SOFTWARE RELEASE NOTICE

GHGC-
01. SRN Number: SRN-283

02. Project Title: Evolution of Near-field Environment :	Project No.: 20.06002.01.072
03. SRN Title: MULTIFLO V1.5.2	
04. Originator/Requestor: Scott Painter	Date:11/12//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	
L Browning	RO	
R. Green	RO	
G. Ofoegbu	RO	
R. Pabalan	RO	
C. Manepally	RO	
M. Seth	RW	

07. Element Manager Approval: S. C. Date: 11/12/2002

08. Remarks:

CNWRA Form TOP-6 (06/95)

SOFTWARE SUMMARY FORM

01. Summary Date: 11/12/2002	02. Summary prepared by (Name and phone) **Scott Painter, 522-3348**	03. Summary Action: **New**
04. Software Date: 11/12//2002	05. Short Title: **MULTIFLO Version 1.5.2**	
06. Software Title: **MULTIFLO Version 1.5.2**		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: 11-12-02

CNWRA Form TOP-4-1

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

Software Title/Name: MULTIFLO Version 1.5.2
Version: 1.5.2
Demonstration workstation: BRAHMA (Room A209, Bldg. 189)
Operating System: UNIX
Developer: S. PAINTER

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

SRD Version: 2.0
SRD Approval Date: 1/12/1999

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: CNWRA SCR-406 utilized.

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

SDP Version: January 2001
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:

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: bwdcond.f

Comments: Includes disclaimer notice, including interfacing arguments & interfacing routines.

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

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: bndcond.f

Comments: Comment lines verified

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: 282E-SCR-406

Comments: Acceptance Tests will be in a CD provided to QA.

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 Nov 4 16:10:46 2002

Name/Version Displayed: MULTIFLO Version 1.5.2 November 2002

Comments:

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 file mainmulti.f

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

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:

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QA 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

Comments: M. Seth's work is reviewed by P.I. S. Painter. Not formally required in SDP.

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?

S. Painter did acceptance Testing on Two computers.

Yes: ☒ No: ☐ N/A: ☐

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

Yes: ☒ No: ☐ N/A: ☐

Computer Platforms: Brahma & Idaho Operating Systems: Solaris & Unix Windows NT

Location of Acceptance Test Results: On a CD in This folder.

Comments:

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

Yes: ☒ No: ☐ N/A: ☐

Computer Platforms: Brahma & Idaho Operating Systems: Solaris & Windows NT

Location of Acceptance Test Results: On a CD in This folder

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: MULTIFLO User Manual 1.5 Dec 2001 Rev 3

Comments: The User's manual will be updated later according to P.I.

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

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

Yes: ☒ No: ☐ N/A: ☐

Location of Instructions: On The CD with the code in a Readme.file - also in User's manual.

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: 11/12/2002

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

Yes: ☒ No: ☐ N/A: ☐

Comments: Copied MULTIFIO 1.5.1 files as they did not change

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

Yes: ☒ No: ☐ N/A: ☐

Location of Source Code: In This folder in the QA Records Room

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: In This folder in the QA Records Room

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: 283

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
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: July 2002 The SVTP for MULTIFLO 1.5.1 will be updated for 1.5.2.

Date Reviewed and Approved via QAP-002: 7/26/2002

Comments: SEE NOTES ABOVE. Working Password MULTIFLO 1.5.2 Validation — To ~~1.5.2~~ 1.6.1. 11/12/02

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:

Additional Comments:

