & 0 \\ 0 & 0 & 0 & 1 \\ \frac{-\alpha_2}{D} & \frac{V_F}{D} & \frac{s+\alpha_2}{D} & 0 \end{bmatrix}$$

c_1 and c_2 are constants calculated so that the boundary conditions at x=0 are met. The calculation of the eigenvalues and eigenvectors is done using a Mathematica script *FloThruDCM.nb*. Once the solution is constructed this way in the Laplace domain, a numerical inverse Laplace transform is performed to obtain the solution in the time domain.

APPENDIX B: ANALYTICAL SOLUTION FOR TEST CASE 7

Consider a one-dimensional system with SiO_2(aq) initially in equilibrium with quartz. At t=0, the concentration at the inlet is decreased by a factor of 10. The pressure drop across the system is held constant. As the mineral dissolves, the permeability and velocity increase as a result. Considered two situations where it is possible to get an approximate solution: in Scenario 1, the mineral is not allowed to fully disappear at the inlet, while in Scenario 2, the problem is advection dominated. In both situations, the quasi-stationary state approximation of Lichtner (1996) was used. Specifically, the characteristic time for mineral dissolution was much larger than the time required for the aqueous concentration to reach equilibrium. Thus the aqueous concentration is assumed to be stationary, or more precisely, to be described by a sequence of quasi-stationary states.

The aqueous concentration $C(x,t)$ is governed by the following equation

$$\frac{\partial}{\partial t}\phi C + v\frac{\partial C}{\partial x} - \phi D\frac{\partial^2 C}{\partial x^2} = -k's\left(C - C_{eq}\right)H\left(x - \ell(t)\right)$$

where ϕ is the porosity, v is the darcy velocity, C_{eq} is the equilibrium concentration, D is the diffusion coefficient, s is the specific surface area, and $k' = k / C_{eq}$, where k is the reaction rate. $H(\cdot)$ is the Heaviside function. Quartz is dissolving and will eventually dissolve fully; $\ell(t)$ is the width of the fully dissolved region.

The mineral volume fraction is given by

$$\frac{\partial \phi_s}{\partial t} = \overline{V_s}k's\left(C - C_{eq}\right)H\left(x - \ell(t)\right)$$

where $\overline{V_s}$ is the molar volume for the mineral. The initial and boundary conditions are:

$$C(x, t = 0) = C_{eq}$$
$$C(x = 0, t) = C_0$$
$$\phi_s\left(x, t = 0\right) = \phi_s^0$$

B.1 Mineral Not Fully Dissolved at Inlet

If the mineral has not fully dissolved at the inlet, $\ell(t) = 0$, the concentration is stationary, and we can neglect the time derivative in the above equation for aqueous concentration. The time required for the mineral to dissolve at the inlet is $\tau_s = \dfrac{\phi_S^0}{k's\Delta C\overline{V_S}}$. The equation has solution

$$C(x,t)-C_{eq}=(C_0-C_{eq})\exp\left[-x\frac{v}{2\phi D}\left(\sqrt{1+\frac{4k's\phi D}{v^2}}-1\right)\right]$$

if advection dominates, this is approximately

$$C(x,t)-C_{eq}=(C_0-C_{eq})\exp\left[-\frac{k's}{v}x\right].$$

These solutions are found on page 631 of Bear (1972). Note, that Bear's λ is $\frac{k's}{v}$. The mineral volume fraction has solution

$$\phi_S^0(x,t)=\phi_S^0\ [1-\exp(-qx)t/\tau_S]$$

where

$$q=\frac{v}{2\phi D}\left[\sqrt{1+\frac{4k's\phi D}{v^2}}-1\right].$$

If no permeability modification is allowed, the velocity is fixed in the above equation.

