

SOFTWARE RELEASE NOTICE

01. SRN Number: SRN- GHC-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 <ul style="list-style-type: none"> <input type="checkbox"/> Release of new software <input checked="" type="checkbox"/> Release of modified software: <ul style="list-style-type: none"> <input checked="" type="checkbox"/> Enhancements made <input type="checkbox"/> Corrections made <input type="checkbox"/> Change of access software <input type="checkbox"/> Software Retirement 		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
Scott Painter Mohan Seth	RW RW	
07. Element Manager Approval: E.C. - [Signature]		Date: 6/20/2002
08. Remarks:		

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: <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module	09. Processing Mode: <input type="checkbox"/> Interactive <input type="checkbox"/> Batch <input checked="" type="checkbox"/> Combination	10. APPLICATION AREA a. General: <input checked="" type="checkbox"/> Scientific/Engineering <input checked="" type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> Other b. Specific: Groundwater multiphase flow and reactive transport model	
11. Submitting Organization and Address: CNWRA 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: Scott Painter, (210) 522-3348	
13. Narrative: The code is used to model multiphase groundwater flow and reactive transport.			
14. Computer Platform SUN	15. Computer Operating System: UNIX	16. Programming Language(s): Fortran 77	17. Number of Source Program Statements: ~70,000
18. Computer Memory Requirements: Problem Dependent	19. Tape Drives: N/A	20. Disk/Drum Units: N/A	21. Graphics: ASCII plot data files
22. Other Operational Requirements Thermodynamic database required.			
23. Software Availability: <input type="checkbox"/> Available <input checked="" type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY		24. Documentation Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Inadequate <input type="checkbox"/> In-House ONLY DRAFT	
Software Developer: <u>Scott Painter</u> Date: <u>6-24-02</u>			

**CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT**

FOR

→ DEVELOPED OR ACQUIRED TO BE MODIFIED SOFTWARE ←

Software Title/Name:	<u>Multifl</u>
Version:	<u>1.5.1</u>
Demonstration workstation:	<u>Spock</u>
Operating System:	<u>Unix / Solaris</u>
Developer:	<u>Scott Painter</u>

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

SRD Version:	<u>2.0</u>
SRD Approval Date:	<u>10/31/2000</u>

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:	<u>2.0</u>
SDP (EM) Approval Date:	<u>2/5/2001</u>

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: bnd card.f, solve.f

Comments: b card.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: *SN 282R*

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: *bnd cond.f solve.f*

Comments: *bcond.f init.f*

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?

Computer Platforms: Solaris PC Operating Systems: NT Unix Yes: ☒ No: ☐ N/A: ☐

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 Transcribed 12/13/01

Comments:

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

Location of Instructions: Readme file on CD. for v. 1.5. Yes: ☒ No: ☐ N/A: ☐
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?

Date of Approval: 6/24/02 Yes: ☒ No: ☐ N/A: ☐

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

Comments: see list. Yes: ☒ No: ☐ N/A: ☐

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

Location of Source Code: See CD v. 1.5.1 Yes: ☒ No: ☐ N/A: ☐
Comments:

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

Location of script/make files: See CD v. 1.5.1 Yes: ☒ No: ☐ N/A: ☐
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?

SRN Number: G HGC - 270 Yes: ☒ No: ☐ N/A: ☐
Comments:

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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 June 14, 2002
Aug. 9, 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 Paine 6-24-02
Software Developer/Date

Ray Paine
Software Custodian/Date 6/24/02

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~~June~~ 2002

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

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Header Information

C VERSION/REVISION HISTORY

```
c $Id$
c $Log$
```

	Date	Author(s)	Comments/Modifications
	April 97	Peter C. Lichtner	Initial Implementation
		Mohan S. Seth	
	May 98		Beta Release
	February 2000	Peter C. Lichtner	1.2 Release
		Mohan S. Seth	
		Scott Painter	
	May 2000		V1.2.1 Minor Bug fixes
	August 2000		V1.2.2 Fix bug related to water density calculation and phase change test
	December 2000		V1.2.3 Fix bug related to dryout in GEM. Also change surface area update in GEM, which was bypassed for secondary minerals. Minor fix to printing errors.
	July 2001		V1.5 Section 5,7,8 of V2.0 SRD
			Also assorted minor fixes
	June 2002		SCR351

> Header Information

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
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.