11-12-02 11/12/2002

Software Developer/Date Software Custodian/Date

```
c*file bndcond.f

c Program Name:          MULTIFLO/GEM
c File/Subroutine Name: bndcond.f

c Release Date:          November 2002
c Release Version:       1.5.2
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
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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
c SCR-351   2002     Mohan S Seth           revised to treat individual
c                                           grid blocks for coupled runs
c
c November 2002       Scott Painter          SCR406 Item 4
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

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.

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c  PURPOSE:
```

```
c  This routine imposes boundary conditions for implicit method,
however,
c  it designed such that it can also be used for op. split and explicit
c  and other methods.

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c  INTERFACING ARGUMENTS:

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

c   nc          Integer                 -number of primary species
c   ppsigl      Array(nc,nb), Real*8    -total concentration in aqueous or
c                                          gaseous phase
c   dpsi        Array(nc,nc,*), Real*8 -partial derivatives of ppsi
c   psiglbnd    Array(nc,6), Real*8     -boundary condition array
c-----------------------------------------------------------------------
c   Externals
c   =========

c   none

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c   INTERFACING ROUTINES

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

c      cehyliq.f
c      cehytwph.f
c      cetvdliq.f
c      cetvdtwp.f
c      cgasos.f
c      cihytwph.f
c      cliqos.f
c      coshyliq.f

c      Called routines       Function
c     ================       =========

c      none

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c   INCLUDE FILES

c      Name                              Description
c      ====                              ============

c      impl.h        -Declares real variables to real*8 and sets
c                       frequently used constants in common.
c      metragem.h    -Variables which are common to both metra and gem
c                       codes.
c      paramtrs.h    -Sets dimension limits for all variables.
c      scalgem.h     -Scalars in common.
c      comgem.h      -Gem-related common blocks.
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c   SYSTEM LIBRARY ROUTINES
```

```
c      Name                                Description
c      ====                                ===========

c      none

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c    OUTPUT UNIT(s)

c    Unit Name(Number)                Description           file name

c      none

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c    REFERENCES

c    none

ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

       subroutine bndcond (nc,ncsq,ncx,ppsi,ppsig,dpsi,dpsig,dpril,
      .           dsecl,cc,cx,cdl,r,vl,vg,ssat,j1c,j2c,ncc,mm2)

       include 'impl.h'
       include 'paramtrs.h'
       include 'metragem.h'
       include 'scalgem.h'
       include 'comgem.h'
       include 'debye.h'
       include 'fields.h'
       include 'iounits.h'

       dimension ppsi(nc,*), ppsig(nc,*), dpsi(ncsq,*), dpsig(ncsq,*),
      .          dpril(ncc,*), dsecl(ncx,*), cc(nc,*), cx(ncx,*),
      .          cdl(ncsq,*), r(nc,*), vl(*), vg(*), ssat(*)

       dimension qk(ncmx),dq2(ncmx*ncmx),psiz(ncmx),dpsiz2(ncmx*ncmx)
cms    .         ,dq0(ncmx*ncmx)

       save cvfac1, theta

       data cvfac1/.018016d0/        ! mw of h20 * 1.e-3
       data theta/0.9d0/

c=====================================================================
c      nc = no of componets for all species
c=====================================================================

       if(mm2.eq.0) then
         nblc1 = 1
         nblc2 =  nblkbc
       else
         nblc1 =  mm2
         nblc2 =  mm2
       endif

c      print *,'iregn ',(iregngem(mm),mm=nblc1,nblc2)

       do 500 mm = nblc1, nblc2
```

```
          ibc = iregngem(mm)
          ibctype = ibndtyp(ibc)

          if(ibctype.ne.1 .and. ibctype.ne.3) go to 500

          m2 = iblkbc(mm)
          if(method.eq.1.or.method.eq.3) then
            im2 = m2
          else
            im2 = 1
          endif

          dist = distbc(ibc)
          area = areabc(mm)

          ql = vl(mm)*area

c         write (*,11) mm,m2,dist,area,vl(mm)
 11       format(1x,'mm nc dist area vl ',2i4,3e10.3)

          if(ibctype.eq.3) then
            do j = j1c, j2c
              qk(j) = zero
            end do

            do jj = 1, ncsq
              dq2(jj) = zero
            end do
            go to 100
          endif

cSCR-351: changed subscript ibc to mm on porlsbc and sgbc

          if(icode.ge.3) porslbc(mm) = por(m2)*(one-sgbc(mm))

          if(idif.eq.0) then
c-------------------------------------------------------------------------
c                                       species-independent diffusion coefs

            td2 = ssat(m2)*por(m2)*dpril(1,m2)
c SCR406 item 4  SP 10.24.02
            if(icode.eq.2) then
             td1 = porslbc(ibc)*dpril(1,m2)
            else
             td1 = porslbc(mm)*dpril(1,m2)

            endif

cSCR-351: changed subscript ibc to mm on porlsbc in above line

c           write (iunit2,'("td1 td2 porsl ssat por dpril ",6e10.3)')
c    .      td1,td2,porslbc(mm),ssat(m2),por(m2),dpril(1,m2)

            if(ihrmc.eq.1) then             ! harmonic
              if(td1+td2.ne.zero) then
                td = two*td1*td2/(td1+td2)
              else
                td = zero
              endif
            else
```

```
            td = half*(td1+td2)           ! arithmetic
          end if

          trdif = td*area/dist

c         write(iunit2,*) 'bndcond2: ',td,td1,td2,area,dist

          if(abs(ql).ge.theta*two*trdif .and. ifor.eq.0) then ! hybrid

            do j = j1c,j2c
              qk(j) = zero
            end do

            do jj = 1,ncsq
              dq2(jj) = zero
            end do
            go to 100
          endif

          trdif = -trdif

          do j = j1c,j2c

            qk(j) = trdif*(ppsi(j,m2)-psibnd(j,ibc))

c           write(iunit2,*) 'bndcond0: ',mm,trdif,delt,
c    .      ppsi(j,m2),psibnd(j,ibc),qk(j)

          end do

          do jj = 1,ncsq
            dq2(jj) = trdif*dpsi(jj,im2)
          end do

        else
c-------------------------------------------------------------------------
c                                        species-dependent diffusion coefs

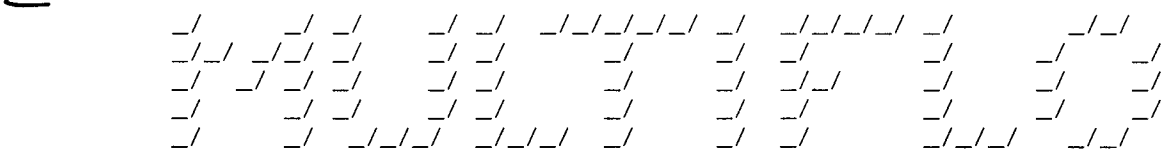
cSCR-351: changed subscript ibc to mm on porlsbc in below
c SCR406 item 4  SP 10.24.02
          if(icode.eq.2) then
           td1 = porslbc(ibc)
          else
           td1 = porslbc(mm)
          end if
          td2 = ssat(m2)*por(m2)

          if(ihrmc.eq.1) then
            trdif = two*td1*td2/(td1+td2)
            trdif = trdif/dist
          else
            trdif = half*(td1+td2)/dist  ! arithmatic avg
          endif

          difmx = zero
          do j = 1,nc
            dif = dpril(j,m2)
            difmx = max (difmx,dif)
          end do

          trdx = difmx*trdif*area
```

This file was created on: Mon Nov 4 16:10:46 2002



Developed for the U.S. NRC

VERSION 1.5.2

November 2002

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:
/net/spock/home/spainter/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.
Courant Number.....COURNR =	5.0000E+05
DELT Reduction Factor.....DTCUTF =	5.000E-01

```
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:          November 2002
c Release Version:       1.5.2
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
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

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  November 2002       Scott Painter          SCR406
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c DISCLAIMER/NOTICE
```

MULTIFLO, 1.5.1 LIST OF FILES, June 21, 2002

V 1.5.2 Lists of files has not changed

Scott Burns
11-12-2002

```
 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
```