If permeability modification is allowed, the velocity will change. The effect of this velocity change can be accounted for in an approximate way by replacing the velocity v with a time averaged velocity $\bar{v}$, which is calculated as follows. At time *t* we have from the condition of fixed pressure gradient in one dimension,

$$\frac{v_0}{v}-\frac{1}{L}\int_0^L\left(\frac{\kappa_0}{\kappa}\right)dx=0$$

where the latter term on the left is the ratio of initial permeability κ_0 to effective permeability at time *t*. The permeability change is calculated from the porosity change according to a power-law (other relationships are possible but are not considered here):

$$\frac{\kappa_0}{\kappa}=\left(\frac{\phi_0}{\phi}\right)^m=\left[\frac{\phi_R-\phi_S^0}{\phi_R-\phi_S^0-\exp(-qx)t/\tau_S}\right]^m$$

where ϕ_R is the reactive volume fraction. The velocity appearing in q here is not $v(t)$ but the time-averaged velocity. This can be approximated as $\bar{v}=(v_0+v)/2$, which implies $v=2\bar{v}-v_0$.

Substituting $v = 2\bar{v} - v_0$ and for $\left(\frac{\kappa_0}{\kappa}\right)$ in the integrand, and then calculating the integral explicitly yields the following equation:

$$\frac{v_0}{2\bar{v} - v_0} + \frac{b + (b + a\exp(Lq))\log(b + a\exp(Lq))}{(b + a\exp(Lq))q} - \frac{b + (b + a)\log(b + a)}{(b + a)q} = 0$$

Here, the effective (time averaged) velocity is to be used in the expression for *q*, not *v(t)*. This equation is then to be solve for $\bar{v}$. This result is specific to the situation $m = 2$. Note $a = \phi_R - \phi_S^0$ and $b = t\overline{V_S}k's\Delta C$.

Once the time-averaged velocity is obtained, it is used in place of V in the expression for the mineral volume fraction.

B.2 Advection Dominated Case

The preceding analysis applies when the mineral has not completely disappeared at the inlet. This analysis is difficult to extend to the more general situation of a moving boundary in the general case, but can be extended if we restrict our consideration to the advection dominated case. The solution in this situation is given, for example, on page 51 of Lichtner (1996)

$$C(x,t) - C_{eq} = (C_0 - C_{eq})\exp\left[-\frac{k's}{v}(x - \ell(t))\right].$$

where

$$\ell(t) = \frac{\overline{V_S}v\Delta C}{\phi_S^0}(t - \tau_S)$$

Similarly, the mineral volume fraction is given by:

$$\phi_S(x,t) = \phi_S^0\left(1 - \exp\left[-\frac{k's}{v}(x - l(t))\right]\right).$$

Continuing as before, the following equation is obtained;

$$\frac{v_0}{2\bar{v} - v_0} - \frac{b + (b + a\exp(L'q))\log(b + a\exp(L'q))}{(b + a\exp(L'q))q} + \frac{b + (b + a)\log(b + a)}{(b + a)q} - \left(\frac{\phi_0}{\phi_R}\right)^m \ell(t) = 0$$

where $q(\bar{v}) = \frac{k's}{\bar{v}}$, $b = \overline{V_s} k's\Delta C$, $L' = L - \ell(t)$, and the time average velocity is to be used in place of v in $\ell(t)$. This equation is to be solved for the time averaged velocity, which replaces the velocity in the equation for the mineral volume fraction.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): **SCR-406**	2. Software Title and Version: **Multiflo V1.5.1**	3. Project No: **20.01402.562**

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

The following are changes needed for Version 1.5.1.

(1) When executing GEM in standalone mode, the matrix porosity and saturation are not retrieved properly from the input file. Change the input format to retrieve these from the ISYS keyword instead of the DCMP keyword.

(2) The fracture-to-matrix relative permeability function, which is nominated on the DCMP keyword, is not activated. Make change to the util.f file to correct.

(3) Time dependent boundary conditions not set properly in METRA.

(4) In GEM, water content (porosity*saturation) is not set properly at boundary. Change bndcond.f file to correct.

(5) In coupled mode, boundary temperatures are not set properly in GEM. Required change to setbcon.f file.

5. Change Requested by: **Scott Painter** Date: **August 13, 2002**	6. Change Authorized by (*Software Developer*): **Scott Painter** Date: **August 13, 2002**

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

All problems corrected. Required change to metra/util.f, metra/setbc.f, metra/bcond., gem/util.f, gem/bndcond.f , gem/setbcon.f, and gem.f. Corrected code will be released as V1.5.2.

8. Implemented by: **Scott Painter**	Date: **November 1, 2002**

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: **November 4, 2002**