[illegible]

C PURPOSE:

```
c  This routine is the main program for the MULTIFLO driver which
c  couples METRA and GEM.
```

[illegible]

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_srffm2.xyp
06/12/02	04:06p		3,371 dcm1_srffm1.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_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	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	VAld_errs
06/12/02	04:11p	5,849	VAld_his.xyp
06/12/02	04:11p	147,995	VAld_out
06/12/02	04:11p	14,567	VAld_press.xyp
06/12/02	04:11p	14,567	VAld_rh.xyp
06/12/02	04:11p	14,567	VAld_sat.xyp
06/12/02	04:11p	14,567	VAld_tmp.xyp
05/06/02	05:19p	14,460	VAldfldf7.xyp
05/06/02	05:20p	14,460	VAldfldf8.xyp
06/12/02	04:11p	14,460	VAldfldf5.xyp
05/06/02	05:19p	14,460	VAldfldf6.xyp
06/12/02	04:08p	14,460	VAldfldm3.xyp
05/06/02	05:19p	14,460	VAldfldm7.xyp
06/12/02	04:09p	14,460	VAldfldm4.xyp
05/06/02	05:20p	14,460	VAldfldm8.xyp
06/12/02	04:11p	14,460	VAldfldm5.xyp
06/12/02	04:06p	14,460	VAldfldm1.xyp
05/06/02	05:19p	14,460	VAldfldm6.xyp
06/12/02	04:06p	14,460	VAldfldm2.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_secml.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	VAldgvt1vz4.xyp
02/21/02	03:22p	13,405	VAldgvt1vz8.xyp
06/12/02	04:40p	13,405	VAldgvt1vz1.xyp
06/12/02	04:45p	13,405	VAldgvt1vz5.xyp
02/21/02	03:22p	13,405	VAldgvt1vz9.xyp
02/21/02	03:22p	14,460	VAldgvt1fldf6.xyp
02/21/02	03:22p	14,460	VAldgvt1fldf7.xyp
02/21/02	03:22p	14,460	VAldgvt1fldf8.xyp
06/12/02	04:45p	14,460	VAldgvt1fldf5.xyp
02/21/02	03:22p	14,460	VAldgvt1fldf9.xyp
06/12/02	04:40p	14,460	VAldgvt1fldm2.xyp
02/21/02	03:22p	14,460	VAldgvt1fldm6.xyp
06/12/02	04:46p	18,987	VAldgvt1_press.xyp
06/12/02	04:43p	14,460	VAldgvt1fldm3.xyp
02/21/02	03:22p	14,460	VAldgvt1fldm7.xyp
06/12/02	04:44p	14,460	VAldgvt1fldm4.xyp
02/21/02	03:22p	14,460	VAldgvt1fldm8.xyp
06/12/02	04:40p	14,460	VAldgvt1fldm1.xyp
06/12/02	04:45p	14,460	VAldgvt1fldm5.xyp
02/21/02	03:22p	14,460	VAldgvt1fldm9.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	gmfmt.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	interp.f
06/12/02	04:58p	11,203	interp.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
06/12/02	04:58p	10,746	masstran.obj
02/21/02	02:07p	2,641	metragem.h
02/21/02	02:07p	77	minrl.h
02/21/02	02:07p	532	ofiles.h
02/21/02	02:06p	66,969	opsplit.f
06/12/02	04:58p	74,743	opsplit.obj
02/21/02	02:06p	57,144	outgem.f
06/12/02	04:58p	89,033	outgem.obj
05/31/02	02:50p	2,639	paramtrs.h
02/21/02	02:06p	8,505	pecletnr.f