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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
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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
```

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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
06/12/02  04:58p            27,720 kinrxnaq.obj
02/21/02  02:06p            16,176 kinrxns.f
06/12/02  04:58p            16,105 kinrxns.obj
02/21/02  02:06p            10,078 linmonod.f
06/12/02  04:58p            13,339 linmonod.obj
02/21/02  02:06p            12,284 luslv.f
06/12/02  04:58p             4,191 luslv.obj
02/21/02  02:06p            24,354 maingem.f
02/21/02  05:23p            30,011 Makefile
02/21/02  02:06p             9,262 massbal.f
06/12/02  04:58p             7,989 massbal.obj
02/21/02  02:06p            14,286 masstran.f
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SOFTWARE VALIDATION REPORT FOR MULTIFLO VERSION 1.5.2

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–02–012

Prepared by

Scott Painter

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

February 2003

ABSTRACT

MULTIFLO is a computer code for modeling coupled thermal-hydrological-chemical processes in partially saturated and strongly heated porous and fractured media. This software may be used in reviewing the license application for the high-level waste repository proposed for Yucca Mountain, Nevada. Eight software validation tests were conducted. These tests cover the expected range of processes and conditions that may need to be reviewed. For all test cases, MULTIFLO Version 1.5.2 successfully reproduced the target results, which were based on analytical, semi-analytical, or previously published solutions to the underlying mathematical models. The successful validation tests suggest that the MULTIFLO Version 1.5.2 software is functioning properly.

CONTENTS

CONTENTS (continued)

FIGURES

TABLES

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–97–009 and NRC–02–02–012. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

The author is grateful to C. Dinwiddie and B. Sagar for their reviews of the manuscript, and to P. Houston for formatting.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No data were generated for this report.

ANALYSES AND CODES: This report documents quality assurance software validation activities for MULTIFLO Version 1.5.2. MULTIFLO was developed under software quality assurance procedure TOP–018. Calculations are documented in Scientific Notebook 282E.

1 INTRODUCTION

This Software Validation Report documents software validation results for the computer code MULTIFLO (Lichtner, 1996; Painter, et al, 2001), a numerical model describing two-phase nonisothermal flow and multicomponent reactive transport in variably saturated porous media. This software may be used in reviewing the license application for the high-level waste repository proposed for Yucca Mountain, Nevada.

The code can be used to analyze the drift scale and repository scale coupled thermal-hydrologic-chemical processes that could affect the performance of the proposed repository. The code can be applied to assess processes such as

- Isothermal and nonisothermal movement of water through unsaturated rock as liquid and vapor
- The evolution of groundwater compositions near and within the engineered barrier system
- Changes in porosity and permeability of the host rock resulting from mineral alteration and the resulting effects on fluid transport
- Transport of aqueous and gaseous radionuclides from the waste package

The software validation tests described in this report are required by the Quality Assurance Procedure TOP–018 and follow the procedure specified in the Software Validation Test Plan for MULTIFLO Version 1.5.1 (Painter, 2002). The validation deviates slightly from that specified in the Software Validation Test Plan in two aspects. First, MULTIFLO Version 1.5.2 is validated instead of the earlier Version 1.5.1 that was specified in the Software Validation Test Plan. Second, some of the input files specified in the Software Validation Test Plan were modified slightly to accommodate different input requirements for the new Version1.5.2 or to correct errors in the input file. Input and output files for the validation are on the accompanying disk.

2 SCOPE OF THE VALIDATION

This software validation is for MULTIFLO Version 1.5.2 which supersedes Version 1.5.1. The MULTIFLO software comprises the METRA and GEM components, which can be used separately or in combination. Details of the software and its functioning can be found in the MULTIFLO User's Manual and in supporting technical material (Lichtner, 1996). 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

3 ENVIRONMENT

Validation tests were performed on the workstation farm directed by the computer known as Idaho, which uses the Solaris 5.8 operating system. The commercial program Mathematica® 4.1, running on the Windows NT (version 4) workstation Brahma, was used for some calculations to establish target solutions to the underlying mathematical equations. No special peripherals were used.

4 TEST CASES

4.1 Test 1: Multiphase Simulations of Doughty and Pruess

4.1.1 Description of the Test

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 2.0). The geometry is one-dimensional cylindrical with a line heat source in the center and correspond to Figure 6 of Doughty and Pruess (1992). They employ a Boltzmann transformation to reduce the partial differential equation to an ordinary differential equation boundary value problem. They then solve the boundary value problem by the shooting method. Two test cases are considered: one with and one without vapor pressure reduction due to capillary effects. Input parameters for the test are presented in Table 1. A grid of 400 computational cells was used for these two tests.

4.1.2 Test Input and Output

Test input files are on the accompanying disk: *TestCase1\novpl.dat* and *TestCase1\vpl.dat*. Output files are in the same directory.

4.1.3 Target Solution

The target solutions for the two simulations can be found in Figure 6 of Doughty and Pruess (1992). They employ the Boltzmann transformation approach, and rescale the radial variable according to the Boltzmann transformation, $z = \mathrm{Ln}\left[r / \sqrt{t}\right]$, with radius r in meters and time t in seconds. The solution then becomes a function of z only, independent of r and t.

4.1.4 Results

The case with no vapor-pressure lowering ran to completion without error. The case with vapor-pressure lowering ran to completion without error after it was modified to terminate at

Table 1. Parameters for Test 1.	
Parameter	**Value**
Heat source	667 W/m (0.237 Horsepower/feet)
Initial gas pressure	1 bar
Initial temperature	18 °C (64.4 °F)
Initial liquid saturation	0.8
Absolute permeability	20×10^{-15} m^2 (2.15×10^{-13} ft^2)
Porosity	0.10
Rock density	2550 kg/m^3 (159.2 lbm/ft^3)
Specific heat	800 J/kg K (0.191 BTU/lbm °F)
Thermal conductivity	2 W/m K (4.54×10^{-4} Horsepower/ft °F)
Tortuosity parameter	0.5
Diffusion coefficient	2.6×10^{-5} m^2/s (2.80×10^{-4} ft^2/s)
van Genuchten α parameter	8.0×10^{-5} Pa^{-1} (8 bar^{-1})
van Genuchten λ parameter	0.45
Residual saturation	9.6×10^{-4}
Capillary pressure cutoff	5.0×10^{8} Pa^{-1} (5×10^{3} bar^{-1})

0.1 year. For longer simulation times, excessively large vapor-pressure reduction factors caused numerical instabilities in the case with vapor-pressure lowering. These instabilities were observed when temperatures exceeded 260 °C [500 °F]. This code is not expected to be used for temperatures of this magnitude during the regulatory reviews.

A comparison between the METRA solution and the Doughty and Pruess (1992) results for liquid saturation is shown in Figure 1 for the case without vapor pressure lowering. The data points are from Doughty and Pruess (1992, Figure 6) and the curves are METRA results at t = 0.1, t = 1, and t = 6 years. The METRA curves were invariant with time, as predicted by the similarity solution, and overlay each other on this scale over most of the range. The agreement with the Doughty and Pruess results is good over the entire range. The small differences in the location of the hot edge of the boiling zone (relative difference of about 2 percent) is believed to be due to numerical discretization errors in the METRA solution.

Saturation profiles for the case with vapor pressure lowering are compared in Figure 2. The data points are the Doughty and Pruess result (Doughty and Pruess, 1992, Figure 6) and the curve is the METRA result at 0.1 year. The relative difference in the location of the dry-out zone, defined here by be the position where saturation is 20 percent, is 21 percent. The agreement is good, but not exact. Exact agreement is not to be expected because of numerical discretization error and because of minor differences in the physics models.

Temperature profiles for the case with vapor pressure lowering are compared in Figure 3. The data points are the Doughty and Pruess result (Doughty and Pruess, 1992, Figure 6) and the

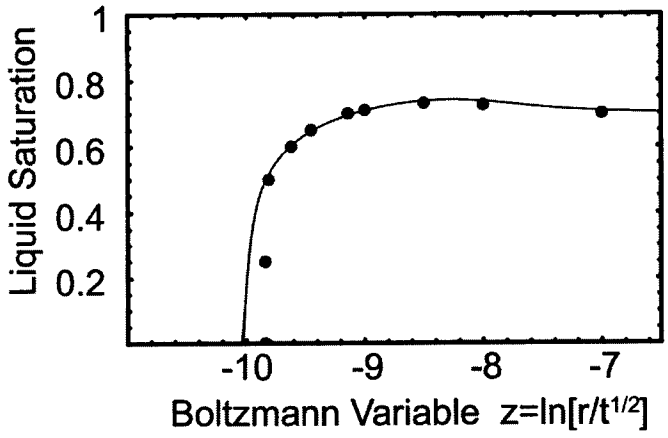

Figure 1: Liquid Saturation Versus Boltzmann Variable for Test 1 Without Vapor Pressure Lowering. The MULTIFLO Simulation Is Plotted as a Solid Line and the Results of Doughty and Pruess [1992] Are Shown as Individual Data Points. The Boltzmann Variable is $\mathrm{Ln}\left[r / \sqrt{t}\right]$ Where r Is Radius in Meters and t Is Time in Seconds.

[Unit Conversion: Multiply by 1.19 to Obtain the Boltzmann Variable with Radius in Feet.]

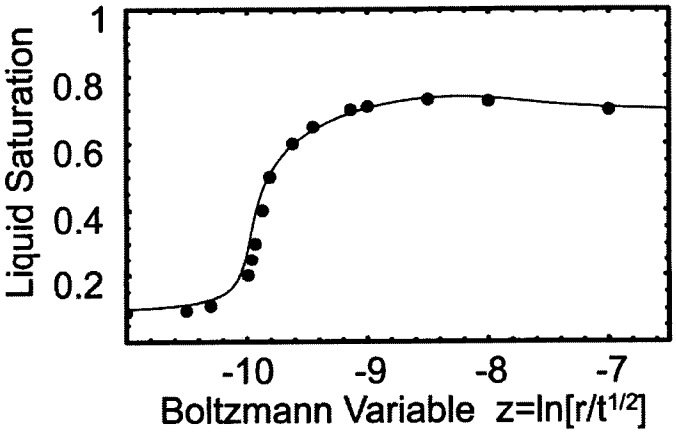

Figure 2: Liquid Saturation Versus Boltzmann Variable for Test 1 with Vapor Pressure Lowering. The MULTIFLO Simulation Is Plotted as a Solid Line and the Results of Doughty and Pruess [1992] Are Shown as Individual Data Points. The Boltzmann Variable is $\mathrm{Ln}\left[r / \sqrt{t}\right]$ Where r Is Radius in Meters and t Is Time in Seconds.

[Unit Conversion: Multiply by 1.19 to Obtain the Boltzmann Variable with Radius in Feet.]

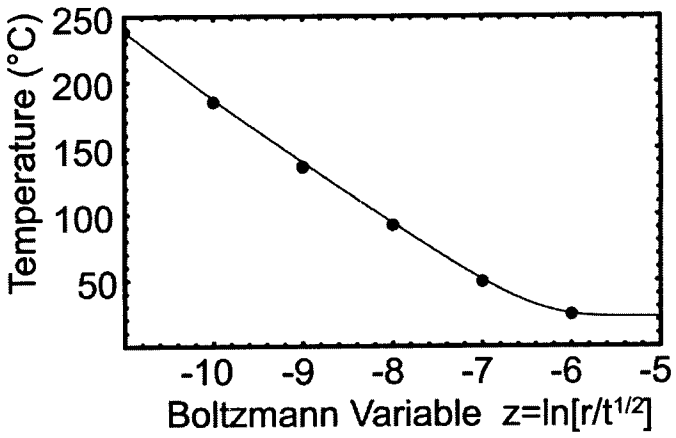

Figure 3: Temperature Versus Boltzmann Variable for Test 1 with Vapor Pressure Lowering. The MULTIFLO Simulation Is Plotted as a Solid Line and the Results of Doughty and Pruess (1992) Are Shown as Individual Data Points. The Boltzmann Variable Is $\mathrm{Ln}\left[r / \sqrt{t}\right]$ Where r Is Radius in Meters and t Is Time in Seconds. Unit Conversion: Multiply by 1.19 to Obtain the Boltzmann Variable with Radius in Feet. [Unit Conversion: Multiply by 9/5 and 32 to Obtain Temperature in Fahrenheit.]