06/12/02	04:58p	5,655	pecletrn.obj
02/21/02	02:06p	17,553	pprcgem.f
06/12/02	04:58p	18,771	pprcgem.obj
06/12/02	03:14p	47,372	read1.f
06/12/02	04:58p	52,220	read1.obj
02/21/02	02:06p	55,443	read2.f
06/12/02	04:58p	78,587	read2.obj
02/21/02	02:07p	1,486	scalgem.h
02/21/02	02:07p	271	scratch.h
02/21/02	02:06p	10,506	setbcon.f
06/12/02	04:58p	13,116	setbcon.obj
02/21/02	02:06p	7,422	setconn.f
06/12/02	04:58p	6,451	setconn.obj
02/21/02	02:06p	7,558	solprd.f
06/12/02	04:58p	6,533	solprd.obj
02/21/02	02:06p	6,897	solprodt.f
06/12/02	04:58p	3,383	solprodt.obj
02/21/02	02:06p	23,242	solve1d.f
06/12/02	04:58p	10,799	solve1d.obj
02/21/02	02:06p	10,700	speciate.f
06/12/02	04:58p	10,150	speciate.obj
02/21/02	02:06p	3,335	srcgem.f
06/12/02	04:58p	4,056	srcgem.obj
02/21/02	02:06p	16,080	startup.f
06/12/02	04:58p	26,619	startup.obj
02/21/02	02:06p	15,846	stdyst.f
06/12/02	04:58p	12,927	stdyst.obj
02/21/02	02:06p	10,690	stepgem.f
06/12/02	04:58p	6,651	stepgem.obj
02/21/02	02:07p	354	surfkin.h
02/21/02	02:07p	300	tdconst.h
02/21/02	02:06p	8,044	textab.f
06/12/02	04:58p	10,099	textab.obj
05/31/02	01:17p	2,209	title.h
02/21/02	02:05p	6,128	tolower
02/21/02	02:06p	11,580	transd.f
06/12/02	04:58p	11,578	transd.obj
02/21/02	02:07p	266	units.h
06/12/02	03:39p	8,808	updtgem.f
06/12/02	04:58p	6,307	updtgem.obj
02/21/02	02:06p	30,439	util.f
02/21/02	02:06p	45,976	watsolv.f
02/21/02	02:07p	388	watsolv.h
02/21/02	02:06p	6,049	zonek.f
06/12/02	04:58p	4,021	zonek.obj
135 File(s)		23,788,585	bytes

Directory of R:\mf101.5.1\metra

06/19/02	11:12a	<DIR>	.
06/19/02	11:12a	<DIR>	..
06/12/02	11:21a		17,203 accm.f
06/12/02	04:56p		8,828 accm.obj
05/31/02	10:17a		2,541 add.h
06/12/02	11:21a		13,245 allot.f
06/12/02	04:56p		5,189 allot.obj
06/12/02	11:23a		30,865 bcond.f