curve is the METRA result at 0.1 year. The agreement is excellent (<3.5 percent difference) over the entire range of the Boltzmann variable.

4.2 Test 2: Infiltration in Dual Permeability Media

4.2.1 Description of the Test

This simulation is designed to test METRA's representation of unsaturated flow in dual permeability media (major capability 2 in Section 2.0). The geometry is one-dimensional vertical with specified saturation at the top and bottom boundaries. The domain size is 10 m [37.8 ft] and is discretized into 100 cells of size 0.1 m (0.328 ft). The saturation at the lower boundary is specified as 100 per cent liquid for both fractures and matrix. The saturation at the top boundary is specified as 20 percent for the matrix and 60 percent for the fractures. van Genuchten's model is used to relate capillary pressure to saturation. The simulation is run until steady state is reached. The main parameters are given in Table 2.

4.2.2 Test Input and Output

Test input file is on the accompanying disk: *TestCase2\sstate1.dat*. Output files are in the same directory.

Table 2. Parameters for Test 2	
Parameter	**Value**
Matrix permeability	4×10^{-14} m^2 ($4.30\ 10^{-13}$ ft^2)
Matrix porosity	0.20
Fracture permeability (intrinsic)	4×10^{-13} m^2 ($4.30\ 10^{-12}$ ft^2)
Fracture porosity	0.001
van Genuchten α parameter for matrix	1.99×10^{-3} Pa^{-1} (199 bar^{-1})
van Genuchten λ parameter for matrix	0.851
van Genuchten α parameter for fracture	1.99×10^{-3} Pa^{-1} (199 bar^{-1})
van Genuchten λ parameter for fracture	0.851
Matrix block size	0.1 m (0.328 ft)
Fracture-to-matrix area reduction factor	10^{-6}

4.2.3 Target Solution

The Richards equation provides an approximation to the physical situation. After setting gas pressure to atmospheric, the mass conservation equations for a single continuum reduce to Richards equation. In steady state and with one spatial dimension the dual permeability Richards equation can be written:

$$q_F = -K_F k_{rF}\left(\frac{\partial h_F}{\partial z} - 1\right)$$

$$\frac{\partial q_F}{\partial z} + S_{FM} = 0$$

$$q_M = -K_M k_{rM}\left(\frac{\partial h_M}{\partial z} - 1\right)$$

$$\frac{\partial q_M}{\partial z} - S_{FM} = 0$$

$$S_{FM} = A_{FM}\ \eta\ K_{Fm}\ k_{rfm}\ \frac{h_F - h_M}{d}$$

where z is depth, K is the saturated hydraulic conductivity, k_r is the relative permeability, h is the water pressure head in meters, and q is the volumetric flux. These are combined with two constitutive relations: one to relate capillary pressure with saturation and the second to relate k_r with saturation. The van Genuchten model is used here. The subscript *F (M)* denotes fracture (matrix) properties. The term S_{FM} describes the flow between fractures and matrix, where A is

the fracture/matrix interfacial area, h is a modifying factor [0,1], and k_{fm} is the conductivity for transfer between matrix and fracture system. In METRA, the relative permeability for fracture-matrix transfer is defined as the upstream value. If flow is from matrix to fracture, the matrix value is used. If flow is in the other direction, the fracture values are used. K_{fm} is taken as the harmonic average of the fracture and matrix after appropriately weighting by the two distances (fracture aperture, and average matrix block size). In practice, this is essentially the same as using the matrix permeability for K_{fm} and one-half the matrix block size for d. This approximation is used in constructing the target solution (but not in METRA).

The author is unaware of analytical solutions to Richards equation in dual-permeability media with van Genuchten's model for capillary pressure. The target solution was constructed numerically using the Mathematica software system. The numerical approach used a shooting method. Specifically, flux and pressure head were specified at the bottom boundary and the in-built solver for initial value ordinary differential equations **NDSolve** was used to solve for pressure head (and thus saturation) in the one-dimensional column. This **NDSolve** calculation was called iteratively within the Mathematica **FindRoot** function so as to adjust the specified flux to cause the liquid saturation to agree with the specified value at the upper boundary, thus solving the boundary value problem. The Mathematica script used to construct the target solution is in the Mathematica Notebook Test2.nb on the attached disk.

4.2.4 Results

The simulation executed to completion without error. Steady-state saturations are shown in Figure 4. The target solution is plotted as solid curves, and the METRA results are shown as individual data points. The agreement between the two is very good for both matrix and fracture systems. The maximum error is 0.5 percent for the matrix and 1.4 percent for the fractures.

4.3 Test 3: Drawdown in an Infinite Confined Aquifer

4.3.1 Description of the Test