06/12/02	04:56p	19,461	bcond.obj
06/12/02	11:21a	8,095	blkdtmet.f
06/12/02	04:56p	242,505	blkdtmet.obj
06/12/02	11:21a	32,384	coefs.f
06/12/02	04:56p	19,857	coefs.obj
05/31/02	10:17a	5,002	com.h
06/12/02	11:24a	21,476	cond.f
06/12/02	04:56p	8,392	cond.obj
06/12/02	11:21a	18,100	dtstep.f
06/12/02	04:56p	4,147	dtstep.obj
06/12/02	11:21a	21,410	ecmtbl.f
06/12/02	04:56p	12,468	ecmtbl.obj
06/12/02	11:24a	23,464	emip.f
06/12/02	04:56p	14,431	emip.obj
06/12/02	11:21a	18,328	equil.f
06/12/02	04:56p	9,565	equil.obj
05/31/02	10:17a	503	frfmt.h
06/12/02	11:21a	12,049	griddat.f
06/12/02	04:56p	6,463	griddat.obj
05/31/02	10:17a	179	impl.h
06/12/02	11:21a	55,377	init.f
06/12/02	04:56p	46,547	init.obj
06/12/02	11:21a	15,956	inpifv.f
06/12/02	04:56p	19,078	inpifv.obj
06/12/02	11:24a	52,459	inpmetra.f
06/12/02	04:56p	62,047	inpmetra.obj
06/12/02	11:25a	22,280	iter.f
06/12/02	04:56p	13,458	iter.obj
06/12/02	11:21a	27,782	mainmtra.f
05/31/02	10:52a	10,328	Makefile
06/12/02	04:57p	1,212,835	metra.exe
06/12/02	04:57p	95,516	metra.map
05/31/02	10:17a	2,641	metragem.h
06/12/02	11:21a	12,907	openfls.f
06/12/02	04:57p	6,826	openfls.obj
06/12/02	11:25a	35,699	outmetra.f
06/12/02	04:57p	32,984	outmetra.obj
05/31/02	10:17a	2,278	para1.h
05/31/02	10:17a	2,639	paramtrs.h
06/12/02	11:22a	29,557	pckr.f
05/31/02	10:17a	1,085	pckr.h
06/12/02	04:57p	16,624	pckr.obj
06/12/02	11:22a	32,961	plots.f
06/12/02	04:57p	43,297	plots.obj
06/12/02	12:59p	20,068	pproc.f
06/12/02	04:57p	23,909	pproc.obj
06/12/02	11:25a	9,354	prints.f
06/12/02	04:57p	5,753	prints.obj
06/12/02	11:22a	27,627	pvt.f
06/12/02	04:57p	18,349	pvt.obj
06/12/02	11:22a	19,446	pvtfunc.f
05/31/02	10:17a	565	pvtfunc.h
06/12/02	04:57p	13,711	pvtfunc.obj
06/12/02	11:22a	29,376	pvth2o.f
06/12/02	04:57p	27,483	pvth2o.obj
05/31/02	10:17a	916	pvttbl.h
06/12/02	11:22a	26,420	pvtvp.f

06/12/02	04:57p	16,221	pvtvp.obj
06/12/02	11:26a	67,434	recdat.f
06/12/02	04:57p	64,769	recdat.obj
06/12/02	11:26a	18,302	rstart.f
06/12/02	04:57p	32,386	rstart.obj
05/31/02	10:17a	1,698	scalars.h
06/12/02	11:26a	13,245	setbc.f
06/12/02	04:57p	6,725	setbc.obj
06/12/02	11:26a	16,320	slvlp.f
06/12/02	04:57p	7,983	slvlp.obj
06/12/02	11:27a	10,045	solve.f
06/12/02	04:57p	2,479	solve.obj
06/12/02	11:22a	10,689	source.f
06/12/02	04:57p	2,788	source.obj
06/12/02	11:27a	13,587	thomas.f
06/12/02	04:57p	4,704	thomas.obj
05/31/02	11:56a	2,165	title.h
06/12/02	11:22a	10,194	trans.f
06/12/02	04:57p	3,677	trans.obj
05/31/02	10:17a	266	units.h
06/12/02	11:27a	8,882	update.f
06/12/02	04:57p	5,182	update.obj
06/12/02	11:22a	15,840	updtpsk.f
06/12/02	04:57p	7,495	updtpsk.obj
06/12/02	11:22a	16,799	updtvpk.f
06/12/02	04:57p	8,419	updtvpk.obj
06/12/02	11:22a	30,439	util.f
06/12/02	04:57p	20,453	util.obj
06/12/02	11:27a	45,737	watsolv.f
05/31/02	10:17a	388	watsolv.h
06/12/02	04:57p	31,789	watsolv.obj
	96 File(s)	3,149,388	bytes

Total Files Listed:

508 File(s)

49,657,974 bytes

0 bytes free

SOFTWARE VALIDATION TEST PLAN FOR MULTIFLO VERSION 1.5.1

Prepared by

Scott Painter

**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. Lichtner, 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\vppl.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 vppl*.
- (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:

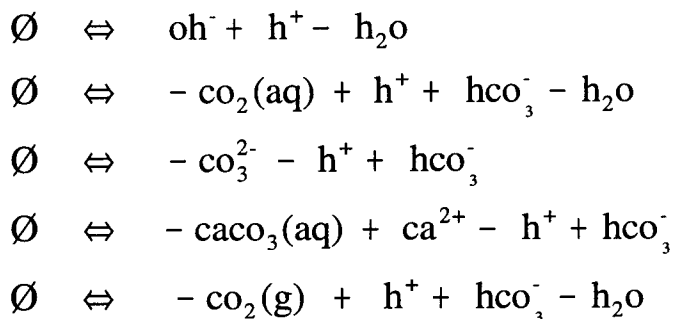
- (1) Execute MULTIFLO by typing *MULTIFLO theis*.
- (2) Enter 1 at the command prompt.
- (3) Verify that the code runs to completion without error.
- (4) Extract results for pressure at 1.e-4 years, convert to equivalent drawdown in meters, and compare with the well-known analytical solution of Theis.

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:



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 $3.15 \text{ m}^2/\text{yr}$ is used. The system size is $40 \times 11 \times 11$ 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 $\text{SiO}_2(\text{aq})$. 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,

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

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

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 $D_F = \phi_F S_F \varepsilon_F D_0$ 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 $\alpha \approx \frac{\phi S D_0 A}{d}$ 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,

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

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

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

$$\alpha_2 = \frac{2DA}{d} \frac{\phi S}{\phi_F S_F \varepsilon_F}$$

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

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

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

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,

$$\bar{\xi}(x,s) = c_1 \mathbf{v}_1 \exp[\lambda_1 x] + c_2 \mathbf{v}_2 \exp[\lambda_2 x]$$

where $\bar{\xi}(x,s) = \left(C, \frac{\partial C}{\partial x}, C_F, \frac{\partial C_F}{\partial x} \right)^T$, λ_1 and λ_2 are the negative eigenvalues, and \mathbf{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 $\text{SiO}_2(\text{aq})$ 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

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

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

$$\frac{\partial \phi_s}{\partial t} = \bar{V}_s k's(C - C_{eq})H(x - \ell(t))$$

where \bar{V}_s is the molar volume for the mineral. The initial and boundary conditions are:

$$C(x, t = 0) = C_{eq}$$

$$C(x = 0, t) = C_0$$

$$\phi_s(x, t = 0) = \phi_s^0$$

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 $\tau_s = \frac{\phi_s^0}{k's\Delta C V_s}$. 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 $b = \bar{V}_s k'_s \Delta C$.

Once the time-averaged velocity is obtained, it is used in place of \bar{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

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

Similarly, the mineral volume fraction is given by:

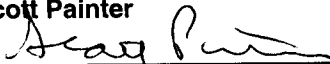
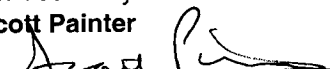
$$\phi_s(x, t) = \phi_s^0 \left(1 - \exp\left[-\frac{k'_s}{v}(x - \ell(t))\right] \right)$$

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 $q(\bar{v}) = \frac{k's}{v}$, $b = \overline{V_s} k's \Delta C$, $L' = L - \ell(t)$, and the time average velocity is to be used in place of \mathcal{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. (<i>Software Developer Assigns</i>): SCR-406	2. Software Title and Version: Multiflo V1.5.1	3. Project No: 20.01402.562
<p>4. Affected Software Module(s), Description of Problem(s):</p> <p>The following are changes needed for Version 1.5.1.</p> <p>(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.</p> <p>(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.</p> <p>(3) Time dependent boundary conditions not set properly in METRA.</p> <p>(4) In GEM, water content (porosity*saturation) is not set properly at boundary. Change bndcond.f file to correct.</p> <p>(5) In coupled mode, boundary temperatures are not set properly in GEM. Required change to setbcon.f file.</p>		
<p>5. Change Requested by: Scott Painter</p> <p>Date: August 13, 2002</p>	<p>6. Change Authorized by (<i>Software Developer</i>): Scott Painter</p> <p>Date: August 13, 2002</p>	
<p>7. Description of Change(s) or Problem Resolution (<i>If changes not implemented, please justify</i>):</p> <p>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.</p>		
<p>8. Implemented by: Scott Painter</p> 	<p>Date: November 1, 2002</p>	
<p>9. Description of Acceptance Tests:</p> <p>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.</p>		
<p>10. Tested by: Scott Painter</p> 	<p>Date: November 4, 2002</p>	