This simulation is designed to test METRA's representation of saturated flow including compressibility effects (major capability 3 in Section 2.0). The geometry is one dimensional radial with specified withdrawal from the center. The permeability of the aquifer is 10^{-11} m^2 ($1.08\ 10^{-10}$ ft^2), the porosity is 0.2, and the specified withdrawal rate is 1 kg/s (2.20 lbm/s). Compressibility of the background formation is set to zero, and the only compressibility considered is that of water.

4.3.2 Test Input

The test input file is on the accompanying disk: *TestCase3\theis.dat.*

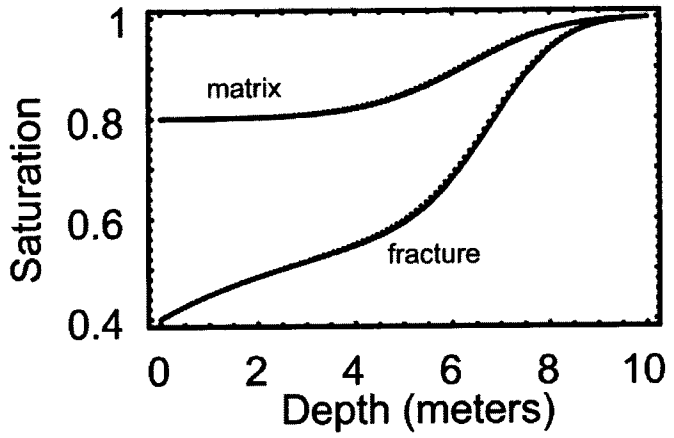

Figure 4: Liquid Saturation Versus Depth (Test 2). The MULTIFLO Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves. The Two Overlay Each Other and Are Indistinguishable on this Scale. [Unit Conversion: Multiply by 3.28 to Convert the x-axis to Feet.]

4.3.3 Target Solution

This configuration has a well-known analytical solution by Theis (1935), which follows directly from an analogy with a classical heat transport problem (e.g., see Domenico and Schwartz, 1990). Drawdown s is given by

$$s = \frac{Q}{4\pi} W(u)$$

where Q is the pumping rate, $u = r^2 S/4Tt$, T is the transmissivity, S is the storativity, r is distance from the well, and t is time. The function $W(u)$ is the exponential integral given by

$$W(u) = \int_u^\infty \frac{e^{-z}}{z} dz$$

4.3.4 Results

The simulation executed to completion without error. Drawdown curves at 52 minutes and 525 minutes are shown in Figure 5. The target solution is plotted as solid curves, and the METRA results are shown as individual data points. The agreement between the two is very good. Normalizing by the maximum drawdown, the relative error is about 9 percent near the origin and decreases with increasing radius. The small difference is most likely due to the fact that the Theis equation requires the compressibility of water to be approximated as a constant, whereas METRA uses the full equation-of-state of water to determine compressibility.

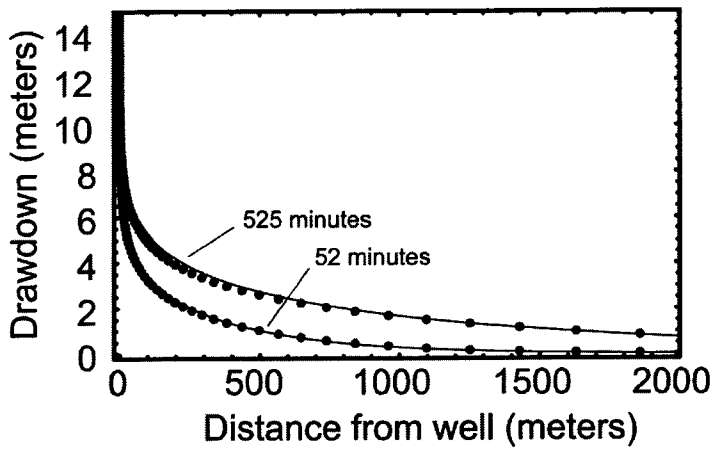

Figure 5: Drawdown Versus Distance from Well at Two Different Times (Test 3). The Multiflo Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves.
[Unit Conversion: Multiply by 3.28 to Convert the meters to feet.]

4.4 Test 4: Equilibrium Speciation in GEM

4.4.1 Description of the Test

This simulation is designed to test GEM's representation of equilibrium speciation for aqueous and gaseous species at 25 °C (77 °F), thus testing major capability 5 in Section 2.0. The reaction system is written in MULTIFLO format as

$$\varnothing \rightleftharpoons -h^+ + h_2o - oh^-$$
$$\varnothing \rightleftharpoons h^+ + hco_3^- - h_2o - co_2(aq)$$
$$\varnothing \rightleftharpoons -h^+ + hco_3^- - co_3^{2-}$$
$$\varnothing \rightleftharpoons ca^{2+} - h^+ + hco_3^- - caco_3(aq)$$
$$\varnothing \rightleftharpoons h^+ + hco_3^- - h_2o - co_2(g)$$

where the symbol $\varnothing$ refers to the null species. 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.

4.4.2 Test Input and Output

The test input and output files are on the accompanying disk in directory *TestCase4.*

4.4.3 Target Solution

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 calculated activities should be consistent with the mass action equations. The mass action equation for the r-th reaction is

$$K_r^{eq} = \prod_{i=1}^{N} a_i^{\nu_{ir}}$$

where K_r^{eq} is the equilibrium constant for the *r*-th reaction, a_i is the activity for the *i*-th species and ν denotes the stochiometric matrix.

Activity coefficients in MULTIFLO/GEM are calculated from an extended Debye-Huckel relation

$$\log \gamma_i = -\frac{z_i^2 A\sqrt{I}}{1+\mathring{a}_i B\sqrt{I}} + \dot{b} I$$

where A, B and $\dot{b}$ are parameters, $\mathring{a}_i$ represents the hydrated ionic radius of the *i*-th species, z_i is the charge of the *i*-th species, and I is the ionic strength of the solution.

4.4.4 Results

The simulation ran to completion without error. Calculated concentrations remain identical to the initial and boundary conditions.

Comparisons between the input value for the equilibrium constants and the equilibrium constants as calculated from the output activities are shown in Table 3. The values are in agreement. The simulation ran to completion without error.

Activity coefficients as calculated from MULTIFLO/GEM are compared with an extended Debye-Huckel relation in Table 4.

4.5 Test 5: Solute Transport in Dual Permeability Media

4.5.1 Description of the Test

This simulation is designed to test GEM's representation of advective/diffusive transport in dual permeability media (major capability 4 in Section 2.0). The configuration involves constant flow

Table 3. Input Values for Equilibrium Constants Compared with Values Calculated from the Simulation Output for Test 4		
Reaction	**Input K^{eq}**	**Calculated K^{eq}**
$oh^- \rightleftharpoons -h^+ + h_2o$	14.00	14.00
$co_2(aq) \rightleftharpoons h^+ + hco_3^- - h_2o$	-6.345	-6.345
$co_3^{2-} \rightleftharpoons -h^+ + hco_3^-$	10.33	10.33
$caco_3(aq) \rightleftharpoons ca^{2+} - h^+ + hco_3^-$	7.002	7.002
$co_2(g) \rightleftharpoons h^+ + hco_3^- - h_2o$	-7.814	-7.814

Table 4. Activity Coefficients from Test 4 Compared with Hand Calculations		
Species	**Activity Coefficient (target)**	**Activity Coefficient (GEM)**
ca^{2+}	0.7063	0.7063
h^+	0.9227	0.9227
$hco3^-$	0.9131	0.9131
cl^-	0.9110	0.9110

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. Parameters for the flow-through problem are given in Table 5.

4.5.2 Test Input and Output

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

4.5.3 Target Solution

The author is unaware of analytical solutions to transport in dual permeability media. A semi-analytical solution was developed, as described in Appendix A. Specifically, a analytical solution was obtained in the Laplace domain. Time-domain solutions were then obtained by numerical inverse Laplace transform. The Mathematica notebook used to obtain the target solution is on the accompanying disk (*Test5.nb*).

Table 5. Hydrological Parameters for Test 5	
Parameter	**Value**
Matrix porosity	0.11
Fracture porosity (internal)	0.11
Fracture volume fraction	0.11
Matrix block size	0.1 m (0.328 feet)
Fracture-to-matrix area reduction factor	10^{-6}
Fracture saturation	0.5
Matrix saturation	0.5
Darcy velocity in fractures	1 m/year (3.28 ft/year)
Diffusion coefficient	31.5 m^2/year (339 ft^2/year)

4.5.4 Results

The test ran to completion without error. Results are shown in Figure 6. The target solutions are shown as curves and the test results are shown as individual data points. The test results overlay the target solution and the two are indistinguishable on this scale. The maximum relative error is 4.6 percent for the fractures and 1.2 percent for the matrix.

4.6 Test 6: Three-Dimensional Advective/Dispersive Transport in GEM

4.6.1 Description of the Test

The test case tests the transport in GEM in three dimensions (major capability 4 in Section 2.0). The velocity field is uniform and constant with flow directed in the x direction. The initial concentration is 0.0008 mol/liter (3.94 10^{-6} mol/in^3). 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 (3.28 ft/yr) in the x direction and a diffusion coefficient of 3.15 m^2/yr (33.9 ft^2/yr) is used. The system size is 40 × 11 × 11 cells, with a nonuniform spacing in each direction.

4.6.2 Test Input and Output

The test input and output files are on the accompanying disk in the directory *TestCase6.* The input file was modified slightly from that specified in the Validation Test Plan to correct an error in the input file in the specification of the boundary condition.

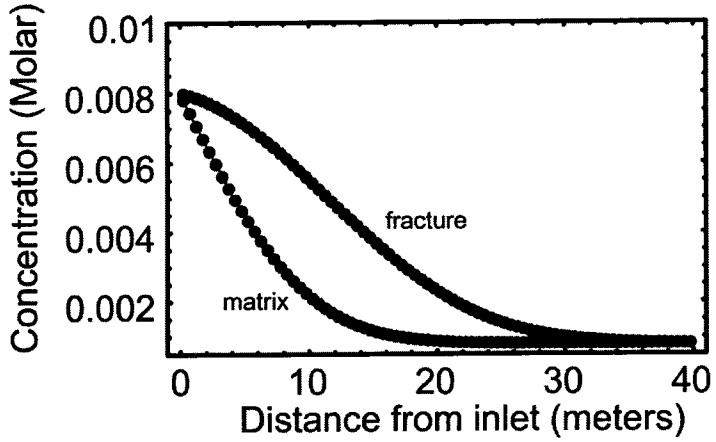

Figure 6: Concentration in Mol/liter in Fractures and Matrix (Test 4). The MULTIFLO Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves. The Two Overlay Each Other and Are Nearly Indistinguishable on this Scale. [Unit Conversion: Multiply by 0.016 to Convert mol/liter to mol/in^3.]

4.6.3 Target Solution

Analytical solutions for the situation of interest are given by Sagar (1982) and Wexler (1991). For a rectangular patch source centered at the origin extending from *(0, Y_1, Z_1)* to *(0, Y_2, Z_2)*, the analytical solution is

$$C(x,y,z,t) = C_0 \, x \exp\left[\frac{vx}{2D}\right] \int_0^t \tau^{-3/2} \exp\left[-\frac{v^2\tau}{4D} - \frac{x^2}{4D\tau}\right]$$

$$\left\{\operatorname{erfc}\left[\frac{Y_1 - y}{2\sqrt{D\,t}}\right] - \operatorname{erfc}\left[\frac{Y_2 - y}{2\sqrt{D\,t}}\right]\right\}\left\{\operatorname{erfc}\left[\frac{Z_1 - z}{2\sqrt{D\,t}}\right] - \operatorname{erfc}\left[\frac{Z_2 - z}{2\sqrt{D\,t}}\right]\right\} d\tau$$

Here D is the diffusion coefficient, v is the transport velocity, and Z is a dummy variable.

4.6.4 Results

The simulation ran to completion without error. One-dimensional traces extracted from the MULTIFLO output are compared with the target solution in Figure 7. When normalized by the maximum concentration, the maximum error is 5 percent. The error is much smaller for most locations. The cause of the error is numerical dispersion on the relatively coarse grids of this simulation.

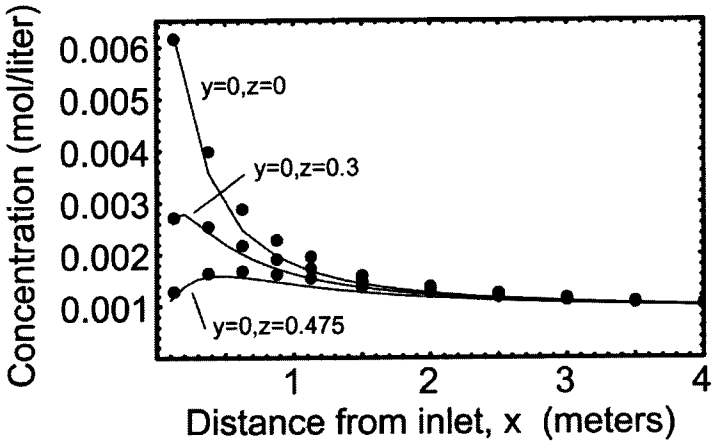

Figure 7: One-Dimensional Traces of Concentration from the Three-Dimensional Flow-Through Test (Test 6). The MULTIFLO Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves. The Two Overlay Each Other and Are Nearly Indistinguishable on this Scale.
[Unit Conversion: Multiply by 0.016 to Convert mol/liter to mol/in^3. Multiply by 3.28 to Convert meters to feet.]

4.7 Test 7: Fully Coupled Flow/Transport with Mineral Dissolution and Permeability Modification

4.7.1 Description of the Test

This simulation tests the coupling between METRA and GEM and kinetically controlled mineral reactions in GEM (major capability 6 in Section 2.0). 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.

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.

In each scenario, the initial quartz fraction is 50 percent, the porosity is 10 percent, and 40 percent of the volume is assumed to be non-reactive. The initial velocity is 3.1 m/yr (10.2 ft/yr).

4.7.2 Test Input and Output

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

4.7.3 Target Solution

A new analytical solution to the coupled flow-through problem with dissolution is described in Appendix B and implemented in the Mathematica notebook, *Test7.nb*, which is on the attached disk.

4.7.4 Results

The tests ran to completion without error. Results are shown in Figure 8a for Scenario 1 and in Figure 8b for Scenarios 2 and 3. The target solution is shown as solid curves and the results of the MULTIFLO simulations are shown as individual data points. The agreement with the target solution is excellent for each scenario. The error relative to the initial mineral abundance is 0.8, 1.5, and 1.4 percent for Scenarios 1, 2, and 3, respectively.

4.8 Test 8: Unstructured Grid Capability

4.8.1 Description of the Test

The test case tests the unstructured grid capability (major capability 7 in Section 2.0). The test case is the same as Test Case 3 of Section 5.3, but implemented as an unstructured grid.

4.8.2 Test Input and Output

The test input and output files are on the accompanying disk in the directory TestCase8.

4.8.3 Target Solution

The target solution is given in Section 5.3.3.

4.8.4 Results

The test ran to completion without error. Results are shown in Figure 9. Agreement with the analytical solution is very good. Discrepancy between the target solution and simulation result is the same as in Test Case 3.

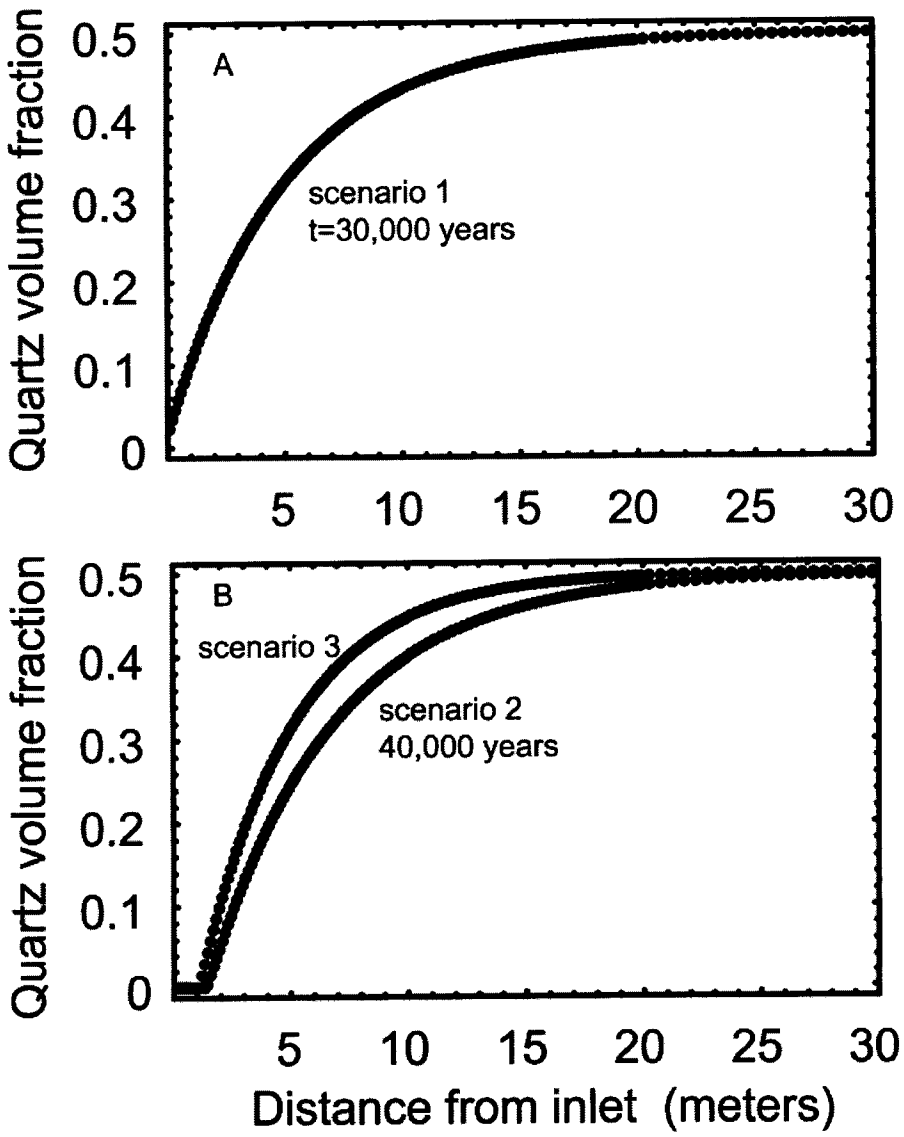

Figure 8: Quartz Volume Fraction Versus Distance from Inlet for the Three Scenarios of Test 6. The MULTIFLO Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves.
[Unit Conversion: Multiply by 3.28 to Convert meters to feet]

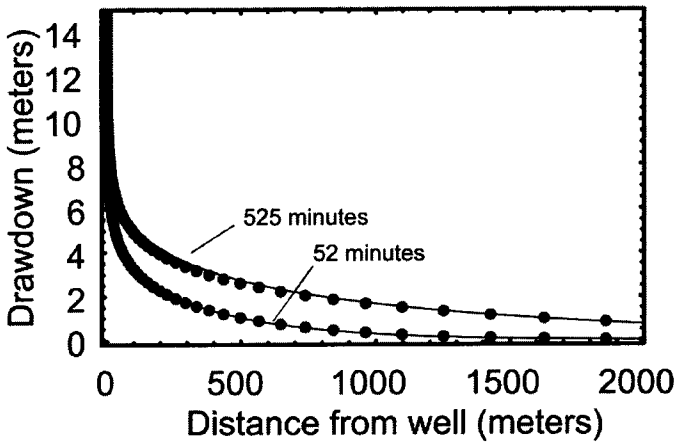

Figure 9: Drawdown Versus Distance from Well at Two Different Times (Test 8). The MULTIFLO Results Are Shown as Individual Data Points and the Target Solution Is Shown as Solid Curves.
[Unit Conversion: Multiply by 3.28 to Convert the meters to feet]

5 KNOWN PROBLEMS

The vapor-pressure lowering variant of Test 1 exhibited a numerical instability at high temperatures. The temperatures at which the instability appears are outside the range expected in the repository proposed for Yucca Mountain, Nevada. Consequently, the instability will have no impact on regulatory activities.

6 CONCLUSIONS

With the minor exception listed in Section 6, results of the validation tests were consistent with the expected results, thereby providing confidence that the major capabilities probed by these tests are correctly implemented in MULTIFLO.

The minor problem noted in Section 6 manifest under conditions different from those expected in the repository proposed for Yucca Mountain, Nevada. Consequently, this problem will have no impact on regulatory activities.

7 REFERENCES

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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 the Mathematica® system (Wolfram, 1999). The mass balance equations in one-dimension are

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

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

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 is a result of 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,

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

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

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

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

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,

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

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_2 are the negative eigenvalues, and $\mathbf{u}_1$ and $\mathbf{u}_2$ 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.

REFERENCE

Wolfram, S. *The Mathematica Book*. 4th Edition. New York City, New York: Wolfram Media/Cambridge University Press. 1999.

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:

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

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 $\tau_s = \frac{\phi_s^0}{k's\Delta C\overline{V}_s}$. 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 in Bear (1972, p. 631). Note, that Bear's λ is $\frac{k's}{v}$. The mineral volume fraction has solution

$$\phi_s(x,t) = \phi_s^0\left[1-\exp(-qx)\,t/\tau_s\right]$$

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 $\overline{V}$, which is calculated as follows. At time *t* we have from the condition of fixed pressure gradient in one dimension,

$$\frac{v_0}{v} - \frac{1}{L}\int_0^L\left(\frac{k_0}{k}\right)dx = 0$$

where the latter term on the left is the ratio of initial permeability k_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):

$$\frac{k_0}{k} = \left(\frac{\phi_0}{\phi}\right)^m = \left[\frac{\phi_R - \phi_S^0}{\phi_R - \phi_S^0 - \exp(-qx)\, t / \tau_S}\right]^m$$

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 $\frac{k_0}{k}$ 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 $b = t\bar{V_S}k's\Delta C$.

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

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, in Lichtner (1996, p. 51)

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

where

$$\ell(t) = \frac{\bar{V}_s v \Delta C}{\phi_s^0}(t - \tau_s)$$

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;

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

where $q(\bar{v})=\frac{k's}{\bar{v}}$, $b=\bar{V}_S k's\Delta C$, $L'=L-\ell(t)$, 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.

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